Ellipsoidal Brownian self-driven particles in a magnetic field

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We study the two-dimensional Brownian dynamics of an ellipsoidal paramagnetic microswimmer moving at a low Reynolds number and subject to a magnetic field. Its corresponding mean-square displacement, showing the effect of a particle’s shape, activity, and magnetic field on the microswimmer’s diffusion, is analytically obtained. Comparison between analytical and computational results shows good agreement. In addition, the effect of self-propulsion on the transition time from anisotropic to isotropic diffusion of the ellipse is investigated.

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I. INTRODUCTION

The study of active (self-propelled) Brownian particles (ABps) has recently received considerable attention [1–4]. These microparticles are able to self-propel due to an internal mechanism which may be based on a light stimulus (thermophoresis) or concentration gradients (diffusophoresis) or by the motion of actuated synthetic filaments [5]. ABps are interesting from a fundamental point of view due to their out-of-equilibrium nature. For example, when ABps interact among each other they may form clusters [6], thus these simple systems may shed light on the way active matter organizes, which eventually will lead to technology based on active materials [3,7]. In addition ABps can be considered as minimalistic models for studying swimming microorganisms [8,9]. Substantial efforts have also focused on the potential biomedical and environmental applications for these small self-driven systems [10–12], such as targeted drug delivery, microsurgery, decontamination, and environmental monitoring, among others [2].

Related works have often considered spherical ABps [9,13–18]. However, it is very common, in nature [19] and in synthetic devices, to find anisotropic particles. Along this line, Han et al. [20] studied the Brownian motion of passive (not self-propelled) ellipsoidal particles. They experimentally and theoretically characterized its anisotropic diffusion. Grima and Yaliraki [21] derived the equations of motion for an ellipsoidal Brownian passive particle under an external force. In particular, they applied their general results to the case of forces derived from a linear and a harmonic potential. Later, Han et al. [22] experimentally investigated the long-time effective diffusion coefficients along the short and long axis of an ellipsoid as well as wall confinement effects on its diffusion.

Inspired by finding methods able to change the direction of microengines, Tierno et al. [23] characterized the dynamics of overdamped paramagnetic ellipsoidal particles immersed in a rotating field and found nonlinear motion of ellipsoids under certain circumstances. Their analytical results were also experimentally tested. A subsequent work [24] then demonstrated the ability of external magnetic fields to guide self-driven microellipsoids by means of a torque created by the external field and the magnetic anisotropy of the ellipsoids. The inclusion of thermal forces on similar systems has been undertaken by Giell and coworkers [25]. They found approximated analytical expressions for the diffusion of an ellipsoidal paramagnetic passive particle under the effect of a rotating field. More recently, ten Hagen et al. [26] found analytical expressions, in two and three dimensions, for the mean-square displacement of a self-propelled ellipsoidal particle. Technological applications of these magnetically torqued ellipsoidal particles have been highlighted in a recent review [27].

Other studies related to the present work are the theoretical and experimental study on the dynamics of a microswimmer with an L shape made by Kummel et al. [8], the treatment of the dynamics of living active particles with a permanent magnetic moment (magnetotactic bacteria) in a rotating field by Cebers and coworkers [28,29], and the report in [30] on the diffusive behavior of magnetotactic bacteria due to the random switching of the microorganisms’ flagellar motors.

Motivated by the latter research, we extend previous investigations to the case of ABps under the presence of a magnetic field, that is, we analyze the effect of the particle’s shape, self-propulsion, and magnetic field on the diffusion of an ellipsoidal self-driven particle. The effect of activity on the transition time from anisotropic to isotropic diffusion is also discussed.

II. MODEL

Let us analyze a self-propelled paramagnetic ellipsoidal particle (swimmer) of semimajor axis a and semiminor axis b. This particle moves in a two-dimensional fluctuating environment at temperature T and is subject to an external magnetic field of the form \( \mathbf{H}(t) = H_0[\cos(\omega_H t), \sin(\omega_H t)] \) (see Fig. 1). In this model, the swimmer is able to rotate along the azimuthal direction \( \theta \), and we represent its center-of-mass position (in Cartesian coordinates) as \( \mathbf{x}(t) = [x_1(t), x_2(t)] \). The self-propulsion of the particle is included by imposing a swimming velocity (along its long axis) of the form \( \mathbf{U}_s = U \mathbf{e}(t) \), where \( \mathbf{e}(t) = [\cos \theta(t), \sin \theta(t)] \) is the instantaneous unit vector in the direction of swimming with its origin at the center of the particle, and \( U \) is the magnitude of the swimming velocity.
velocity, which is taken to be constant here, for simplicity. Thermal fluctuations in translation, $f(t) = [f_1(t), f_2(t)]$, and rotation, $g(t) = g(t)\mathbf{k}$, are modeled as zero-mean random variables whose correlations are given by [20]

$$\langle f_i(t) f_j(t') \rangle = 2D_{ij}(t) \delta(t-t'), \tag{1}$$

$$\langle g(t) g(t') \rangle = 2D_m \delta(t-t'), \tag{2}$$

where

$$D_{ij}(t) = \langle \mathbf{D}_i \rangle + \frac{1}{2}\Delta D \begin{bmatrix} \cos 2\theta(t) & \sin 2\theta(t) \\ \sin 2\theta(t) & -\cos 2\theta(t) \end{bmatrix}. \tag{3}$$

Note that $\mathbf{D} = 1/2(D_a + D_b)$ and $\Delta D = D_a - D_b$, where $D_a = k_b T/R_a$, $D_b = k_b T/R_b$, and $D_m = k_b T/R_m$; here $R_a$ and $R_b$ are the resistance coefficients to translation along semiaxes $a$ and $b$, respectively, while $R_m$ is the resistance coefficient to rotation and $k_b$ is the Boltzmann constant.

In a low-Reynolds-number environment, and in the laboratory reference frame, the balance of forces on the ellipsoidal Brownian particle leads to the following Langevin equation for translation [26]:

$$\frac{dx}{dt} = Ue(t) + f(t). \tag{4}$$

Similarly, the director vector, $\mathbf{e}$, follows the dynamics [31]

$$\frac{d\mathbf{e}}{dt} = \Omega(t) \times \mathbf{e}(t), \tag{5}$$

where $\Omega(t)$ represents the swimmer’s angular velocity. The latter equation can be further simplified by using the torque-balance condition on the ellipse: $\tau_m + \tau_H = \mathbf{g}$, where $\tau_H = -R_m \Omega(t) \mathbf{k}$ represents the hydrodynamic torque, $\tau_H = \mu_w \mathbf{m} \times \mathbf{H}$ is the magnetic torque ($\mu_w$ is the magnetic susceptibility of water), and $\mathbf{g} = \mathbf{g}(t) \mathbf{k}$ is the stochastic torque. $[\mathbf{g}] = g(t)$. The magnetic moment is related to the magnetic field by $\mathbf{m} = V \chi \mathbf{H}$, where $V = (4/3)\pi ab$ and $\chi$ is a second-order tensor representing the susceptibility of the ellipse. For the situation where there is a preferred magnetization direction, the susceptibility tensor may be expressed as $\chi = \chi_{\perp} I + \Delta \chi \mathbf{e} \mathbf{e}$, where $\Delta \chi = \chi_{||} - \chi_{\perp}$ and $\chi_{||}$ ($\chi_{\perp}$) is the susceptibility component parallel (normal) to $\mathbf{e}$. The mentioned torque balance condition together with Eq. (5) finally leads to

$$\frac{d\theta}{dt} = \omega_c \sin[2(\omega t - \theta(t))] + g(t), \tag{6}$$

where we have defined $\omega_c = \mu_w V \Delta \chi H^2/2R_m$. Note that the stochastic differential equations (4) and (6) describe the dynamics of the active ellipsoidal swimmer. The solution of these equations will enable us to find the swimmer’s effective diffusion, as detailed in the following section.

### III. MEAN-SQUARE DISPLACEMENT

To find analytical expressions for the swimmer’s effective diffusion, we need to calculate its mean-square displacement. Let us integrate Eq. (4) with respect to time, square it, and perform an ensemble average to that result. The resulting equations in components read

$$\langle \chi^2_1(t) \rangle = U^2 \int_0^t \int_0 ^t \langle \cos \theta(t') \cos \theta(t'') \rangle dt'' dt', \tag{7}$$

and

$$\langle \chi^2_2(t) \rangle = U^2 \int_0^t \int_0 ^t \langle \sin \theta(t') \sin \theta(t'') \rangle dt'' dt', \tag{8}$$

Clearly, one can see that in order to integrate Eqs. (7) and (8), the explicit expressions for the correlations $\langle \cos \theta(t') \cos \theta(t'') \rangle$, $\langle \cos \theta(t') \sin \theta(t'') \rangle$, and $\langle \sin \theta(t') \sin \theta(t'') \rangle$ are needed. One way of calculating these correlations is to use the corresponding joint probability distribution, $G(\theta_1,t_1;\theta_2,t_2) = P(\theta_1,t_1|\theta_2,t_2)P(\theta_2,t_2)$, which is obtained after solving the respective Smoluchowski equation for Eq. (6). In this way one can use that

$$\langle \cos \theta(t') \cos \theta(t'') \rangle = \langle \cos \theta_1 \cos \theta_2 \rangle = \int \int \cos \theta_1 \cos \theta_2 P(\theta_1,t_1|\theta_2,t_2) \times P(\theta_2,t_2) d\theta_1 d\theta_2, \tag{9}$$

where the conditional and unconditional PDFs are $P(\theta_1,t_1|\theta_2,t_2)$ and $P(\theta_2,t_2)$, respectively. Unfortunately, the joint probability distribution $G$ for the nonlinear Eq. (6) cannot be explicitly obtained. Hence, a further approximation is required to make some progress. Based on numerical observations of the solution of Eq. (6), it is proposed that its solution is approximately given by [25]

$$\theta(t) \approx \theta_0(t) + \sigma B_t, \tag{10}$$
where \( \theta_d(t) \) is the corresponding deterministic solution to Eq. (6). \( B_t \) is the classical Brownian motion, and \( \sigma = \sqrt{2D_c} \).

One should note that, depending on the ratio \( \gamma = \omega_c/\omega_H \), the rotational deterministic dynamics of the ellipsoidal particle is different. For example, for the case \( \gamma > 1 \), the deterministic solution to Eq. (6) is

\[
\theta_d(t) = \omega_H t + \arctan[-\gamma + c_2 \tanh(c_2 \omega_H t + c_4)],
\]

(11)

where \( c_2 = \sqrt{\gamma^2 - 1} \) and \( c_4 = \tanh^{-1}(\tan(\theta_0 + \gamma/c_2)) \). The behavior of Eq. (11) can be appreciated in Fig. 2(a). This dynamics represents the case where the ellipsoidal particle rotates synchronously with the magnetic field. For the case \( \gamma < 1 \), the deterministic solution to Eq. (6) is

\[
\theta_d(t) = \omega_H t - \arctan[\gamma + c_1 \tan(c_1 \omega_H t - c_3)],
\]

(12)

where \( c_1 = \sqrt{1 - \gamma^2} \) and \( c_3 = \arctan(\tan(\theta_0 + \gamma/c_1)) \). The behavior of Eq. (12) is shown in Fig. 2(b). For this case, the ellipsoidal swimmer performs a back-and-forth rotational motion while it is trying to follow the rotation of the magnetic field. This state can be considered as an asynchronous state.

Once we have established Eqs. (11) and (12), we use Eq. (10) to show that

\[
\langle \cos \theta(t) \rangle = e^{-4D_c t} \cos \theta(t).
\]

(13)

In the same way,

\[
\langle \cos \theta(t') \cos \theta(t'') \rangle = \langle \cos[\theta_d(t') + \sigma B_t] \rangle \times \cos[\theta_d(t'') + \sigma B_{t''}] + \cos[\theta_d(t'') - \theta_d(t')] \rangle.
\]

(14)

After certain manipulation and by defining \( \Theta \equiv \theta_d(t'') + \theta_d(t') + 2\theta_0 \), it can be shown that

\[
\langle \cos \theta(t') \cos \theta(t'') \rangle = \frac{e^{-\sigma^2(t'-t'')/2}}{2}[e^{-2n^2r^2} \cos \Theta(t) + \cos[\theta_d(t'') - \theta_d(t')] \rangle.
\]

(15)

Similarly, the correlation

\[
\langle \sin \theta(t') \sin \theta(t'') \rangle = \langle \sin[\theta_d(t') + \sigma B_t] \rangle \times \sin[\theta_d(t'') + \sigma B_{t''}] \rangle.
\]

(16)

can be simplified as

\[
\langle \sin \theta(t') \sin \theta(t'') \rangle = \frac{e^{-\sigma^2(t'-t'')/2}}{2}[-e^{-2n^2r^2} \cos \Theta + \cos[\theta_d(t'') - \theta_d(t')] \rangle.
\]

(17)

The latter results allow us to have implicit analytical expressions for the effective diffusion coefficients as we see in the next section.

IV. EFFECTIVE DIFFUSION

By definition, the diffusion coefficient along the \( x_i \) direction \((i \in \{1, 2\})\) is

\[
D_{x_i}(t, \theta_0) = \frac{\langle \dot{\theta}^2(t) \rangle}{2t}.
\]

(18)

Thus if one includes Eq. (7) together with Eqs. (13) and (15) in Eq. (18), we get

\[
D_{x_1}(t, \theta_0) \approx \dot{D} + \frac{\Delta D}{2t} + \int_{t_0}^{t} e^{-4D_c t'} \cos 2\theta_d(t') dt' \times \left[ e^{-4D_c t''} \cos \Theta + \cos[\theta_d(t'') - \theta_d(t')] \right] dt' dt''.
\]

(19)

Similarly, using Eqs. (8) and (17) one can show that the diffusion along the \( x_2 \) direction is

\[
D_{x_2}(t, \theta_0) \approx \dot{D} + \frac{\Delta D}{2t} + \int_{t_0}^{t} e^{-4D_c t'} \cos 2\theta_d(t') dt' \times \left[ e^{-4D_c t''} \cos \Theta + \cos[\theta_d(t'') - \theta_d(t')] \right] dt' dt''.
\]

(20)

Note that the latter two expressions provide a way of analytically quantifying the effects of the activity \((U)\), swimmer’s shape \((D, \Delta D)\), and strength of the magnetic field on the diffusion of a paramagnetic ellipsoidal swimmer. Therefore Eqs. (19) and (20) represent an extension of the works of Grima and Yaliraki [21], Güell et al. [25], and ten Hagen et al. [26], among others, to the case of active matter under external fields.

For the case \( \gamma > 1 \) it is possible to find an asymptotic expression for its long-term effective diffusion coefficient. To do this, one can show that for long times, Eq. (6) reduces to the Langevin equation \( d\theta/dt = \omega_H + g(t) \) with a given initial orientational angle \( \theta_0 \). The latter Langevin equation corresponds to a conditional PDF of the form

\[
P(\theta_1, t_1|\theta_2, t_2) = \frac{1}{\sqrt{4\pi D_c t}} e^{-\frac{(\theta_1 - \theta_2)^2}{4D_c t}},
\]

(21)

where \( \tau = t_1 - t_2 \), here \( t_1 > t_2 \). Thus with the use of Eq. (9), one can find the swimmer’s orientation correlations exactly.
After performing the indicated integrals in Eqs. (7) and (8), using Eq. (18), and applying the limit \( t \to \infty \), one gets that the ellipsoidal swimmer long-time diffusive behavior is

\[
D_x = D_y = \bar{D} + \frac{D_0 U^2}{D_0 + \omega_H^2},
\]

which is exactly the same expression as for a spherical particle under an external torque [32]. In other words, after a long time the ellipsoidal particle statistically behaves like a sphere. For comparison purposes, Eq. (22) is plotted in Fig. 3(a) and discussed in the next section.

V. COMPARISON AMONG NUMERICAL AND ANALYTICAL RESULTS

In order to check how accurately the analytical Eqs. (19) and (20) describe the effective diffusion coefficients, we perform Brownian dynamics simulations. (A stochastic Runge-Kutta algorithm was used. The particle always started at the origin with an initial angular orientation \( \theta_0 = 0 \), and 20 000 realizations were used to perform the averages.) In these simulations, we consider an ellipsoidal swimmer with translational diffusivities \( D_a = 0.18 \mu m^2/s \) and \( D_b = 0.044 \mu m^2/s \) (typical experimental values [20]), immersed in water at \( T = 300 \) K, and simulate the cases \( \gamma > 1 \) and \( \gamma < 1 \). Figure 3(a) shows the effective diffusion coefficients along the \( x_1 \) and \( x_2 \) directions of an ellipsoidal particle swimming at speed \( U = 3 \mu m/s \) with \( \gamma > 1 \). The theoretical results are represented by dashed green and black lines; the Brownian dynamics results, by solid blue and red lines. A good agreement between theory and numerics can be appreciated. The asymptotic long-time diffusive coefficient dictated by Eq. (22) is also plotted as the light-red dashed line for comparison. Since the rotating nature of the magnetic field does not break the overall isotropy of the problem and the initial anisotropic translational motion of the particle will eventually be washed out by rotational diffusion, after a period of time, isotropic diffusion is recovered and both diffusive coefficients \( (D_{x_1}, D_{x_2}) \) tend to the same constant value dictated by Eq. (22). Figure 3(b) shows the same particle swimming at the same speed \( (U = 3 \mu m/s) \) but with \( \gamma < 1 \). Once again, the theoretical results appear as dashed green and black lines, while the Brownian simulations appear as solid red and blue lines. A good agreement between theory and numerical results is also obtained in this regime. From the latter comparisons one can see that Eqs. (19) and (20) provide a good description of the effective diffusion of a magnetically torqued swimmer at both short and long times. One can also see that for long times, both cases \( (\gamma > 1, \gamma < 1) \) tend to a constant value, that is, the system tends to display an isotropic behavior as expected.

A. Transition time to isotropic diffusion

We finally show the effect of the swimming velocity \( U \) and magnetic frequency \( \omega_H \) on the transition time the ellipsoidal particle takes to develop isotropic diffusion. To this end, we use Eqs. (19) and (20) and fix the Brownian diffusive constants as \( D_a = 0.18 \mu m^2/s \) and \( D_b = 0.044 \mu m^2/s \), as well as the frequency \( \omega_c = 14.7 \) s\(^{-1} \) for all simulations. In the first numerical experiment, we vary the magnetic-field frequency as \( \omega_H = \{1 \) s\(^{-1} \), \( 3 \) s\(^{-1} \), \( 5 \) s\(^{-1} \), \( 7 \) s\(^{-1} \), \( 9 \) s\(^{-1} \), \( 11 \) s\(^{-1} \), \( 13 \) s\(^{-1} \), \( 15 \) s\(^{-1} \), \( 17 \) s\(^{-1} \), \( 19 \) s\(^{-1} \), \( 21 \) s\(^{-1} \), \( 23 \) s\(^{-1} \)\} and repeat the procedure for three swimming velocities: \( U = \{0 \mu m/s, 3 \mu m/s, 4 \mu m/s\} \). In Fig. 4, for \( \gamma > 1 \), one can see that a higher swimming velocity and lower magnetic frequency lengthen the transition time. A similar dependence on the magnetic frequency has been reported for passive ellipsoidal particles [25]. The increase in transition time due to self-propulsion can be understood as a result of the enhanced directionality memory of the particle’s long axis, along which
the active particle translates for a longer time compared with a passive one. For $\gamma < 1$, while the particle self-propulsion has the same effect of lengthening the transition time, the transition time also increases with the magnetic frequency due to the back-and-forth motion, similarly to the case of passive particles [25]. In our second numerical experiment, we further explore the dependence of transition time on swimming velocity. In Fig. 5, the transition time is plotted against the typical microswimmer velocity from $U = 0$ to $U = 10 \, \mu m/s$ at two magnetic frequencies selected in the synchronous and asynchronous regimes, namely, $\omega_H = 7$ and $21 \, s^{-1}$. The simulations for the case $\omega_H = 7 \, s^{-1}$ are represented by red squares, while the case $\omega_H = 21 \, s^{-1}$ is shown by blue circles. Solid blue and red lines represent a quadratic fitting curve, suggesting a quadratic scaling between the transition time and the swimming velocity as $t_{\text{trans}} \sim CU^2$, where $C$ is a constant.

Finally, typical paths of paramagnetic ellipsoidal microswimmers during 150 s are shown in Fig. 6. A swimmer with $U = 6 \, \mu m/s$ and subject to a magnetic frequency $\omega_H = 7 \, s^{-1}$ ($\gamma < 1$) is shown in Fig. 6(a), while a swimmer with $U = 6 \, \mu m/s$ under $\omega_H = 21 \, s^{-1}$ ($\gamma > 1$) is shown in Fig. 6(b). Figure 6(c) represents typical paths for a swimmer without a magnetic field. One can appreciate the rotational motion the swimmers perform when they are subject to an external rotating magnetic field. This rotation reduces the swimmer’s effective diffusion. In the absence of external fields the ellipsoidal swimmer samples longer distances [see Fig. 6(c)]. One can also observe in Figs. 6(a) and 6(b) that for higher magnetic frequencies ($\gamma > 1$), the swimmer reaches distances longer than those reached at $\gamma < 1$.

VI. CONCLUDING REMARKS

In summary, we have found analytical expressions able to characterize the effect of a particle’s shape, self-propulsion, and external magnetic fields on the diffusion of ellipsoidal particles for both short and long times. A comparison among analytical and computational results was also made and good agreements were obtained. The particle activity offers an additional mechanism to control the crossover from anisotropic to isotropic diffusion, and it was found that the transition time increases with the self-propulsion velocity.

As a remark, although a paramagnetic microswimmer is considered in this work, similar dynamics is expected for ferromagnetic microswimmers (e.g., magnetotactic bacteria) under the same setup. Despite the differences in the ferromagnetic and paramagnetic moments, the two-dimensional rotating magnetic-field setup renders similar mathematical structures in the equation of motion in these different cases. Under a rotating magnetic field, a ferromagnetic microswimmer hence also displays synchronous and asynchronous behaviors similar to those of a paramagnetic microswimmer [29,30]. Finally, it may be biologically relevant to investigate the effects of the run-and-tumble motility of bacterial cells on the transition from anisotropic to isotropic diffusion. Qualitatively, we would expect the run-and-tumble behavior to shorten the transition time since it introduces an additional mechanism to wash out the directionality of the particle. The quantitative aspect may be an interesting topic for future analysis.

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