Noisy swimming at low Reynolds numbers

Jörn Dunkel and Irwin M. Zaid
Rudolf Peierls Centre for Theoretical Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, United Kingdom
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Small organisms (e.g., bacteria) and artificial microswimmers move due to a combination of active swimming and passive Brownian motion. Considering a simplified linear three-sphere swimmer, we study how the swimmer size regulates the interplay between self-driven and diffusive behavior at low Reynolds number. Starting from the Kirkwood-Smoluchowski equation and its corresponding Langevin equation, we derive formulas for the orientation correlation time, the mean velocity and the mean square displacement in three space dimensions. The validity of the analytical results is illustrated through numerical simulations. Tuning the swimmer parameters to values that are typical of bacteria, we find three characteristic regimes: (i) Brownian motion at small times, (ii) quasi-ballistic behavior at intermediate time scales, and (iii) quasi-diffusive behavior at large times due to noise-induced rotation. Our analytical results can be useful for a better quantitative understanding of optimal foraging strategies in bacterial systems, and they can help to construct more efficient artificial microswimmers in fluctuating fluids.

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I. INTRODUCTION

Biological [1, 2, 3] and artificial microswimmers [1, 4, 5, 6, 7] move through a fluid by performing a series of self-induced shape changes [8, 9]. Handicapped by their tiny size (typically a few micrometers for a bacterium [10]), they are forced to swim at very low Reynolds numbers \( R \ll 1 \) [11, 12, 13]. Hence, in order to account for the resulting lack of inertia, the swimming strategies of microorganisms are very different from those operative at human length scales. More precisely, since the fluid flow is reversible at low Reynolds number, locomotion in this regime is possible only if the swimming stroke violates certain time-reversal symmetries [8, 13, 14, 15, 16].

Stimulated by experimental advances [1, 2, 3, 4, 17], in recent years considerable progress was achieved in understanding the dynamics of deterministic microswimmers models [10, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29]. Yet, comparatively little is known quantitatively about the complex interplay between active self-motion, hydrodynamic interactions, and thermal fluctuations in the surrounding fluid [29, 30, 31, 32]. Very recently, first steps towards clarifying these issues were made by Howse et al. [6], who measured in their experiments the first steps towards clarifying these issues were made by Howse et al. [6], who measured in their experiments the fluid flow. Although the analytical and numerical results in this paper refer to the case of a quasi-linear 3-sphere swimmer \((p = 3)\), the formalism can be easily generalized to more complex models (e.g., flexible \( p \)-sphere swimmer chains). Therefore, this approach can be generally very useful for studying Brownian motion effects and hydrodynamic interactions in active biological systems at low Reynolds numbers. Furthermore, since it is straightforward to implement an external confinement (e.g., tweezer or lattice potentials), the Kirkwood-Smoluchowski scheme can help to construct and optimize arrays [33] of, e.g., micro-pumps that work efficiently on those scales where thermal fluctuations in fluid become

*Electronic address: jorn.dunkel@physics.ox.ac.uk*
non-negligible.

Thus, purpose and content of the present paper can be summarized as follows: First, we will discuss a convenient formalism that allows to simulate active microswimming by means of Langevin equations and interaction potentials (Sec. II). Subsequently, we derive analytic results for the diffusion of a single swimmer (Sec. III), thereby extending recent work of Golestanian and Ajdari [23] on deterministic swimmers. A thorough analysis of the single-swimmer case is instructive for a number of reasons: (i) Exact analytical results provide a useful test of numerical simulations, cf. Sec. IV. (ii) Recently, Leoni et al. [4] were able to experimentally realize an individual 3-sphere system similar to those considered here. (iii) Understanding the noise-induced behavior of a single swimmer is a prerequisite for understanding complex behavior and pattern formation in, e.g., self-assembling bacterial systems [10]. (iv) Dynamical calculations as those presented below may provide a "microscopic" justification for purely probabilistic models of bacterial motility [40]. (v) Depending on the swimmer size, we find a rather sharp transition from purely Brownian to quasi-ballistic motions. From a (bio-)physical perspective, it is remarkable that the transition occurs when the 3-sphere ballistic motions are encoded in the 'off-diagonal' components \( \mathcal{H}(\alpha \beta) \), \( \alpha \neq \beta \). If these hydrodynamic interactions are neglected, corresponding to the (infinitely dilute) limit case \( \mathcal{H}(\alpha \beta) = 0 \), Eq. (1) reduces to an 'ordinary' Smoluchowski equation with a diffusion constant \( D_\alpha = k_B T / \gamma_\alpha \) for each sphere.

Here, we are interested in the effects of hydrodynamic interactions, corresponding to \( \mathcal{H}(\alpha \beta) \neq 0 \). A simple approximation for \( \mathcal{H}(\alpha \beta) \), obtained by solving the Stokes equation for a point-like source, is the Oseen-tensor [44, 45]

\[
\mathcal{H}_O^{\alpha \beta} = \frac{1}{8 \pi \mu r_{\alpha \beta}} \left( \delta_{ij} + \frac{r_{\alpha \beta} \mathbf{r}_{\alpha \beta}}{r_{\alpha \beta}^2} \right), \quad \alpha \neq \beta, \tag{2b}
\]

where \( r_{\alpha \beta} \) is the distance between the center of mass of the \( \alpha \)th swimmer and that of the \( \beta \)th swimmer. However, the associated diffusion tensor \( D^O := k_B T \mathcal{H}_O \) is not necessarily positive definite, leading to unphysical behavior if sphere separations become too small [42, 43]. In our numerical simulations we shall therefore use the improved approximation

\[
\mathcal{H}_M^{\alpha \beta} = \mathcal{H}_O^{\alpha \beta} + \frac{(\sigma_\alpha^2 + \sigma_\beta^2)}{24 \pi \mu r_{\alpha \beta}^3} \left( \delta_{ij} - 3 \frac{r_{\alpha \beta} \mathbf{r}_{\alpha \beta}}{r_{\alpha \beta}^2} \right), \tag{2c}
\]

which was derived by Mazur [44]. The additional term on the right-hand side of Eq. (2c) can be understood as the next-order correction in a radius-over-distance expansion of the mobility tensor for two spheres [45]. For spheres of equal size \( a_\alpha = a_\beta \), the tensor \( \mathcal{H} = \mathcal{H}_M \) defined by Eqs. (2a) and (2c), reduces to the Rotne-Prager-Yamakawa tensor [44, 46]. While Eq. (2c) gives a more accurate description than Eq. (2b) at moderate densities, both expressions become invalid if the distance between spheres becomes very small. At very high densities, when sphere-sphere collisions dominate the dynamics, near-field hydrodynamics and lubrication effects must be modeled more carefully [47]. In the present paper, however, we focus on systems that can be described by Eq. (2c).

Unlike the Oseen tensor \( \mathcal{H}_O \) from Eq. (2b), the tensor \( \mathcal{H} = \mathcal{H}_M \) is positive definite for \( r_{\alpha \beta} > a_\alpha + a_\beta \) and thus can be Cholesky-decomposed in the form

\[
\mathcal{H}(\alpha \beta) = \frac{1}{2} C(\alpha \beta)(\gamma k) C(\beta \gamma)(\gamma k), \tag{3}
\]

The decomposition (3) is crucial if one wishes to find a Langevin representation for the stochastic process.
\( \{X_{(a)}(t)\} \) described by the KSE \( \mathcal{H} \): Upon noting that \( \{14\} \)

\[ \partial_{(a)} \mathcal{H}_{(a)(\beta j)} \equiv 0 \quad (4) \]

holds (for both \( \mathcal{H}^{\text{O}} \) and \( \mathcal{H}^{\text{M}} \), one finds that the KSE \( \mathcal{H} \) corresponds to the following Ito-Langevin equation \( \{15\} \)

\[ dX_{(a)}(t) = \mathcal{H}_{(a)(\beta j)}F_{(\beta j)} \, dt + \left( k_B \mathcal{T} \right)^{1/2} C_{(a)(\gamma k)} \xi_{(\gamma k)}(t). \quad (5) \]

Here, \( \{F_{(\beta j)}\} := \{-\partial_{(\beta j)} U\} \) comprises the deterministic forces acting on the spheres, and \( \{B_{(\gamma k)}(t)\} \) is a collection of standard Wiener processes; i.e., the increments \( dB_{(\gamma k)}(t) := B_{\gamma k}(t+dt) - B_{\gamma k}(t) \) are independent Gaussian random numbers with distribution

\[ \mathcal{P}\{dB_{(\gamma k)}(t) \in [u, u + du]\} = \frac{e^{-u^2/2dt}}{(2\pi dt)^{1/2}} \, du, \quad (6) \]

and, according to the Ito scheme \( \{16\} \), the coefficients \( C_{(a)(\gamma k)} \) are to be evaluated at time \( t \). For completeness, we still note that, upon formally dividing by \( dt \), the stochastic differential equation \( \{15\} \) can be rewritten as a `standard' Langevin equation:

\[ \dot{X}_{(a)}(t) = \mathcal{H}_{(a)(\beta j)}F_{(\beta j)} + \left( k_B \mathcal{T} \right)^{1/2} C_{(a)(\gamma k)} \xi_{(\gamma k)}(t), \quad (7a) \]

where \( \dot{X}_{(a)}(t) := dX_{(a)}(t)/dt \) denotes the velocity, and \( \xi_{(\gamma k)}(t) := dB_{(\gamma k)}(t)/dt \) represents Gaussian white noise, i.e.,

\[ \langle \xi_{(\alpha)}(t) \rangle = 0, \quad \langle \xi_{(\alpha)}(t)\xi_{(\beta)}(t') \rangle = \delta_{\alpha\beta} \delta(t-t'). \quad (7b) \]

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**B. Swimming mechanism**

Having discussed how to implement fluctuations, we still need to specify the swimming mechanism. To this end, consider two spheres \( \alpha \) and \( \beta \) that form the leg of a swimmer. We assume that the internal forces between beads \( \alpha \) and \( \beta \), which generate the swimming stroke, can be derived from a time-dependent potential of the form

\[ U_{\text{leg}}(t, d_{\alpha\beta}) = \frac{k_0}{2} \{d_{\alpha\beta} - [\ell + \lambda_{\alpha\beta} \sin(\varphi t + \varphi_{a\beta})]\}^2, \quad (8a) \]

with \( d_{\alpha\beta}(t) := |X_\alpha(t) - X_\beta(t)| \) denoting the distance between the spheres, \( \lambda_{\alpha\beta} \) the approximate amplitude of the stroke, and \( \ell > a_\alpha + a_\beta + \lambda_{\alpha\beta} \) the mean length of the leg. The potential \( U_{\text{leg}} \) gives rise to two characteristic time-scales: the driving period \( T_\omega := 2\pi/\omega \) and, for a sphere of mass \( M_\alpha \), the oscillator period \( T_0 := 2\pi/\sqrt{k_0/M_\alpha} \). Since we are interested in the over-damped regime, these time scales must be long compared to the characteristic damping time \( T_\gamma := M_\alpha/\gamma_\alpha \). More precisely, we have to impose

\[ T_\gamma \ll T_0 \ll T_\omega \quad (8b) \]

corresponding to slow driving and fast relaxation. The constraint \( \{17\} \) ensures that our swimmers behave similar to a shape-driven swimmer \( \{18\} \).

In the remainder, we shall focus on 3-sphere swimmers, representing the smallest self-swimming system within our approach (two-sphere swimmers can achieve active locomotion only due to collective effects \( \{19\} \)). We consider three spheres \( \{\alpha, \beta, \gamma\} \) forming a swimmer with central sphere \( \beta \), e.g., in the case of a single swimmer \( \{\alpha, \beta, \gamma\} = \{1, 2, 3\} \) with middle sphere \( \beta = 2 \). The legs are given by \( d_{\alpha\beta} := X_\beta - X_\alpha \) and \( d_{\beta\gamma} := X_\gamma - X_\beta \), and we still define normalized connectors

\[ n_{\alpha\beta} := d_{\alpha\beta}/d_{\alpha\beta} , \quad n_{\beta\gamma} := d_{\beta\gamma}/d_{\beta\gamma} . \]

In order to ensure that the swimmer moves quasi-linearly \( \{22\} \), we introduce a stiffness potential

\[ U_{\text{lin}} = \frac{K}{2} \ell^2 (n_{\alpha\beta} \cdot n_{\beta\gamma} - 1)^2, \quad (9) \]

which, for \( K \gg k_0 \), penalizes bending. The resulting force components \( F_{\alpha k}^{\text{lin}} := -\partial_{(\alpha)} U_{\text{lin}} \) read explicitly

\[ F_{\alpha k}^{\text{lin}} = -\frac{Q}{d_{\alpha\beta}} (\delta_{ik} - n_{\alpha\beta} n_{\alpha\beta k}) n_{\beta\gamma i}, \quad (10a) \]

\[ F_{\gamma k}^{\text{lin}} = \frac{Q}{d_{\beta\gamma}} (\delta_{ik} - n_{\beta\gamma} n_{\beta\gamma k}) n_{\alpha\beta i}, \quad (10b) \]

\[ F_{\beta k}^{\text{lin}} = -(F_{\alpha k}^{\text{lin}} + F_{\gamma k}^{\text{lin}}), \quad (10c) \]

where \( n_{\alpha\beta i} := d_{\alpha\beta i}/d_{\alpha\beta} \) and

\[ Q := K \ell^2 (n_{\alpha\beta} \cdot n_{\beta\gamma} - 1) . \quad (10d) \]

Equations \( \{8\} \) and \( \{13\} \) provide a convenient way of modeling and simulating rigid or flexible \( p \)-sphere swimmers by means of potentials. We note that, by construction, the sum over the internal swimmer forces is zero. The total potential \( U \) appearing in the KSE \( \{14\} \) is obtained by summing over all effective interaction potentials \( \{8\} \) and \( \{13\} \).

**III. ANALYTICAL RESULTS**

We next summarize formulae for the correlation time of the orientation vector, the mean swimmer velocity and the spatial mean square displacement of an isolated 3-sphere swimmer. These analytical results can be obtained from the Langevin equation \( \{15\} \) by using the Oseen approximation \( H \simeq H^{\text{O}} \), and their explicit derivation is discussed in the Appendix \( \{20\} \).

A swimmer’s motion can be characterized by its geometric center

\[ R(t) := \frac{1}{3}(X_1 + X_2 + X_3) \quad (11a) \]

and the orientation vector

\[ N(t) := \frac{X_3 - X_1}{|X_3 - X_1|} \quad (11b) \]
We are interested in determining the mean square displacement
\[ D_R(t) := \langle [R(t) - R(0)]^2 \rangle, \]
and the correlation function
\[ D_N(t) := \langle N(t)N(0) \rangle, \]
where the average is taken over fluctuations in the fluid (i.e., over all realizations of the Wiener process).

It is convenient to discuss \( D_N(t) \) first. For a deterministic initial state \( N(0) = (N_k(0)) \), we can write \( D_N(t) = \langle N_k(t) \rangle N_k(0) \) with a summation over equal indices. To obtain an analytical formula for \( \langle N_k(t) \rangle \), we assume that Eq. (8a) holds true and that bending is negligible, \( K \gg k_0 \). Then the swimmer behaves like a stiff, shape-driven Najafi-Golestanian \[20\] swimmer and we can approximate
\[ d_{12} := X_2 - X_1 \approx N \, d_{12}, \]
\[ d_{23} := X_3 - X_2 \approx N \, d_{23}, \]
\[ d_{13} := X_3 - X_1 \approx N \, (d_{12} + d_{23}), \]
where, cf. Eq. (8a),
\[ d_{12} = \ell + \lambda_{12} \sin(\omega t + \varphi_{12}), \]
\[ d_{23} = \ell + \lambda_{23} \sin(\omega t + \varphi_{23}). \]
Adopting the Oseen approximation \( \mathcal{H} \approx \mathcal{H}^O \), one can derive from the Langevin equations (5) the following linear evolution equation (see App. A)1
\[ \langle \dot{N}_k \rangle = -\frac{k_B T}{2\pi \mu d_{13}^2} \left[ \frac{2}{3} \left( \frac{d_{13}}{a_1} + \frac{d_{13}}{a_3} \right) - 1 \right] \langle N_k \rangle, \]
where \( \langle \dot{N}_k \rangle := \langle dN_k(t)/dt \rangle \). The \( 1/a_\alpha \)-parts are contributions to the rotation rate due to noise on the spheres, whereas the \( 1/d_{13}^2 \)-contribution is a correction due to hydrodynamic interactions. Equation (14) can be solved exactly. The solution exhibits an exponentially decaying oscillatory behavior due to the periodicity of the swimming stroke \( d_{13} \). However, for \( \ell \gg \max(\lambda_{a\beta}) \) it suffices to approximate \( d_{13} \approx 2\ell \), yielding an exponential decay \( D_N(t) \approx \exp(-t/\tau_N) \) with orientation correlation time
\[ \tau_N \approx \left\{ \frac{k_B T}{16\pi \mu \ell^3} \left[ \frac{4}{3} \left( \frac{\ell}{a_1} + \frac{\ell}{a_3} \right) - 1 \right] \right\}^{-1}. \]

The time parameter \( \tau_N \) not only determines the temporal correlation of the orientation vector, it also plays an important role for the dynamics of the geometric center \( R(t) \). As shown in App. A, the mean swimmer velocity \( \langle \dot{R}(t) \rangle \) is governed by the equation
\[ \langle \dot{R}_k \rangle = \frac{A_1}{3} \langle F_{(1k)} \rangle + \frac{A_3}{3} \langle F_{(3k)} \rangle, \]
where
\[ \langle F_{(1k)} \rangle = -\frac{B_3 \langle d_{23k} \rangle + C \langle d_{23k} \rangle}{B_3 B_3 - C^2}, \]
\[ \langle F_{(3k)} \rangle = \frac{C \langle d_{12k} \rangle + B_3 \langle d_{23k} \rangle}{B_1 B_3 - C^2}, \]
are the noise-averaged internal forces on the first and third sphere (the force on the central sphere can be eliminated by virtue of \( F_{(1k)} + F_{(2k)} + F_{(3k)} \equiv 0 \), respectively, and
\[ \langle \dot{d}_{12k} \rangle = \langle \dot{N}_k \rangle d_{12} + \langle N_k \rangle \dot{d}_{12}, \]
\[ \langle \dot{d}_{23k} \rangle = \langle \dot{N}_k \rangle d_{23} + \langle N_k \rangle \dot{d}_{23}, \]
the mean change of the leg vectors due stochastic rotations and swimming strokes, with abbreviations
\[ A_1 := \frac{1}{\gamma_1} - \frac{1}{\gamma_2} + \frac{1}{4\pi \mu} \left( \frac{1}{d_{13}^2} - \frac{1}{d_{23}^2} \right), \]
\[ A_3 := \frac{1}{\gamma_3} - \frac{1}{\gamma_2} + \frac{1}{4\pi \mu} \left( \frac{1}{d_{13}^2} - \frac{1}{d_{13}^2} \right), \]
\[ B_1 := \frac{1}{\gamma_1} + \frac{1}{\gamma_2} - \frac{1}{2\pi \mu d_{12}}, \]
\[ B_3 := \frac{1}{\gamma_2} + \frac{1}{\gamma_3} - \frac{1}{2\pi \mu d_{23}}, \]
\[ C := \frac{1}{\gamma_2} + \frac{1}{4\pi \mu} \left( \frac{1}{d_{13}^2} - \frac{1}{d_{23}^2} - \frac{1}{d_{13}^2} \right). \]
Since the quantities \( \langle N_k \rangle, \langle \dot{N}_k \rangle, d_{a\beta} \), and \( d_{a\beta} \) are known, Eqs. (10) provide a closed analytical result for the mean velocity \( \langle R_k \rangle \) of a shape-driven swimmer (within the Oseen approximation). In particular, Eqs. (10) generalize the corresponding velocity formulas for a deterministic swimmer, recently obtained by Golestanian and Ajdari [27], to the ”noisy swimming” regime.

For realistic swimmer parameters the orientation correlation time \( \tau_N \) is typically much larger than the driving period \( T_\omega = 2\pi/\omega \). In this case, the rather lengthy result (10) can be considerably simplified (see last part of App. A for details) to read
\[ \langle \dot{R}(t) \rangle = \dot{V} \langle N(t) \rangle. \]
Finally, let us still consider the mean square displacement $D_R(t) := \langle [R(t) - R(0)]^2 \rangle$ for a stiff, shape-driven 3-sphere swimmer described by Eqs. (14). As discussed in App. A21 by starting from the Langevin equation for $R(t)$, one can show that $D_R(t)$ decomposes into the form

$$D_R(t) = D_R^p(t) + D_R^\tau(t), \quad \text{(20a)}$$

where the first part

$$D_R^p(t) = \frac{1}{9} \frac{k_B T}{\pi \mu} \left( \frac{1}{a_1} + \frac{1}{a_2} + \frac{1}{a_3} \right) t + \frac{2}{9} \frac{k_B T}{\pi \mu} \int_0^t ds \left( \frac{1}{d_{12}} + \frac{1}{d_{23}} + \frac{1}{d_{13}} \right) \quad \text{(20b)}$$

comprises passive Brownian motion contributions due to thermal diffusion of the spheres (first line) and hydrodynamic Oseen interactions between them (second line), while the second part

$$D_R^\tau(t) \simeq \bar{V} \int_0^t ds \int_0^s du \langle N(s)N(u) \rangle \quad \text{(20c)}$$

is the contribution due to active self-swimming. Similar to Eq. (17), the expression (20c) is valid if the orientation correlation time is much larger than the stroke period, $\tau_N \gg \tau_w$. Inserting the above result $\langle N(t)N(s) \rangle \simeq \exp(-t/\tau_N)$ and approximating $d_{12} = d_{23} = d_{13}/2 \simeq \bar{t}$, we obtain for the spatial mean square displacement

$$D_R(t) \simeq \frac{1}{9} \frac{k_B T}{\pi \mu} \left( \frac{1}{a_1} + \frac{1}{a_2} + \frac{1}{a_3} + \frac{5}{\bar{t}} \right) t + 2 \bar{V}^2 \tau_N \left[ t + \tau_N (e^{-t/\tau_N} - 1) \right]. \quad \text{(21)}$$

The approximate result (21) provides a coarse-grained stroke-averaged description of the translational diffusion (details of the swimming stroke are encoded in $\bar{V}$). An analogous formula can be used to describe the diffusion of a spherical, chemically driven microswimmer [6]. By virtue of Eq. (21), we can readily distinguish three distinct regimes:

(i) For $t \ll \tau_N$ we can expand the exponential term to linear order and find

$$D_R(t) \simeq D_R^p(t), \quad \text{(22a)}$$

i.e., passive Brownian motion dominates on very short time scales.

(ii) For $t \lesssim \tau_N$ we need to include terms quadratic in $t/\tau_N$ and obtain

$$D_R(t) \simeq D_R^p(t) + \frac{\bar{V}^2 t^2}{\tau_N}, \quad \text{(22b)}$$

i.e., ballistic motion can dominate on intermediate time scales provided $\bar{V}^2/\tau_N$ is large enough (cf. examples below).

(iii) For $t \gg \tau_N$, we recover diffusive behavior

$$\lim_{t \to \infty} \frac{D_R(t)}{t} = \frac{D_R^p(t)}{t} + 2\bar{V}^2 \tau_N. \quad \text{(22c)}$$

If the swimmer is constructed such that $2\bar{V}^2 \tau_N \gg D_R^p(t)/t$, then its diffusive behavior at large times is due to noise-induced rotation (with persistence time $\tau_N$).

In a sense, the above results provide a ‘microscopic’ justification for the assumptions made by Lovely and Dahlquist [31], who studied purely probabilistic models of bacterial motion. We also note that the asymptotic behavior for $t \gg \tau_N$ and $2\bar{V}^2 \tau_N \gg D_R^p(t)/t$ agrees qualitatively with results reported by Lobaskin et al. [32] for triangular swimmers in the moderate Reynolds number regime $R \sim 1$. In this context, we also mention recent work by Golestanian et al. [50], who discuss similar scaling relations for the diffusion of phoretic swimmers.

In the remainder, we are going to compare the analytical predictions with results of computer simulations, based on a direct numerical integration of the Langevin equations (5) for the spheres. Our main focus is on the transition from the passive Brownian motions to the active swimming regime.

**IV. SWIMMER TUNING & NUMERICAL SIMULATIONS**

We simulate a single 3-sphere swimmer described by the interaction potentials (5) and (9) and governed by the Langevin equation (5). We consider identical spheres of radius $a_\alpha = a$, mass $M_\alpha = M$, and equal stroke amplitudes $\lambda_{12} = \lambda_{23} = \lambda$. The density of the spheres is chosen as $\rho = 10^3$ kg/m$^3$ (water), and the fluid is water at room temperature [$\mu = 10^{-3}$ kg/(m$\cdot$s), $T = 300$ K]. By fixing the parameters of the spring and bending potentials as $k_0 = 10^{-4}$ kg/s$^2$, $\omega = 10^3$ Hz and $K = 10k_0$, we satisfy the time scale condition [33] while ensuring that the swimmer behaves approximately stiff and shape-driven.

The velocity $\bar{V}$ of the swimmer is optimized by choosing $\Delta \phi = \pi/2$, cf. Eq. (23a). We are primarily interested in understanding how a change of the swimmer size may affect the diffusive behavior. We therefore fix the ratios $\ell/a = \ell/\lambda = 10$ and only vary the leg length $\ell$ from 1 to 10 $\mu$m in our simulations (i.e., the mean swimmer length is $\Lambda = 2\ell$). Put differently, we scale the swimmer proportionally by varying $\ell$. Having specified all parameters, it is useful to summarize the relevant formulae for our choice:

$$\bar{V} \simeq \frac{7}{24} \omega \left( \frac{\lambda^2}{\ell^2} \right) \sin \Delta \phi = 0.292 \frac{\ell}{s}, \quad \text{(23a)}$$

$$\tau_N \simeq \frac{16 \pi \mu \ell^3}{k_B T} \left( \frac{8\ell}{3a} - 1 \right)^{-1} = 0.473 \frac{\ell^3 s}{\mu \text{m}^3}, \quad \text{(23b)}$$

$$\frac{D_R^p}{t} \simeq \frac{1}{9} \frac{k_B T}{\pi \mu} \left( \frac{3}{a} + \frac{5}{\bar{t}} \right) = 5.127 \frac{\text{mm}^3}{\ell s}. \quad \text{(23c)}$$
It is remarkable that increasing the swimmer size by one order of magnitude increases the correlation time by three orders of magnitude.

and

\[ 2 \bar{V}^2 \tau_N = 0.080 \frac{\ell^5}{\mu m^5 s}. \]  

(23d)

It is remarkable that increasing the swimmer size by one order of magnitude increases the orientation correlation time \( \tau_N \) by three orders of magnitude.

Figures 1 and 2 depict the results of numerical simulations (symbols) of the Langevin equations (5) and also the corresponding theoretical predictions (dashed lines). The numerical data points represent averages over 100 trajectories with identical initial conditions. More precisely, at time \( t = 0 \) the swimmer is pointing along the \( x_3 \)-axis with the first sphere being located at the origin, i.e., \( X_1(0) = 0 \), \( X_2(0) = \ell N(0) \), and \( X_3(0) = [2\ell - \lambda \sin(\Delta \psi)] N(0) \), where \( N(0) = (0, 0, 1) \).

As evident from the diagrams in Fig. 1 and 2 the results of the numerical simulations are very well matched by the theoretical curves over several orders of magnitude in time. In particular, for a leg length in the range \( \ell \sim 5 \mu m \) (red ‘+’/green ‘x’-symbols) one readily observes the three aforementioned regimes: (i) Brownian diffusion at small time scales \( t \ll \tau_N \), (ii) ballistic behavior at intermediate time scales, and (iii) quasi-diffusive behavior due to noise-induced rotation for \( t \gg \tau_N \).

We conclude the discussion of the numerical results by addressing a few technical aspects that might be relevant and helpful for future simulations. When considering ensembles with \( N > 1 \) swimmers the computationally most expensive step is the Cholesky decomposition of the diffusion tensor, see Eq. (3), which is approximately of the order \( O[(pN)^3] \) \( 30 \). It is also worthwhile to briefly comment on the choice of the time step \( dt \) in the Langevin simulations. Ideally, one would like to choose \( dt \) smaller than the smallest dynamical time scale in the system, which for our model is given by the damping time \( T_\gamma = M/(6\pi \mu a) \). For the swimmer parameters considered here we find \( T_\gamma \sim 2 \times 10^{-9} (\ell/\mu m)^2 \)s, which means that adopting \( dt \sim T_\gamma \) would not allow us to simulate experimentally accessible time scales in the seconds range. Since we are not interested in the dynamical details at very short time scales, we choose in our simulations the time step larger than \( T_\gamma \), but much smaller than the period \( T_\omega \) of a swimming stroke by fixing \( dt = 10^{-3} T_\omega \) for \( \ell < 5 \mu m \) and \( dt = 10^{-2} T_\omega \) if \( \ell \geq 5 \mu m \). We verified, however, that for intermediate time scales (of the order of a few stroke periods \( T_\omega \sim 6 \times 10^{-3} \)s) the numerical results for the mean square displacement and other statistical observables agree with those obtained for very short time steps \( dt = 0.1 T_\gamma \). Generally, a satisfactory resolution of the bending and relaxation dynamics of the legs/spheres would require \( dt \ll (M/K)^{1/2} \) and \( dt \ll (M/k_0)^{1/2} \), respectively.

V. CONCLUSIONS

Understanding the interplay between Brownian motion, hydrodynamic interactions, and self-propulsion is a prerequisite for understanding the dynamics of bacteria and artificial swimming devices at the microscale. In the first part, we discussed how one can model these phenomena by means of stochastic processes (overdamped
Langevin equations). Subsequently, as a first application, we focussed on the size-dependence of diffusive behavior at low Reynolds numbers ($\mathcal{R} \ll 1$) for a quasi-linear 3-sphere swimmer model. Our theoretical analysis complements a recent experimental study by Howse et al. [47], who investigated the diffusion of chemically driven, spherical colloids, and theoretical work by Lobaskin et al. [52], who considered the Brownian dynamics of an artificial triangular microswimmer at moderate Reynolds numbers ($\mathcal{R} \sim 1$).

Starting from the Kirkwood-Smoluchowski equation [34, 35, 36, 37], we derived analytical results for the orientation correlation time, the mean velocity, and the mean square displacement of an overdamped, quasi-linear 3-sphere swimmer [24, 25]. Analytical formulae as derived here are useful for testing numerical simulations and (in)validating simplified probabilistic models [33]. Moreover, they provide detailed insight into the size-regulated transition from predominantly random to quasi-ballistic motions.

The proposed method of modeling swimmers by effective potentials within a Langevin scheme can be readily extended to study complex behavior in larger swimmer ensembles. However, at high swimmer densities, collisions and near-field hydrodynamics affect the diffusive behavior [47, 51, 52] and it will be necessary to modify the hydrodynamic interaction tensor accordingly. Generally, a useful dimensionless quantifier for the efficiency of active swimming relative to diffusion is given by the ratio

$$\epsilon = \frac{\tau_N}{\Lambda/\mathcal{V}}.$$  \hspace{1cm} (24)

The denominator corresponds to the time needed by a unperturbed swimmer of velocity $\mathcal{V}$ to move one body length $\Lambda$, and the swimmer geometry is encoded in the orientation correlation time $\tau_N$. For $\epsilon \gg 1$ ($\epsilon \ll 1$) self-propulsion is effective (non-effective). For non-isolated swimmers, $\tau_N$ is not only determined by thermal effects, but also by collisions with other swimmers [51, 52].

With regard to future studies we note that the combination of thermal fluctuations and hydrodynamic coupling might also lead to interesting behavior in simple arrangements of microswimmers. For example, experiments have shown that colloidal spheres localized in an array of optical traps create memory effects [53] and driven vibrations [54]. Our formalism provides a starting point for the investigation of many self-propelled bodies in separate potentials, which could be helpful for interpreting experimental data of trapped bacteria or for constructing pumps from a collection of microswimmers.

To summarize, the above results may provide guidance for constructing artificial microswimmers or pumps that work efficiently in the critical transition region that separates Brownian from quasi-deterministic motions. In particular, by tuning the parameters to the narrow cross-over region one could construct swimmers that explore with high probability a maximized volume fraction within a given period of time. The fact that many bacteria live near or exactly in this niche [10] suggests that this may indeed be a useful strategy. Thus, exploiting the interplay between noise and active self-motion could lead to novel applications [55], e.g., with regard to the controlled transport [56] and distribution of chemical and biological substances in small scale technical devices or even within the human body.

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**APPENDIX A: CALCULATIONS**

This appendix provides derivations of analytical results for the orientation correlation function, the mean velocity, and the spatial mean square displacement from the Langevin equation [43]. Our calculations are based on the following simplifying assumptions:

(i) The motion of the 3-sphere swimmer is approximately stiff and shape-driven, i.e.,

$$d_{12} := X_2 - X_1 \simeq N d_{12},$$ \hspace{1cm} (A1a)

$$d_{23} := X_3 - X_2 \simeq N d_{23},$$ \hspace{1cm} (A1b)

$$d_{13} := X_3 - X_1 \simeq N (d_{12} + d_{23}),$$ \hspace{1cm} (A1c)

where

$$d_{12} = \ell + \lambda_{12} \sin(\omega t),$$ \hspace{1cm} (A1d)

$$d_{23} = \ell + \lambda_{23} \sin(\omega t - \Delta \varphi).$$ \hspace{1cm} (A1e)

In this case the internal forces, which generate the swimming strokes, point along the swimmer’s axis and we may write

$$F_{1i} = g_1 N_i, \quad F_{3i} = g_3 N_i$$ \hspace{1cm} (A2a)

and, with $F_{3i} + F_{2i} + F_{1i} = 0$,

$$F_{2i} = -(g_1 + g_3) N_i,$$ \hspace{1cm} (A2b)

where $g_\alpha$ is the force amplitude, and $N_i$ denotes a component of the orientation vector

$$N(t) := \frac{X_3 - X_1}{|X_3 - X_1|}.$$ \hspace{1cm} (A2c)

(ii) We adopt the Oseen approximation, i.e., $\mathcal{H} \simeq \mathcal{H}^O$, where

$$\mathcal{H}^{O(\alpha)(ij)} := \frac{1}{8\pi \mu d_{\alpha \beta}} \left( \delta_{ij} + \frac{d_{\alpha \beta} d_{\alpha \beta}}{d_{\alpha \beta}^2} \right),$$ \hspace{1cm} (A3)

$$\simeq \frac{1}{8\pi \mu d_{\alpha \beta}} (\delta_{ij} + N_i N_j).$$ \hspace{1cm} (A3)

The second line follows from assumption (A1).
1. Orientation correlation function

Given a deterministic initial state $N(0) = (N_k(0))$, we are interested in $D_N(t) := \langle N(t)N(0) \rangle = \langle N_k(t)N_k(0) \rangle$. The first step is to find the stochastic differential equation (SDE) for the orientation vector $N(t)$. This can be achieved by virtue of the Ito formula [49, 57], yielding

$$dN_k(t) = \frac{\partial_{(\alpha)}N_k}{d_{13}} dX_{(\alpha)} + D_{(\alpha)(\beta)} \partial_{(\alpha)} \partial_{(\beta)} N_k dt,$$  \hspace{1cm} (A4)

where $dX_{(\alpha)}(t)$ is governed by Eq. [5], and the diffusion tensor is given by $D := k_B T \mathcal{H} \simeq k_B T \mathcal{H}^O$.

To determine $\langle \dot{N}(t) \rangle$, we use that $\langle C(\alpha_i)(\gamma_k) dB(\gamma_k) \rangle = 0$ for an Ito SDE, and therefore

$$d(X_{(\alpha)(\beta)}) = \langle H_{(\alpha)(\beta)} F_{(\beta)} \rangle dt.$$ \hspace{1cm} (A5)

Taking the average of Eq. (A4) and inserting (A5), we obtain

$$\langle \dot{N}(t) \rangle = \langle H_{(\alpha)(\beta)} F_{(\beta)} \rangle \partial_{(\alpha)} N_k + \langle D_{(\alpha)(\beta)} \partial_{(\alpha)} \partial_{(\beta)} N_k \rangle,$$ \hspace{1cm} (A6)

where $d(\dot{N}(k)) := \langle dN_k(t) \rangle dt$. We next evaluate the two terms the rhs. of Eq. (A6) separately. To this end we note that

$$\partial_{(\alpha)} N_k = \frac{1}{d_{13}} (\delta_{3\alpha} - \delta_{1\alpha}) (\delta_{jk} - N_j N_k),$$ \hspace{1cm} (A7)

yielding for the first term

$$\mathcal{H}_{(\alpha)(\beta)} F_{(\beta)} \partial_{(\alpha)} N_k = \left[ \mathcal{H}_{(3\alpha)(\beta)} - \mathcal{H}_{(1\alpha)(\beta)} \right] \times \frac{F_{(\beta)}}{d_{13}} (\delta_{ik} - N_i N_k).$$ \hspace{1cm} (A8)

Using Oseen approximation [A3], we find

$$\mathcal{H}_{(3\alpha)(\beta)} F_{(\beta)} = \left[ \frac{g_3}{\gamma_3} + \frac{g_1}{4 \pi \mu d_{31}} - \frac{(g_3 + g_1)}{4 \pi \mu d_{32}} \right] N_i,$$

and, similarly, $\mathcal{H}_{(1\alpha)(\beta)} F_{(\beta)} \propto N_i$. Taking into account that

$$N_i (\delta_{ik} - N_i N_k) \equiv 0,$$ \hspace{1cm} (A9)

the first term on the rhs. of Eq. (A6) vanishes, and Eq. (A6) reduces to

$$\langle \dot{N}(t) \rangle = \langle D_{(\alpha)(\beta)} \partial_{(\alpha)} \partial_{(\beta)} N_k \rangle.$$ \hspace{1cm} (A10)

By virtue of Eq. (A7), we find

$$\partial_{(\alpha)} \partial_{(\beta)} N_k = \frac{1}{d_{13}} (\delta_{3\beta} - \delta_{1\beta}) (\delta_{3\alpha} - \delta_{1\alpha}) \times$$

$$3 N_j N_k N_i - N_j \delta_{ik} - N_k \delta_{ij} - N_i \delta_{jk}).$$ \hspace{1cm} (A11)

To obtain the rhs. of (A10), we still need to contract with the diffusion tensor $D_{(\alpha)(\beta)}$. This results in two contributions: From the diagonal part we get

$$k_B T \sum_{(\alpha)(\beta)} \frac{1}{\gamma_{\alpha}} (\delta_{3\alpha} - \delta_{1\alpha}) (\delta_{3\beta} - \delta_{1\beta}) \times$$

$$\frac{1}{d_{13}} (3 N_j N_k N_i - N_j \delta_{ik} - N_k \delta_{ij} - N_i \delta_{jk})$$

$$= -k_B T \left( \frac{1}{\gamma_1} + \frac{1}{\gamma_3} \right) \frac{2 N_k}{d_{13}},$$ \hspace{1cm} (A12a)

while the hydrodynamic off-diagonal terms give

$$k_B T \sum_{(\alpha)(\beta)} (1 - \delta_{\alpha\beta}) (\delta_{3\alpha} - \delta_{1\alpha}) (\delta_{3\beta} - \delta_{1\beta}) \times$$

$$\frac{\delta_{ij} + N_i N_j}{8 \pi \mu d_{\alpha\beta}} \times$$

$$\frac{1}{d_{13}} (3 N_j N_k N_i - N_j \delta_{ik} - N_k \delta_{ij} - N_i \delta_{jk})$$

$$= \frac{k_B T}{2 \pi \mu d_{13}^3} N_k.$$ \hspace{1cm} (A12b)

Combining the two contributions we find

$$\langle \dot{N}(t) \rangle = \left[ -k_B T \left( \frac{1}{\gamma_1} + \frac{1}{\gamma_3} \right) \frac{2 N_k}{d_{13}} + \frac{k_B T}{2 \pi \mu d_{13}^3} \right] (N_k),$$

which for $\gamma_\alpha = 6 \pi \mu a_i$ gives Eq. (13).

2. Motion of the geometric center

Following a similar procedure, we can derive analytical expression for the mean velocity $\langle \dot{R}(t) \rangle$ and the mean square displacement $\mathcal{D}(R)(t)$.

a. Mean velocity

First, we would like to determine the mean velocity $\langle \dot{R}(t) \rangle$ of the swimmer’s geometric center

$$\dot{R}(t) := \frac{1}{3} (X_1 + X_2 + X_3).$$ \hspace{1cm} (A13)

Averaging the stochastic differential equation

$$dR(t) := \frac{1}{3} (dX_1 + dX_2 + dX_3)$$ \hspace{1cm} (A14)

with respect to the underlying Wiener process and dividing by $dt$, we obtain

$$\langle \dot{R}(t) \rangle = \frac{1}{3} \sum_{\alpha=1}^3 \left\langle \mathcal{H}_{(\alpha)(\beta)} F_{(\beta)} \right\rangle$$

$$= \frac{1}{3} \sum_{\alpha=1}^3 \left\langle \frac{F_{(\alpha)}}{\gamma_{\alpha}} + (1 - \delta_{\alpha\beta}) \mathcal{H}_{(\alpha)(\beta)} F_{(\beta)} \right\rangle.$$ \hspace{1cm} (A15)
Considering as before a stiff, shape-driven swimmer and Oseen interactions \( \mathcal{H} = 3 \mathcal{C}^O \), we have \( F_(\beta_j) \simeq g_\beta N_j \) and, therefore,

\[
(1 - \delta_\alpha \beta) \mathcal{H}(\alpha_i)(\beta_j) F_(\beta_j) \simeq \sum_\beta \left( \frac{\delta_\alpha \beta + N_\beta N_j}{8\pi \mu d_\alpha \beta} \right) g_\beta N_j
\]

\[
= N_j \sum_\beta \frac{g_\beta}{4\pi \mu d_\alpha \beta}.
\] (A16)

Inserting this into Eq. (A15) gives

\[
\langle \dot{R}_i(t) \rangle = \frac{1}{3} \left( N_i g_1 \right) \left[ \frac{1}{\gamma_3} - \frac{1}{\gamma_2} \right] g_2 + \frac{1}{4\pi \mu d_{21}} + \frac{1}{4\pi \mu d_{13}}\right) + \frac{g_1}{4\pi \mu d_{12}} + \frac{g_3}{4\pi \mu d_{23}} \right)
\]

\[
\langle \dot{R}_i(t) \rangle = \frac{1}{3} \left( N_i g_1 \right) \left[ \frac{1}{\gamma_3} - \frac{1}{\gamma_2} \right] g_2 + \frac{1}{4\pi \mu d_{21}} + \frac{1}{4\pi \mu d_{13}}\right) + \frac{g_1}{4\pi \mu d_{12}} + \frac{g_3}{4\pi \mu d_{23}} \right)
\]

\[
= \frac{A_1}{3} \langle N_i g_1 \rangle + \frac{A_3}{3} \langle N_i g_3 \rangle.
\] (A17)

Consequently, to find \( \langle \dot{R}_i(t) \rangle \), we still need to determine the mean forces \( \langle F_(\beta_j) \rangle = \langle N_i g_\beta \rangle \) on the first and last sphere, \( \beta = 1, 3 \). This can be achieved as follows: Equation (A11) implies that

\[
\langle \dot{d}_{12k} \rangle = \langle N_k d_{12} \rangle + \langle N_k d_{12} \rangle, \quad \langle \dot{d}_{23k} \rangle = \langle N_k d_{23} \rangle + \langle N_k d_{23} \rangle.
\] (A18a)

(A18b)

On the other hand, from the definition of the vectors \( d_\alpha \beta \) and the Langevin equations for \( d_\alpha \), we have

\[
\langle \dot{d}_{12k} \rangle = \langle \mathcal{H}(2k)(\beta_j) F_(\beta_j) - \mathcal{H}(1k)(\beta_j) F_(\beta_j) \rangle, \quad \langle \dot{d}_{23k} \rangle = \langle \mathcal{H}(2k)(\beta_j) F_(\beta_j) - \mathcal{H}(2k)(\beta_j) F_(\beta_j) \rangle.
\] (A19a)

(A19b)

Inserting the explicit expressions for \( \mathcal{H}(\alpha_i)(\beta_j) \) and \( F_(\beta_j) \), Eqs. (A19) can be rewritten as

\[
\langle \dot{d}_{12k} \rangle = - \left[ \frac{1}{\gamma_1} + \frac{1}{\gamma_2} - \frac{1}{2\pi \mu d_{12}} \right] \langle N_k g_1 \rangle - \left[ \frac{1}{\gamma_2} - \frac{1}{4\pi \mu} \left( \frac{1}{d_{12}} + \frac{1}{d_{23}} - \frac{1}{d_{13}} \right) \right] \langle N_k g_3 \rangle
\]

\[
= -B_1 \langle N_k g_1 \rangle - C \langle N_k g_3 \rangle
\] (A20a)

and

\[
\langle \dot{d}_{23k} \rangle = \left[ \frac{1}{\gamma_2} - \frac{1}{4\pi \mu} \left( \frac{1}{d_{12}} + \frac{1}{d_{23}} - \frac{1}{d_{13}} \right) \right] \langle N_k g_1 \rangle + \left[ \frac{1}{\gamma_3} - \frac{1}{4\pi \mu} \right] \langle N_k g_3 \rangle
\]

\[
= C \langle N_k g_1 \rangle + B_3 \langle N_k g_3 \rangle.
\] (A20b)

Hence, in order to obtain the unknown expectation values \( \langle N_k g_1 \rangle \), we have to solve the linear system

\[
\langle \dot{d}_{12k} \rangle = -B_1 \langle N_k g_1 \rangle - C \langle N_k g_3 \rangle, \quad \langle \dot{d}_{23k} \rangle = C \langle N_k g_1 \rangle + B_3 \langle N_k g_3 \rangle,
\] (A21a)

(A21b)

with lhs. given by Eqs. (A19). This is easily done and we may summarize the result for the mean velocity:

\[
\langle \dot{R}_k(t) \rangle = \frac{A_1}{3} \langle N_k g_1 \rangle + \frac{A_3}{3} \langle N_k g_3 \rangle,
\] (A22a)

where

\[
\langle N_k g_1 \rangle = - \frac{B_3 \langle \dot{d}_{12k} \rangle + C \langle \dot{d}_{23k} \rangle}{B_1 B_3 - C^2}, \quad \langle N_k g_3 \rangle = C \langle \dot{d}_{12k} \rangle + B_1 \langle \dot{d}_{23k} \rangle \quad \frac{B_1 B_3 - C^2}{B_1 B_3 - C^2},
\] (A22b)

(A22c)

with

\[
\langle \dot{d}_{12k} \rangle = \langle N_k d_{12} \rangle + \langle N_k d_{12} \rangle, \quad \langle \dot{d}_{23k} \rangle = \langle N_k d_{23} \rangle + \langle N_k d_{23} \rangle.
\] (A22d)

(A22e)

Since the quantities \( \langle N_k \rangle \), \( \langle N_k \rangle \), \( \langle N_k \rangle \), \( \langle N_k \rangle \), \( A_1 \), \( B_1 \), and \( C \) are known we have thus obtained a closed analytical result for the mean swimmer velocity within the Oseen approximation. Analogous calculations can be performed for \( \mathcal{H}^M \), but do not yield much additional insight (for a single swimmer).

**Additional simplifications** If the orientation correlation time \( \tau_N \) is larger than the driving period \( T = 2\pi/\omega \) then

\[
\langle \dot{d}_{12k} \rangle \simeq \langle N_k \rangle \dot{d}_{12}, \quad \langle \dot{d}_{23k} \rangle \simeq \langle N_k \rangle \dot{d}_{23}.
\] (A23)

In this case, we may simplify

\[
\langle \dot{R}_k(t) \rangle \simeq \langle N_k(t) \rangle \dot{V}(t) \langle N_k(t) \rangle,
\] (A24a)

where

\[
V(t) = - \frac{A_1}{3} \left( \frac{B_3 \dot{d}_{12} + C \dot{d}_{23}}{B_1 B_3 - C^2} \right) + \frac{A_3}{3} \left( C \dot{d}_{12} + B_1 \dot{d}_{23} \right) \quad \frac{B_1 B_3 - C^2}{B_1 B_3 - C^2}
\] (A24b)

is a periodic function, \( V(t) = V(t + T_N) \). Since we assumed \( \tau_N \gg T_N \), we can achieve further simplification by replacing \( V(t) \) with its stroke-average

\[
\bar{V} := \int_t^{t+T_N} ds \langle V(s) \rangle,
\] (A25)

so that

\[
\langle \dot{R}_k(t) \rangle \simeq \bar{V} \langle N_k(t) \rangle.
\] (A26)
For example, when considering equal-sized beads with $a_\alpha = a$ and $\ell \gg \max\{a, \lambda_{12}, \lambda_{23}\}$, then
\[
\mathcal{V}(t) = \frac{a_\omega \lambda_{12}}{\ell} \cos(\omega t + \varphi_{12}) + \frac{a_\omega \lambda_{23}}{\ell} \cos(\omega t + \varphi_{23}) + \bar{V},
\]
where
\[
\bar{V} = \frac{7}{24} a_\omega \left( \frac{\lambda_{12} \lambda_{23}}{\ell^2} \right) \sin \Delta \varphi
\]  
(A27)
and $\Delta \varphi := \varphi_{12} - \varphi_{23}$, and higher order terms have been neglected.

b. Spatial diffusion

Using the result for $dR(t)$ from above, we may rewrite the mean square displacement $\mathcal{D}_R(t)$ as
\[
\mathcal{D}_R(t) := \langle [\mathbf{R}(t) - \mathbf{R}(0)]^2 \rangle = \int_0^t ds \int_0^t du \left\langle \left[ \frac{A_1}{3} N_k g_1 + \frac{A_3}{3} N_k g_3 \right]_s \times \left[ \frac{A_1}{3} N_k g_1 + \frac{A_3}{3} N_k g_3 \right]_u \right\rangle + \frac{1}{9} \sum_{\alpha, \alpha'}^3 \int \langle [C_{(ak)(\gamma n)}]_s dB_{(\gamma n)}(s) \times [C_{(ak')(\gamma' n')}][u dB_{(\gamma' n')}(u)] \rangle. \]  
(A28)

Here, we have again used that $\langle f(X_\alpha) dB_{(\gamma n)}(t) \rangle = 0$ holds for Itô integrals. We consider the two remaining integrals in Eq. (A28) separately, starting with the second one. We find
\[
\mathcal{D}_R^{\beta}(t) := \frac{1}{9} \sum_{\alpha, \alpha' = 1}^3 \int \langle [C_{(ak)(\gamma n)}]_s dB_{(\gamma n)}(s) \times [C_{(ak')(\gamma' n')}][u dB_{(\gamma' n')}(u)] \rangle
\]
\[
= \frac{2}{9} \sum_{\alpha, \alpha' = 1}^3 \int_0^t ds \langle D_{(ak)(\alpha k')} \rangle
\]
\[
= \frac{2}{9} k_B T \sum_{\alpha, \alpha' = 1}^3 (1 - \delta_{\alpha \alpha'}) \int_0^t ds \mathcal{H}_{(ak)(\alpha k')}^{Q},
\]
where
\[
\mathcal{H}_{(ak)(\alpha k')}^{Q} = \frac{\delta_{kk} + N_k N_k}{8 \pi \mu d_{\alpha \alpha'}} = \frac{1}{2 \pi \mu d_{\alpha \alpha'}}. \]  
(A29)

For spherical particles we have $\gamma = 6 \pi \mu a_\alpha$ and, therefore,
\[
\mathcal{D}_R^{\beta}(t) = \frac{1}{9} k_B T \left( \frac{1}{a_1} + \frac{1}{a_2} + \frac{1}{a_3} \right) t + \frac{2}{9} k_B T \left( \frac{1}{a_1} + \frac{1}{a_2} + \frac{1}{a_3} + \frac{5}{\ell} \right) t.
\]
(A30)

It remains to determine the first (double) integral in Eq. (A28), reading
\[
\mathcal{D}_R^{\alpha}(t) := \int_0^t ds \int_0^t du \left\langle \left[ \frac{A_1}{3} N_k g_1 + \frac{A_3}{3} N_k g_3 \right]_s \times \left[ \frac{A_1}{3} N_k g_1 + \frac{A_3}{3} N_k g_3 \right]_u \right\rangle.
\]

The subscripts indicate the time arguments in the bracketed expressions, respectively. Upon recalling that $F_{(ai)} = g_a N_i$ is the internal force acting on sphere $\alpha$, we see that the contribution $\mathcal{D}_R^{\alpha}(t)$ is essentially determined by the force-force correlation functions. However, instead of calculating these correlation functions exactly, we may approximate, for $\tau_N \gg T_\omega$, the integrand by [cf. Eqs. (A17) and (A26)]
\[
\langle [...]_s [...]_u \rangle \simeq \bar{V}^2 \langle N_k(s)N_k(u) \rangle,
\]
where $\bar{V}$ is the stroke-averaged velocity of the corresponding deterministic swimmer, cf. Eqs. (A24)–(A26). Adopting this approximation we find
\[
\mathcal{D}_R^{\alpha}(t) \simeq \bar{V}^2 \int_0^t ds \int_0^t du \langle N_k(s)N_k(u) \rangle
\]
\[
= \bar{V}^2 \int_0^t ds \int_0^t du \exp(-|u - s|/\tau_N)
\]
\[
= 2 \bar{V}^2 \tau_N \left[ t + \tau_N (e^{-t/\tau_N} - 1) \right],
\]
and thus the final result
\[
\mathcal{D}_R(t) = \mathcal{D}_R^{\beta}(t) + \mathcal{D}_R^{\alpha}(t)
\]
\[
\simeq \frac{1}{9} k_B T \left( \frac{1}{a_1} + \frac{1}{a_2} + \frac{1}{a_3} + \frac{5}{\ell} \right) t + 2 \bar{V}^2 \tau_N \left[ t + \tau_N (e^{-t/\tau_N} - 1) \right]. \]  
(A31)

The first part represents passive (thermal) diffusion, the second part is due to active swimming (note that $\tau_N$ is temperature dependent as well).
