KINEMATIC MATRIX THEORY, CHIRAL DIFFUSION AND
CHROMATOGRAPHY OF SELF-PROPELLERS

A Dissertation in
Physics
by
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Submitted in Partial Fulfillment
of the Requirements
for the Degree of

Doctor of Philosophy

December 2014
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Abstract

In recent years, much attention across the physics and chemistry communities has been attracted by biotic and abiotic self-propellers exhibiting a basic deterministic motion significantly perturbed by stochastic elements. I study the interplay of orientational diffusion and powered rotation in an analytically solvable model and show that it produces an effective translational diffusion with an unusual chiral character. I present a methodology using periodic soft potentials to guide and sort chiral self-propellers based on their dynamical properties such as chirality, rectilinear and angular velocities as well as orientational and translational diffusivities. In the remainder I study the ensemble properties of self-propellers. These quantities are traditionally investigated by differential-equation-based Fokker-Planck and Langevin formalisms which can be cumbersome to apply, especially in complex situations of the sort now attracting attention. I present a simple yet powerful alternative matrix-based approach for self-propellers with uncorrelated noises where the kinematic parameters for the elementary dynamical processes are summarized in a matrix, called kinematrix, from which many ensemble properties of the self-propellers can be obtained by simple matrix algebra. The clarity of kinematrix formalism reveals universalities in self-propellers that previously had been hidden behind complexity of the traditional formalisms. Then, I extend the formalism to include correlated Gaussian noises and obtain a governing equation for the time-evolution propagator, which has exact solution in two dimensions and obtains the necessary information solely from the noise autocorrelation. To demonstrate the utility of this formalism, I analyze the ensemble behaviors of 2D self-propeller with velocity fluctuations and persistent turning curvature, using Ornstein-Uhlenbeck process as the correlated Gaussian noise. The interplay of orientational and inertial time scales generates an emergent disorientation time scale which, with the speed fluctuation time scale, determines a variety of dynamical regimes.
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Acknowledgments

I am looking forward to finish the school marathon by making this my fourth and final dissertation of a very long academic career: two B.Sc.’s in Polymer Engineering & Solid State Physics, one M.Sc. in Theoretical Foundations of Physics and two Ph.D.’s in Chemical Engineering & Physics. I see myself in a transition, where I am concluding a long journey and beginning a new one. As I leave school in capacity as a student I am looking back at a roller coaster ride that my life has been for a better part of last two decades. The path of this ride has been significantly influenced by a multitude of individuals in both professional and personal capacity. I find this journey quite enlightening and I am confident that I have clearer picture of both life and society and particularly my own future in it.

First of all I would like to express my sincere gratitude for Paul (Dr. Lammert), my Ph.D. adviser and mentor, for his intelligent advice, scientific discussions, kindness, patience and life lessons. A person with his qualities is whom I dreamt to work with and learn from long before getting in to a Ph.D. program. My gratitude extends to Vin (Dr. Crespi), my Ph.D. co-adviser and supervisor, for his brilliant ideas, tireless brainstorming, immense support and for giving me the opportunity to be a member of his research group. Since there is not enough space nor is this a forum to discuss all we have been through and all that he has done for me, I would simply like to say that it has been a great experience working for Vin and it has been an honor being his friend.

It was a great opportunity to speak with Moses (Dr. Chan) and hear his points of views which helped me to think deeply about my life experiences. I would like to thank the rest of my dissertation committee: Drs. Borhan, Jain and Samarth for giving their time to this dissertation. I tried my best to make the text as concise as possible so that they do not have to read through pages of text filled with boring bed time stories.

I would like to thank my friends Curtis (Dr. Swagler) and Ken (Dr. Hurd) for their encouragement and for the brilliant quality time they gave me. My sincere thanks go to Damon (Dr. Sims, VP Student Affairs) for his sincerity and kind
support. I would like to acknowledge Dr. Manouchehr Khorassani, Dr. Mehdi Golshani and Dr. Ahmad Fahimifar for their significant influence on my academic career. It is a blessing to have such amazing people in my life.

Finally, my greatest acknowledgment goes to my beloved family, especially my parents, whom I have not seen in seven years, who supported me and encouraged me to continue my education with their sacrifices and patience.
Dedication

To my beloved parents
Self-propellers and active brownian particles are motile non-equilibrium systems [1–4] whose motion is a result of coupling between deterministic and stochastic dynamics, leading to a variety of spreading patterns and ensemble behavior. (see Fig. 1.1) These autonomous movers appear at different length scales. In macroscopic self-propellers, such as insects [5–7], fish [8–11], and other animals [12–16], as well as humans [17] and traffic [18], the majority of stochastic dynamics arise from the decision making processes. At microscale, thermal noises also enter into the dynamics of cells [19–29], bacteria [30–34], and artificial nanomotors [35–39].

In recent years the development of autonomous artificial micro- and nanoswimmers that move autonomously by transducing chemical energy to mechanical motion has defined a fascinating new field in colloid science [38–42]. These systems provide a platform for studying and simulating the physics arising from the coupling of deterministic and stochastic dynamics. In ordinary unpowered colloidal particles even under external driving the translational and orientational dynamics are weakly coupled. However, in self-propellers a stochastic orientation can strongly influence the direction of powered motion. This interplay is of fundamental interest, but is also important to the interpretation of experimental data and designing motors.

The standard methods for theoretical modeling of self-propellers are Langevin or Fokker-Planck formalisms [1,4,17,24–26,43–56]. A self-propeller’s motion naturally decomposes into distinct deterministic (translation and rotation) and stochastic (e.g. orientational diffusion, flipping about an axis, or tumbling) elementary
Figure 1.1. The coupling of deterministic and stochastic elements can give rise to many kinds of distinctive motion and spreading patterns, such as a rectilinear swimmer with speed fluctuation [51] and persistent turning [10, 11], a nanorotor with flipping [45], E. coli circle swimming [32, 84] or magnetotactic bacteria with occasional velocity reversal [63-66]. Nourhani et al., Phys. Rev. E, 90, 062304 (2014). Copyright (2014) by the American Physical Society.

processes whose phenomenological kinematic parameters are typically obtained by comparing experimental observations to theoretical models. The differential-equation-based Langevin and Fokker-Planck formalisms grow more cumbersome as the number of elementary processes increases, and for modeling we may need a menu of methods depending on the nature of the elementary process.

Another interesting feature of self-propellers which appear is rotary self-propellers is their handedness. Chirality, the lack of mirror symmetry, is of fundamental and practical importance over a wide range of disciplines including physics, biotechnology, medicine, and nanotechnology. Particles with structural chirality such as enantiomeric molecules may have radically differing biological activity. Hence, several techniques have been developed for the efficient separation of chiral molecules [57] and nano- and micro particles [58–61]. On the other hand, rotary self-propellers, such as biological and artificial circle swimmers, represent dynamically chiral particles that may be, geometrically, almost achiral. Sorting such chiral active matter is essential to select self-propellers with velocities and functions for specific tasks such as increasing the chance of artificial fertilization by spermatozoa
or using an artificial microswimmer for a fine task in microfluidics.

In this dissertation, I study the interplay of deterministic and stochastic dynamics on the behavior of self-propellers. In chapter 2 I demonstrate that the coupling of orientational diffusion with powered rotation in a nanorotor creates an effective translational diffusion with medium-term chiral bias: the motor is not equally likely to wander left or right from its position during one period; chiral symmetry of traditional diffusion is broken. [48]

In chapter 3, I develop a method to separate chiral self-propellers using a periodic potential which is realizable experimentally by acoustic lattices. The interaction of potential strength and finesse with the dynamical properties of the self-propeller – such as chirality, linear speed, angular speed as well as orientational and translational diffusivities – leads to self-propellers’ chirality-dependent drift in multiple directions, and provides a utility to guide and sort the rotary self-propellers, i.e. a chiral chromatography.

In chapter 4 I develop a kinematrix theory for self-propellers [62] in the white noise limit (uncorrelated stochastic noise) based on matrix algebra as an alternative to Fokker-Plank and Langevin differential-equation-based formalism. This new approach “treats all elementary motive processes on an equal footing and remains tractable for complex motor behavior, and by inspection, compiles the kinematic effects of the elementary processes into a matrix, called the kinematrix. Then, the ensemble behavior of self-propellers is immediately obtain by simple matrix algebra. The kinematrix consolidates the behavior of many classes of self-propellers [29, 33, 46–48, 53, 63–67] into a single unified form with newly emergent composite timescales, thus revealing universalities in the ensemble behavior of diverse self-propellers that had previously been considered ‘different’ systems. The analytical and computational simplicity of the kinematrix should also facilitate further advances in the analysis of large complex datasets, such as the inverse problem of extracting the correct elementary motive processes from complex trajectory data. The effects of active fluctuations and rotation-translation coupling at the level of ensemble properties can be recast as effectively additive contributions arising from independent self-propellers.” [62]

In chapter 5 I advance the kinematic matrix theory to include correlated Gaussian fluctuations – colored noise. Although the approximation of a neg-
ligible stochastic correlation time has been used extensively to model self-propellers [1,45,46,48,53,54,62,68–70], many physical systems suffer environmental noise in the form of forces that act directly on generalized momenta. Such noise is filtered through the inertia of the system and thus becomes colored [71–74]. A similar picture holds for any system with a non-negligible response time, whether or not it fits into traditional mechanical descriptions. Invoking the Central Limit Theorem, we can reasonably expect a large fraction of such noises to be approximately Gaussian. After developing the theory, I demonstrate its utility by analyzing a rectilinear self-propeller with velocity fluctuations and orientational inertia and discuss the interplay of finite correlation times of the involved noises, leading to an emergent disorientation time scale and a variety of dynamical regimes.

I conclude the dissertation in chapter 6 and suggest further research venues.


Chapter 2

Chiral Diffusion of Rotary Self-propellers

2.1 Introduction

In this chapter, we demonstrate that the coupling of orientational diffusion with powered periodic deterministic motion yields an emergent translational diffusion. We demonstrate that this effective translational diffusion can easily dominate the ordinary thermal translational diffusion for experimentally relevant nanomotors, and that this effective diffusion is chiral. Unpowered chiral particles do not exhibit chiral diffusion, but a rotary self-propeller has both a handedness and an instantaneous direction of powered motion, thus – unlike an unpowered particle – its diffusional motion can distinguish left from right. The contents of this chapter is published in Phys. Rev. E 87, 050301(R) (2013) and some passages have been quoted verbatim from it.

2.2 Problem Formulation

Neither a powered non-diffuser nor an unpowered purely orientational diffuser exhibits translational diffusion. However, when a rotary self-propeller undergoes orientational diffusion, the stochastic orientational motion causes the particle to deviate from its deterministic circular path into a quasi-circular one, as shown
Figure 2.1. At time $t$, the nanorotor is instantaneously on a circular path at velocity $v(t)$ about the guiding center $c(t)$ with position $p(t)$ relative to that center. Orientational diffusion results in the trajectory deviating from a circular path to a quasi-circular path at moderate diffusion coefficient. One cycle $T$ later, the motor is instantaneously on a circular trajectory about a new center $c(t+T)$. As in the figure, the direction of powered velocity of laboratory nanorotors and their geometrical axes are generally expected to differ; our theory makes no assumptions about the relationship between the two. Nourhani et al., Phys. Rev. E 87, 050301(R) (2013). Copyright (2013) by the American Physical Society.

In Fig 2.1 for a typical nanorotor; the result at long time is an effective translational diffusion. A nanorotor close to a flat substrate (the typical experimental geometry) moves in a plane at speed $v$ in a direction which both rotates at a deterministic constant angular velocity $\omega$ and wanders due to orientational Brownian motion with orientational diffusion coefficient $D_o$. For a rectilinear self-propeller (i.e. with $\omega = 0$), the induced effective diffusion represents a degradation of the self-propeller’s ability to get from one place to another, but for a rotary self-propeller the effect is quite opposite. We will solve this problem exactly for the effective diffusion coefficient $D_{eff}$ in terms of the fundamental parameters $D_o$, $v$ and $\omega$. $D_{eff}$ is an asymptotic property. Correlations at arbitrary times, and not merely the asymptotic behavior, are also of interest, may be easier to compare to experiment, and suffice to calculate $D_{eff}$. These are studied through a stroboscopic sampling of the motion at integer multiples of the period, under which a purely deterministic rotary motion becomes invisible. Interestingly, even under stroboscopic sampling the chirality manifests itself. For example, after one period, the expected displacement has a chirality-dependent part which can be as large as half the orbit radius.
As illustrated in Fig. 2.1, the particle is at all times on an instantaneous circular trajectory (called the \(c\)-frame circle) of radius

\[ R = \frac{v}{\omega} \quad (2.1) \]

about an instantaneous center \(c(t)\). We will treat two-dimensional vectors as complex numbers, so that the location of the particle with respect to \(c(t)\) on the \(c\)-frame circle is \(p(t) = R\mathbf{u}(t) = Re^{i\theta(t)}\) and its instantaneous velocity is \(\mathbf{v} = iv\mathbf{u}\). Thus, the increment in position \(\mathbf{x}\) in the laboratory frame for an infinitesimal time \(dt\) is

\[ d\mathbf{x} = iv\mathbf{u}dt. \quad (2.2) \]

The position of the particle \(\mathbf{x}\), its instantaneous center \(c\), and its \(c\)-frame location \(p\) are related by

\[ \mathbf{x}(t) = c(t) + p(t). \quad (2.3) \]

In the absence of orientational Brownian motion \((D_o = 0)\), \(c\) is constant. In the presence of orientational diffusion, the self-propeller orientation evolves according to the stochastic differential equation

\[ d\theta = \omega dt + \sigma dW \quad (2.4) \]

where \(W(t)\) is a normalized Weiner process; hence, \(W(t) - W(t')\) is normally distributed, with mean zero and variance \(|t-t'|\), and increments for non-overlapping intervals are independent. The orientational diffusion coefficient is \(D_o = \sigma^2/2\) and the orientation, which is central to the following calculations, is given by

\[ \mathbf{u}(t) = e^{i[\omega t + \sigma W(t)]}. \quad (2.5) \]

The velocity autocorrelation function measures how rapidly the motor forgets its orientation and is an essential ingredient for the derivation of the effective diffusion coefficient. Up to a constant factor \(v^2\), the velocity autocorrelation function is the same as the \(\mathbf{u}\) autocorrelation function. Using Eq. (2.5) and

\[ \langle e^{i\sigma(W(t) - W(t'))} \rangle = e^{-\sigma^2|t-t'|/2}, \quad (2.6) \]
which is a consequence of the Gaussian nature of $W(t) - W(t')$, it follows that

$$C_{uu^*}(t) := \langle u(t)u(0)^* \rangle = e^{i\omega t - D_o |t|}, \quad (2.7)$$

where the orientational correlation time is $D_o^{-1} = 2/\sigma^2$. In $\langle \cdot \rangle$, we average over the initial orientation $u(0)$ as well as perturbation realization $W$. The number of periods of deterministic motion required for the particle’s orientation to become scrambled is about $(2\pi |\tau|)^{-1}$, where $|\tau|$ is the ratio of the deterministic time scale $|\omega|^{-1}$ to the orientation correlation time $D_o^{-1}$, i.e.

$$\tau = \frac{\omega^{-1}}{D_o^{-1}} = \frac{\sigma^2}{2\omega}. \quad (2.8)$$

The parameters $\omega$, $v$, and $\tau$ are all signed quantities to allow for both chiralities. The loss of orientational correlation drives long-term diffusive behavior of $c$ and $x$. 

Figure 2.2. Dimensionless mean square increments in the center of mass $\xi = x$ (dotted) and the center of rotation $\xi = c$ (dashed) across one period $t = T$ of the rotary motion, $\langle |\xi(T) - \xi(0)|^2 \rangle / |\omega|^2 R^2 T$, are shown as a function of the ratio of the time scales of orientational diffusion and rotation. The gray curve shows the long time ($t \to \infty$) common asymptotic behavior of $x$ and $c$, i.e.

$$D_{\text{eff}} / |\omega|^2 R^2 = \lim_{n \to \infty} \langle |\xi(nT) - \xi(0)|^2 \rangle / 4 |\omega|^2 R^2 nT$$

as the effective translational diffusion coefficient. The positive deviations of mean square increments across one period from that asymptote in different regions of $|\tau|$ indicate anticorrelations between changes of $\xi$ over different periods, as depicted in Fig. 2.3. Nourhani et al., Phys. Rev. E 87, 050301(R) (2013). Copyright (2013) by the American Physical Society.
2.3 Effective Diffusivity (asymptotic behavior)

The effective diffusion coefficient $D_{\text{eff}}$ does not depend on the initial conditions on $\boldsymbol{u}$, since they are forgotten exponentially fast. Finite-time calculations require more care, as will be described later. In two dimensions, the effective diffusion coefficient is $4D_{\text{eff}} = \lim_{t \to \infty} t^{-1} \langle |\boldsymbol{x}(t) - \boldsymbol{x}(0)|^2 \rangle$. It follows from Eqs. (2.2) and (2.7) that

$$
\lim_{t \to \infty} \frac{1}{t} \langle |\boldsymbol{x}(t) - \boldsymbol{x}(0)|^2 \rangle = \lim_{t \to \infty} \frac{1}{t} \int_0^t \int_0^t dt' dt'' \langle \boldsymbol{v}(t') \boldsymbol{v}(t'')^\ast \rangle = 2v^2 \Re \left\{ \int_0^\infty dt' C_{\boldsymbol{uu}}(t') \right\} = \frac{2v^2 D_o}{\omega^2 + D_o^2} \tag{2.9}
$$

where $\Re$ extracts the real part; hence,

$$
D_{\text{eff}} = \frac{v^2}{2\omega} \left( \frac{\tau}{1 + \tau^2} \right) \tag{2.10}
$$

The effective diffusion coefficient $D_{\text{eff}}$, represented by the thick solid gray curve in Fig. 2.2, varies non-monotonically with $D_o$ and attains a peak value of $v^2/4|\omega|$ for $|\tau| = 1$, i.e. when the deterministic and stochastic time scales are equal. Note how an intrinsically one-dimensional diffusional process—orientational diffusion in a fixed plane—generates a two-dimensional effective translational diffusion through coupling to the powered motion. The guiding center $\boldsymbol{c}$ has the same asymptotic diffusion coefficient as $\boldsymbol{x}$, since the two are constrained by $|\boldsymbol{c} - \boldsymbol{x}| = R$. However, their motions differ markedly across one period $T = 2\pi|\omega|^{-1}$ of the deterministic rotation: $\langle |\boldsymbol{\xi}(T) - \boldsymbol{\xi}(0)|^2 \rangle / T$ for $\boldsymbol{\xi} = \boldsymbol{x}$ and $\boldsymbol{\xi} = \boldsymbol{c}$ both deviate from $4D_{\text{eff}}$, but in different regimes, as shown in Fig. 2.2.

For $|\tau| \gg 1$, the particle forgets its orientation so rapidly that the deterministic rotational motion is irrelevant and the effective diffusion coefficient $D_{\text{eff}} \approx v^2/2D_o$ is independent of $\omega$: the self-propeller might as well be moving straight at speed $v$, except that its direction changes after time $D_o^{-1}$. Thus, it follows a random walk with steps of length $v/D_o$ and duration $D_o^{-1}$, with a diffusion coefficient proportional to $(\text{step-length})^2/(\text{step-duration})$. In this regime, $\boldsymbol{x}$ barely moves and $\boldsymbol{c}$ diffuses rapidly on a circle centered at $\boldsymbol{x}$. This diffusion on a circle explains why $\langle |\boldsymbol{x}(T) - \boldsymbol{x}(0)|^2 \rangle / T$ is very close to $4D_{\text{eff}}$ when $|\tau| \gg 1$, whereas $\langle |\boldsymbol{c}(T) - \boldsymbol{c}(0)|^2 \rangle / T$
is much larger. Motion on a circle cannot contribute to long-term diffusion. Such finite-time effects are discussed more systematically later.

When the stochastic time scale is much larger than the deterministic time scale ($|\tau| \ll 1$), the effective diffusion coefficient $D_{\text{eff}} \approx v^2 D_o/2\omega^2$ is linear in $D_o$. In this regime, the circular orbit is only slightly perturbed. In a small time interval $\Delta t$, the random change in orientation ($\sim \sqrt{D_o \Delta t}$) leads to a random shift in $c$ by $\sim R \sqrt{D_o \Delta t}$ (recall that $c$ is not moved by the deterministic orientation change). Applying the random walk formula again leads to a diffusion coefficient for $c$ that is proportional to $R^2 D_o = v^2 D_o/\omega^2$. The random motion of $c$ is always on a circle about the instantaneous position $x$, but in this regime $c$ changes only a little before $u$ has changed significantly, causing the curvature of the motion about $x$ to disappear. Therefore, this motion is nearly along a time-dependent axis, and $\langle |c(T) - c(0)|^2 \rangle/T$ closely reflects the effective diffusion coefficient.

We now apply Eq. (2.10) to some recent experiments on catalytic nanorotors to determine whether this coupled effective diffusion is a significant contributor to the overall translational diffusion of real submicron-scale objects. A typical “slow” rotor [75] moves with an average angular velocity of $\omega_{\text{slow}} \approx 2.3 \text{ rad/s}$ and an orientational diffusion coefficient of $D_{\text{slow}}^o \approx 0.1 \text{ rad}^2/\text{s}$, while a typical “fast” rotor [76] has $\omega_{\text{fast}} \approx 30 \text{ rad/s}$ and $D_{\text{fast}}^o \approx 0.5 \text{ rad}^2/\text{s}$. Both nanorotors operate in the regime of weak orientational diffusion, $|\tau| \equiv |\omega|^{-1}/D_{\text{o}}^{-1} \ll 1$. The linear velocity of the slow nanomotor is $v_{\text{slow}} \sim 10 \mu\text{m/s}$ [77], which yields an effective diffusion coefficient of $D_{\text{eff}}^\text{slow} \approx 0.9 \mu\text{m}^2/\text{s}$. For the fast rotor, $v_{\text{fast}} \sim 30\mu\text{m/s}$ [78] and $D_{\text{eff}}^\text{fast} \approx 0.2 \mu\text{m}^2/\text{s}$. The passive translational diffusion coefficient for a similarly-sized (2 $\mu\text{m}$ long) unpowered nanorod in water is about $D_{\text{t}} = 0.4 \mu\text{m}^2/\text{s}$ [77]. For the slow rotor, the effective diffusion is twice as strong as passive translational diffusion.

More generally, when orientational diffusion is weak (i.e. $\tau \ll 1$), effective diffusion $D_{\text{eff}}$ scales linearly in $D_o$. Since $D_{\text{t}} \propto L^{-1}$ but $D_o \propto L^{-3}$, this means that the ratio of the effective effective diffusion to standard translational diffusion scales as $L^{-2}$. For typical rotary nanomotors synthesized to date, effective diffusion will dominate at scales smaller than $\sim 1$ micron.
2.4 Finite Time Scale Behavior

Equation (2.10) applies at long times compared to the period of rotation. The effective diffusion coefficient for shorter times depends on the time interval of the measurement and the initial conditions. We denote expectations under specific initial conditions $c(0) = 0$, $u(0) = e^{i\theta_0}$ by $\mathbb{E}_{\theta_0}[\cdot]$, and the expectation under a uniform distribution of $\theta_0$ (still with $c(0) = 0$) by $\langle \cdot \rangle = \frac{1}{2\pi} \int \mathbb{E}_{\theta_0}[\cdot] d\theta_0$. Passage from $\mathbb{E}_{\theta_0}$ to $\langle \cdot \rangle$ is straightforward, as is the reverse. For example, for a set of variables $\xi, \cdots, \zeta$ generically denoting any of $c$, $u$, or $x$ (not necessarily different), $\mathbb{E}_0$ can be obtained from $\langle \cdot \rangle$ using $\mathbb{E}_0[\xi(t)\cdots\zeta(t')^*] = \mathbb{E}_0[\xi(0)^*\cdots\zeta(t')^* u(0)]$.

Passage from $\mathbb{E}_0$ to $\mathbb{E}_{\theta_0}$ is then provided by the covariance of $\mathbb{E}_{\theta_0}$:

$$\mathbb{E}_{\theta_0}[\xi(t)\cdots\zeta(t')^*] = \mathbb{E}_0[\xi(t)\cdots\zeta(t')^*] e^{-i(n-\overline{n})\theta_0}, \quad (2.11)$$

where $n$ ($\overline{n}$) denotes the number of unconjugated (complex conjugated) variables among $\xi(t), \cdots, \zeta(t')^*$. Thus, $\langle \xi(t)\cdots\zeta(t')^* \rangle$ vanishes unless $n = \overline{n}$ since $\int_0^{2\pi} e^{-i(n-\overline{n})\theta_0} d\theta_0 = \delta_{n\overline{n}}$. This covariance is just a consequence of the fact that the path starting at $\theta_0 \neq 0$ under a particular realization of the noise $W(t)$ is just the corresponding trajectory starting at $\theta(0) = 0$ rotated by $\theta_0$. The expectation $\langle \cdot \rangle$ has two technical advantages over $\mathbb{E}_d[\cdot]$; it is time-translation invariant, assuming we only take differences of $c$'s or $x$'s, and it has the simple time-reversal property $\langle \xi(t)\cdots\zeta(t')^* \rangle = \langle \xi(-t)^*\cdots\zeta(-t') \rangle$.

The short-time behavior is most interesting if examined stroboscopically at discrete multiples of $T$, the period of the rotor. If $D_o = 0$, then nothing happens along this sequence: stroboscopic sampling renders the purely deterministic motion invisible and thereby highlights the effects of orientational diffusion. We label the time argument along this sequence as an integer subscript, $\xi_j := \xi(jT)$, and denote increments over one period as $\Delta \xi_j := \xi((j+1)T) - \xi(jT)$. The rotated increments $\hat{\Delta} \xi_j := \Delta \xi_j u_j^*$ are of great value as they are independent and identically distributed. Therefore, $\hat{\Delta} \xi_j$’s are identically distributed and $\hat{\Delta} \xi_j$ is independent of $\hat{\Delta} \zeta_k$ for $j \neq k$. Thus, for $n \geq 1$, we have the reduction

$$\Delta \xi_0^* \Delta \zeta_n = \Delta \xi_0^* u_n \hat{\Delta} \zeta_n = (\Delta \xi_0^* u_1)(\mathcal{R}_1 \cdots \mathcal{R}_{n-1}) \hat{\Delta} \zeta_n$$
into independent factors, where $R_j := u_{j+1}u_j^*$ is the rotation of the orientation from time $jT$ to $(j+1)T$. Taking an expectation yields

$$\langle \Delta \xi_0^* \Delta \zeta_n \rangle = \langle \Delta \xi_0^* u_1 \rangle \hat{C}^{n-1} \langle \hat{\Delta} \zeta_n \rangle,$$

(2.12)

where [see Eq. (2.7)]

$$\hat{C} := \langle R_j \rangle = C_{uu^*}(T) = e^{-D_0 T} = e^{-2\pi |\tau|}.$$  

(2.13)

Using the time-reversal (TR) and time-translation (TT) invariances of $\langle \cdot \rangle$, the first factor on the right-hand side of Eq. (2.12) can be written as

$$\langle \Delta \xi_0^* u_1 \rangle^\text{TR} \langle (\Delta \xi_{-1}^*) u_{-1}^* \rangle^\text{TT} - \langle \Delta \xi_0^* u_0^* \rangle = -\mathbb{E}_0 [\Delta \xi_0].$$

Defining the one-period-increment expectation of $\xi$ as

$$F_\xi := \mathbb{E}_0 [\Delta \xi_0] = \langle \Delta \xi_0^* u_0^* \rangle \equiv \langle \hat{\Delta} \xi_0 \rangle,$$

(2.14)

we have

$$\langle \Delta \xi_j^* \Delta \zeta_{j+n} \rangle = -F_\xi F_\zeta \hat{C}^{n-1}, \quad n \geq 1.$$  

(2.15)

This shows more explicitly how the decays of all correlations are controlled by that of the orientation given in Eqs. (2.7) and (2.13). The one-period-increment expectations, $F_\xi$, are easy to obtain; $F_u$, that of the orientation $u$ with respect to the instantaneous center $c$, follows from Eq. (2.7), $F_x = iv \int_0^T C_{uu^*}(t) \, dt$ for the self-propeller position $x$, and for the center $c$, $F_c$ follows from $F_c + RF_u = F_x$:

$$F_u = \hat{C} - 1, \quad F_x = \frac{RF_u}{1 + i\tau}, \quad F_c = \frac{-i\tau RF_u}{1 + i\tau}.$$  

(2.16)

Covariances among all of the basic variables take the form

$$\langle (\xi_n - \xi_0)^* (\zeta_n - \zeta_0) \rangle = \sum_{j=0}^{n-1} \sum_{k=0}^{n-1} \langle \Delta \xi_j^* \Delta \zeta_k \rangle$$

$$= \left[ \langle \Delta \xi_0^* \Delta \zeta_0 \rangle + 2 \Re \left\{ F_\xi F_\zeta \right\} \right] n + 2(1 - \hat{C}) \frac{\Re \left\{ F_\xi F_\zeta \right\}}{F_u^2}.$$  

(2.17)
The first term on the right-hand side represents the diffusive contribution; the second is relatively negligible at large times.

The various factors in Eq. (2.17) could be determined in an experimental setting using short-time measurements. The terms containing $F_\xi$ can be calculated in terms of $\tau = \omega^{-1}/D_o^{-1}$ and $R = v/\omega$ using Eq. (2.16), and the one-period correlators $\langle \Delta \xi_0 \Delta \xi_0^* \rangle$ can be evaluated from integrals such as $\langle \Delta x_0 \Delta x_0^* \rangle = v^2 \int_0^T \int_0^T C_{u u^*}(t - s) dt ds$. However, it will be less cumbersome to use Eqs. (2.16) and (2.17) to calculate $\langle \Delta \xi_0 \Delta \xi_0^* \rangle$, noting that the coefficient of $n$ in Eq. (2.17) must be $4D_{\text{eff}}$ when $\xi$ and $\zeta$ are any combination of $x$ and $c$, and zero otherwise (i.e. if either $\xi$ or $\zeta$ is $u$). Thus,

$$\langle \Delta \xi_0^* \Delta \xi_0 \rangle = 4D_{\text{eff}} - 2 \Re \left\{ F_\xi F_\zeta \right\}/F_u, \quad \xi, \zeta \in \{c, x\}. \tag{2.18}$$

Using this result to recast Eq. (2.17) for $\xi, \zeta \in \{c, x\}$ yields

$$\frac{\langle (\xi_n - \xi_0)^*(\zeta_n - \zeta_0) \rangle}{nT} = 4D_{\text{eff}} + \frac{2(1 - \hat{C}^u)}{nT} \Re \left\{ F_\xi F_\zeta \right\}/F_u^2. \tag{2.19}$$

Also,

$$\langle \Delta u_0^* \Delta \zeta_0 \rangle = -2 \Re \left\{ F_\xi \right\}, \quad \zeta \in \{u, c, x\}. \tag{2.20}$$

Combined with Eq. (2.15), this gives us all the pair-correlators of single-period increments.

Although one might expect that correlations between successive increments would vanish in the limit of strong orientational diffusion ($|\tau| \to \infty$), they do not. The plots of $\Re \langle \Delta c_0^* \Delta c_1 \rangle/R^2$, $\Re \langle \Delta x_0^* \Delta x_1 \rangle/R^2$, and $\Re \langle \Delta u_0^* \Delta u_1 \rangle$ shown in Fig. 2.3 reveal a strong anticorrelation between successive increments of $u$ and $c$. Surprisingly, it is strongest in the limit $|\tau| \to \infty$ for which the motion is most disordered. This phenomenon, like the gap between the dotted ($x$) and dashed ($c$) curves in Fig. 2.2, is related to the fact that $|\sum_{i=0}^n \Delta u_i|$ can never exceed 2 because $u$ is trapped on a circle. Hence, when the individual summands become large at large $|\tau|$, there must be strong anticorrelations. More concretely, conditional on the value of $u_1$, the expected values of both $u_0$ and $u_2$ are close to zero for $|\tau| \gg 1$ since they are distributed nearly uniformly over the circle. As a result, the conditional expectations of both $u_0 - u_1$ and $u_2 - u_1$ are close to $-u_1$, i.e. nearly collinear
independently of \( u_1 \). This is also reflected in \( \Delta c \) correlations because \( x \) is barely moving when \( |\tau| \gg 1 \), so that the motion of \( c \) is mostly common with that of \( Ru \).

Going back to Eqs. (2.15) and (2.16), we see that correlations between \( \Delta c_i \) across periods are much weaker than those between \( \Delta x_i \) for \( |\tau| \ll 1 \) (and stronger for \( |\tau| \gg 1 \)). Hence for \( |\tau| \ll 1 \), the mean-square single-period increment in \( c \) should track \( D_{\text{eff}} \) more accurately than does the corresponding increment in \( x \) (and less accurately for \( |\tau| \gg 1 \)). Fig. 2.2 reflects this behavior.

### 2.5 Chiral Diffusion

Since the purely deterministic motion is not visible in the stroboscopic sampling, one might naively expect that sampling at integer multiples \( nT \) of the rotation period would not display any chirality. But it does. Since \( \xi \cdot \zeta = \xi \cdot \zeta^* + i \hat{z} \cdot (\xi \times \zeta) \) (where \( \xi \) is the vector counterpart of the complex number \( \xi \), and \( \hat{z} \) defines the plane of motion), the chirality manifests itself through the imaginary parts of correlators, \( \hat{z} \cdot (\xi \times \zeta) = \Im \{ \langle \xi^* \zeta \rangle \} \). For example, according to Eq. (2.16)

\[
\langle \Delta x_0 u_0^* \rangle = \frac{RF_u}{1 + \tau^2} (1 - i\tau),
\langle \Delta c_0 u_0^* \rangle = \frac{RF_u}{1 + \tau^2} (-\tau^2 - i\tau).
\]
Thus, if the chirality is positive ($\tau > 0$), with respect to an initial orientation $\mathbf{u}_0 = 1$, the expected position $\mathbf{x}(T)$ after one period is to the right and down while the expectation of the instantaneous center $\mathbf{c}(T)$ is to the left and down. To our knowledge, this is the first observation of a chiral stochastic diffusion. Furthermore, from Eq. (2.15) we obtain

$$\dot{\hat{z}} \cdot \langle \Delta \vec{x}_j \times \Delta \vec{x}_{j+n} \rangle = \frac{2R^2F_u^2\tau}{(1 + \tau^2)^2} \hat{C}^{m-1}. \quad (2.21)$$

The positive proportionality to $\tau$ in Eq. (2.21) shows that the stroboscopically sampled path of the motor position has the same chirality as the hidden deterministic motion. The expected value of displacement after $n$ period, given the dynamics starts at $\theta_0 = 0$, is

$$\langle (\xi_n - \xi_0)\mathbf{u}_0^* \rangle = \sum_{j=0}^{n-1} \langle \Delta \xi_j \mathbf{u}_0^* \rangle = \sum_{j=0}^{n-1} \langle \hat{\Delta} \xi_j \hat{u}_j \mathbf{u}_0^* \rangle = \sum_{j=0}^{n-1} \langle \hat{\Delta} \xi_j (\mathcal{R}_{j-1} \cdots \mathcal{R}_0) \rangle$$

$$= \sum_{j=0}^{n-1} \hat{C}^j \langle \Delta \xi_0 \mathbf{u}_0^* \rangle = \sum_{j=0}^{n-1} \hat{C}^j F_{\xi} = - \left( 1 - \hat{C}^m \right) \frac{F_{\xi}}{F_u} \quad (2.22)$$

$F_{\xi}$ is the chirality-dependent displacement after one period, the total displacement is the sum of a sequence of vectors whose magnitude is fixed and their direction changes based on the chirality of the system. Therefore, the displacements in short periods of time are chiral. Similarly, the distribution of $\xi_n - \xi_0$ has a mean which is chirality-dependent. In the asymptotic limit,

$$\langle (\xi_n - \xi_0)\mathbf{u}_0^* \rangle \xrightarrow{n \to \infty} - \frac{F_{\xi}}{F_u}, \quad (2.23)$$

giving

$$\langle (\mathbf{x}_n - \mathbf{x}_0)\mathbf{u}_0^* \rangle \xrightarrow{n \to \infty} \frac{-R}{1 + i\tau} = \frac{R}{1 + \tau^2}(-1 + i\tau), \quad (2.24)$$

$$\langle (\mathbf{c}_n - \mathbf{c}_0)\mathbf{u}_0^* \rangle \xrightarrow{n \to \infty} \frac{i\tau R}{1 + i\tau} = \frac{R\tau}{1 + \tau^2}(i + \tau). \quad (2.25)$$
Again, the dependence on the sign of \( \tau \) reflects chirality. Rewriting Eq. (2.24) in terms of the initial velocity \( \mathbf{v}_0 \) and c-frame location \( \mathbf{p}_0 \) yields

\[
\langle (\mathbf{x}_n - \mathbf{x}_0)u_0^* \rangle \xrightarrow{n \to \infty} \frac{\omega^2}{D_o^2 + \omega^2} \left( -\mathbf{p}_0 + \frac{1}{D_o} \mathbf{v}_0 \right),
\]

where we see that the chiral component of the average ensemble displacement is in the direction of the the initial velocity. We define *asymptotic chiral angle* \( \phi_\infty \) as the angle between the initial velocity \( \mathbf{v}_0 \) and the asymptotic ensemble average displacement \( \lim_{n \to \infty} \langle (\mathbf{x}_n - \mathbf{x}_0)u_0^* \rangle \),

\[
\tan \phi_\infty = \tau = \frac{D_o}{\omega},
\]

which is positive (negative) for counterclockwise (clockwise) chirality, as demonstrated in Fig. 2.4.

### 2.6 Concluding remarks

Powered nanoscale motors are now a laboratory reality. However, at such a small scale, deterministic powered motion is significantly perturbed by thermal fluctuations, especially orientational diffusion. Powered rotational motion combined with orientational diffusion produce a strong effective translational diffusion with an unusual chiral character. For example, for a pair of nanorotors in close proximity...
the chiral bias of the random motion could give a misleading appearance of hydro-
dynamic interactions between them. The stroboscopically sampled position $x_n$ of
a rotor is *not* a Markovian process: an orientational hidden variable ($u_n$) biases
the increments in $x$ and provides the memory for $x_n$ to behave like a persistent
random walk, i.e a “time-domain semiflexible polymer”. These effects should be
readily apparent for individual rotors.
3.1 Introduction

In this chapter, we present a systematic methodology for programmable controlled drift and sorting chiral self-propellers based on their dynamical properties including chirality, linear and angular velocities as well as orientational and translational diffusivities. The pioneering separation methods for chiral self-propellers are based on interaction of the microswimmers with hard obstacles – equi-armed L-shaped [79] and pinwheel shaped [80] – of patterned substrates. However, the fixed substrate pattern in these approaches limit their control in guiding particles in desired directions. The discreteness of the rotor/substrate interaction for hard walls leads to sharp discontinuities in the drift response of these rotors as a function of various structural or motive characteristics, and the well-defined subpopulations (in terms of drift direction and speed) wash out into a continuum of behaviors in the presence of stochastic forces. In contrast, dynamics of rotors in a smooth external potential, as could be imposed by an undulating substrate or periodic acoustic/optical fields, is likely to be dominated by a small set of attractors in phase space; thus it is more likely to yield well-defined subpopulations, even under stochastic perturbation. Further richness can be obtained by tuning the strength of the potential – straightforward for acoustic and optical fields – including the ability to steer pop-
ulations of rotors to arbitrary points in a plane through a judicious sequence of drifts.

A chiral self-propeller rotates either clockwise or counterclockwise, and in the absence of thermal noise or external potential returns to its original position after each period of rotation. Addition of orientational diffusion results in an effective translational diffusion [48], but not a steady drift. To obtain a chiral drift from motion of an active particle in a potential, we design a family of periodic force fields, realizable by optical or acoustic lattices, by superposing three standing waves. The key property is lack of rotation and inversion symmetry in the potential. By modulating the potential’s strength and finesse we guide the particle into different chirality-dependent trajectory attractors with distinct directions (directionally variable ratchet effect) in an overdamped dynamical regime. In this way, a circle swimmer can be guided from one specific position in the plane to any other. This technique can be used not only for separation and sorting applications, but also for directing cargo carrying circle swimmers for tasks such as targeted drug delivery or guiding a rotary spermatozoa to an ovum for fertilization. Random perturbation in the form of orientational diffusion suppresses or enhances the drift, or alters the direction. We discuss these effects and map out partial “drift phase diagrams”.

In using a soft potential for separating (inert) structurally chiral particles, the unpowered particle is set to motion by an external field (such as steady fluid flow), thus breaking the symmetry of the periodic square lattice potential. However, chiral self-propellers are autonomous and require only a static chiral potential. Such a potential should lack some symmetries to provide a chirality-dependent drift. In order to have a drift in one specific direction, the potential clearly should have no rotation symmetry, and must also lack inversion symmetry. [If a rotary self-propeller had a drift velocity in an inversion-symmetric potential, under inversion, chirality and the potential are unchanged yet the drift is reversed, which is a contradiction. ] Now suppose that the potential lacks inversion symmetry, but has one mirror symmetry. This reflection preserves the potential, but reverses the handedness of the chiral self-propeller such that the drift of a right-handed autonomous particle is the reflection through this line of the drift of a left-handed particle and guarantees that self-propellers with different chiralities part ways.
3.2 Problem Formulation

In our model, in the absence of a potential a chiral self-propeller moves with velocity \( \mathbf{v}_0 = v_0 \hat{v}_0 \) and rotates with angular velocity \( s_{\omega} \omega \) where \( \omega > 0 \) and \( s_{\omega} \) is the handedness: \(-1\) for clockwise and \(1\) for counter-clockwise rotation. The presence of a static external potential \( V(\mathbf{r}) \) in the overdamped regime results in an additive contribution \(-\mu \nabla V(\mathbf{r})\) to the velocity where \( \mu \) is the Stokes mobility of the self-propeller. We design the potential as a superposition of standing waves \( \mu V(\mathbf{r}) = C \sum_{i=1}^{3} c_i \cos(K \hat{k}_i \cdot \mathbf{r} + \delta_i) \), where \( \sum_{i=1}^{3} c_i^2 = 1 \). \( K \) and \( C \) determine the finesse and strength of the potential, respectively. The shape and symmetry properties are determined by the directions of the unit vectors \( \hat{k}_i \), the ratios of the \( c_i \) and phase offsets \( \delta_i \). Including orientational \( (D_o) \) and translational \( (D_t) \) diffusivities, and working in units of \( \omega^{-1} \) for time and \( v_0/\omega \) for length, the equations of motion are

\[
\frac{d\mathbf{v}}{dt} = \dot{\mathbf{v}}_0(\theta) + \mathbf{\xi}(t) + \alpha \sum_{i=1}^{3} c_i \sin(\beta \hat{k}_i \cdot \mathbf{r} + \delta_i) \\
\frac{d\theta}{dt} = s_{\omega} + \zeta(t). \tag{3.1}
\]

Here, \( \alpha = CK/v_0 \), \( \beta = Kv_0/\omega \), and \( \zeta \) and \( \xi_i \) are independent zero-mean Brownian white noises with strengths \( \gamma_o = D_o/\omega \) and \( \gamma_t = D_t \omega/v_0^2 \). For typical nanorotors \( \gamma_o \sim 10^{-2} \) and \( \gamma_t \sim 10^{-3} - 10^{-2} \) [35].

We begin by studying the fully deterministic system, then we add orientational diffusion and finally translational diffusion. In our numerical simulations, we take \( \hat{k}_1 = (-1, 0) \), \( \hat{k}_2 = (-1/2, \sqrt{3}/2) \) and \( \hat{k}_3 = \hat{k}_2 - \hat{k}_1 \) as shown in Fig. 3.1a. We set \( \delta_1 = \delta_2 = 0 \), \( \delta_3 = 1.3 \), and \( c_1 = 0.256 \), \( c_2 = c_3 = 0.683 \). The unequal amplitudes and phase offset ensure that inversion and rotation symmetries are broken while maintaining a mirror-line parallel to the x-axis. Figure 3.1b illustrates the periodic potential consisting of local maxima and minima and “mountain passes” \( T_1 \), \( T_2 \), \( T_1 \) and \( T_2 \) that connect a local minimum to its four neighboring local minima. At very small values of \( \alpha \) the self-propeller has no trouble riding over the potential maxima. However, at larger \( \alpha \), these maxima are unreachable and the chiral self-propeller transits from one local potential minimum to a neighboring one through a mountain passes. Since the dynamics of a counter-clockwise self-propeller is the
reflection of that of a clockwise one about \( x \)-axis, we give results only for the latter \((s_\omega = -1)\).

### 3.3 Deterministic Trajectory Attractors

The fully deterministic case \((\gamma_t = \gamma_o = 0)\) itself has realizations for swimmers of length scale \( \sim 100 \mu m \) where the potential-free trajectories are almost perfect circles [81]. We solved the equations of motion (3.1) for 12 different initial positions in the potential unit cell for 100 periods of rotation on a grid with resolutions \( \Delta \alpha = 0.01 \) and \( \Delta \beta = 0.5 \). This revealed the “drift phase diagram” shown in Fig. 3.1(c). At both small and large values of \( \alpha \) there are regions where the chiral self-propeller executes closed orbits with no net drift. In between, there are a variety of different steady drifts. While the direction of drift changes with variation of \( \alpha \) and \( \beta \), in most of the drift domain the drift speed \( v_d \) is equal to one potential lattice constant per one period of rotation, that is,

\[
v_\beta = \frac{2}{\beta \sqrt{3}} v_0 \tag{3.2}
\]

for each \( \beta \), independent of \( \alpha \), and variation of potential strength mostly changes the direction of the drift. Except a small leftward motion window (light blue region) in the drift phase diagram (see Fig. 3.1c), the potential guides the rotary-self-propellers to the right. For most \((\alpha, \beta)\), the 12 trajectories with different initial conditions eventually collapse to a single attractor. However, in the white region of the diagram, trajectories repeat only after many orbital periods and may be sensitivity to initial conditions. This possibly chaotic behavior washes out in the presence of stochastic noise, as discussed later. But it remains an aspect in need of further exploration.

To gain a clearer picture of the trajectory attractors and guiding directions, we consider the particular case of \( \beta = 7.00 \) (recall that \( \beta \) is the wavevector of the potential in inverse units of the free self-propeller’s orbit radius). Representative trajectories are shown in Fig. 3.1d–3.1j. With zero potential strength \( \alpha = 0 \), trajectories are perfect circles. Turning the potential on \((\alpha = 0.3)\) distorts the circular trajectory and as we increase the potential strength \((\alpha = 1.10)\) the chiral
Figure 3.1. (a) Three unit wave vectors that defines the periodicity of the potential. (b) The potential has translation symmetry. For each local minimum, there are four neighbor local minima. To go from one local minima to another, the rotor performs on the depicted T1, T2, T1 or T2 transitions through a pass between two neighbor local maxima. The arrows show the additive velocity due to the potential. (c) The drift phase diagram for drift speed and direction. There are localized regimes (ellipse glyphs) at both small and large potential strength. For a given $\beta$ with change of potential strength $\alpha$ we can change the direction of motion. (d)-(j) Trajectory attractors for clockwise rotor. The arrows on the trajectories show the direction of motion.

self-propeller performs all four mountain pass transitions in one period and we have a closed loop (Fig. 3.1e). As we increase the potential further, the rotor cannot make some of these transitions; this opens the trajectory from its closed state and the rotor experiences a net displacement after each period of rotation thus leading to directionally variable ratchet effect as a function of potential strength. At a higher potential strength, $\alpha = 1.22$ chiral self-propeller cannot perform T1 transition, so it turns back into the local minimum and does a T1, leading to a downward $-90^\circ$ drift. At $\alpha = 1.30$ the chiral self-propeller enters the local minima through a T1 transition, but it cannot continue with a T2, so it climbs back by a T1 to its initial local minimum and then performs a T2 transition, leading to a net upward drift of $30^\circ$. At higher potential $\alpha = 1.40$, after a T1 transition,
Figure 3.2. Phase diagrams in the dimensionless potential strength ($\alpha$) - wave vector ($\beta$) plane for experimentally-relevant orientational diffusivities $\gamma_o = 0.01$ and 0.10 for a clockwise rotary self-propeller. In the presence of diffusion, the small-$\alpha$ localized regime becomes diffusion (squiggles). At intermediate values of $\alpha$, a variety of steady drift behaviors occur. Diffusion induce a wide window where the drift direction is to the left. With increase in orientational diffusivity the size of the leftward motion domain and the drift speed in that domain decreases.

The chiral self-propeller cannot go back to its original local minima by a $T_1$; it is turned back and does another $T_1\bar{T}$, resulting in a downward $-30^\circ$ drift. Finally, at higher potential strength $\alpha = 2.00$ the chiral self-propeller cannot even perform a $T_1\bar{T}$, so it is trapped in a local well and follows a closed orbit whose size is much smaller than the diameter of the free-motion circle.
Figure 3.3. Phase diagrams in the dimensionless potential strength (\(\alpha\)) - wavevector (\(\beta\)) plane for various values of the dimensionless translational diffusivities \(\gamma_t = 0.001\) and \(0.010\) for a clockwise self-propeller. The similar pattern of behavior for only-orientational-diffusion noise in Fig. 3.2 is observed.

3.4 Guiding in the Presence of Stochastic Noise

Next we add stochastic noise to the deterministic dynamics to study the effect of the coupling and deviation from the purely deterministic case. We start with orientational diffusion. As we discussed in chapter 2, for a free chiral self-propeller (i.e. \(\alpha = 0\)), the powered motion transmutes orientational diffusion into an effective translational diffusion which can easily be significantly larger than ordinary thermal translational diffusion. Figures 3.2a and 3.2b show the effect of two different experimentally-relevant strengths of orientational diffusion in the presence of the periodic potential.

Several deviations from the deterministic drift phase diagram appears. At low
The yellow region in the deterministic drift phase diagram (Fig. 3.1) – where drift is one lattice constant per period at a heading of $-30^\circ$ – is fairly robust to small-to-medium values of $\gamma$. The direction remains $-30^\circ$, but the average drift speed is reduced, since occasionally a well-to-well transition is missed. Also the domain of $-30^\circ$ drift is extended to the part of the settled region in the deterministic diagram at higher $\alpha$ since occasional stochastic kick may lead to well-to-well transitions.

Surprisingly, the stochastic noise develops a new region where the drift is to the left in a wide window. The corresponding domain is the deterministic limit is mostly closed orbits. Between the leftward drift and $-30^\circ$ rightward drift, the
drift is to the right, as at $\gamma_0 = 0$, but the direction shows significant dependence on $\alpha$ and $\beta$. With increase in orientational diffusion though, the size of leftward drift window, and the drift is not as strong and straight as before, but more like a guided Brownian diffuser. These states are marked by squiggly arrow $\nearrow\searrow$ in the figures.

Similarly, the addition of purely translational diffusivity to the deterministic dynamics shows almost the same pattern as the addition of orientational diffusion, as illustrated in Fig. 3.3. Slight perturbation opens a wide window of leftward drift, but as the strength of the noise increases as the domain shrinks and the motion is like a guided Brownian diffuser.

In an actual physical scenario both orientational and translational diffusivities exist. Figure 3.4 shows the effect of variation of orientational diffusivity for a given translational diffusivity for some experimentally relevant values. As before with increase in stochasticity the leftward motion window shrinks. Comparing Figure 3.4a with Figs. 3.2a and 3.3b shows that addition of small orientational diffusion in the presence of translational diffusion have small impact of the drift speed.

It is interesting that orientational and translational diffusion provides something useful to one who wants to controllably move things around. For example, we designed the potential such that the vertical motion of counterclockwise chiral self-propellers will be opposite that of the clockwise chiral self-propellers. If, instead, we wanted to separate according to speed or angular velocity, but not chirality, we could use values $(\alpha, \beta)$ corresponding to $(1.2, 7)$ in Fig. 3.4(a) and $(1.3, 8)$ in Fig. 3.4(b) where the chiral direction is almost zero. Recall that $\alpha$ and $\beta$ depend not only on the potential itself, but also $v$ and $\omega$ of the chiral self-propeller.

### 3.5 Concluding Remarks

Rotary self-propellers are important ingredient of powering at nano and micro scale. While the majority of research of artificial rotary swimmers has been on developing different geometries and structures, very little attention has been given to separating these particles or guide them. The proposed mechanism of guiding and sorting in this chapter could be realized experimentally by acoustic tweezers
and lattices. The separated chiral swimmer could later be used as ingredient of bigger structure or used for do useful tasks such as carrying cargo to specific targets.

### 3.6 Appendix: Periodic Potential

Let’s assume the general case of unit vectors

\[
\hat{k}_1 = \{\cos \phi_1, \sin \phi_1\} \\
\hat{k}_2 = \{\cos \phi_2, \sin \phi_2\}.
\]

These are related to the potential lattice vectors \(\mathbf{a}_i\) (in units of \(v/\omega\)) by

\[
\beta \hat{k}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij} \quad \text{for } i, j = 1, 2.
\]

Solving for \(\mathbf{a}_1\) and \(\mathbf{a}_2\) we obtain

\[
\mathbf{a}_1 = \frac{2\pi}{\beta \sin(\phi_2 - \phi_1)} \{\sin \phi_2, -\cos \phi_2\} \\
\mathbf{a}_2 = \frac{2\pi}{\beta \sin(\phi_2 - \phi_1)} \{-\sin \phi_1, \cos \phi_1\}
\]

To obtain a periodic potential \(\mathbf{k}_3\) should satisfy the following relation for arbitrary integers \(n_1, n_2\)

\[
\mathbf{k}_3 \cdot (n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2) = n \frac{2\pi}{\beta} 
\]

where \(n\) is an integer and in contrast to \(\hat{k}_1\) and \(\hat{k}_2\), the vector \(\mathbf{k}_3\) is not necessarily a unit vector. Any choice of \(\mathbf{k}_3\) that satisfies this relation leads to a periodic potential. We can write any vector \(\mathbf{k}_3\) in terms of a linear combination of \(\hat{k}_1\) and \(\hat{k}_2\), that is, \(\mathbf{k}_3 = m_1 \hat{k}_1 + m_2 \hat{k}_2\). Then, Eq. (3.8) becomes \(m_1 n_1 + m_2 n_2 \in \mathbb{Z}\) which holds for any values of \(n_1\) and \(n_2\) if \(m_1, m_2 \in \mathbb{Z}\).

To build our potential we set

\[
\phi_1 = \pi \leadsto \hat{k}_1 = \{-1, 0\} \\
\phi_2 = \frac{2\pi}{3} \leadsto \hat{k}_2 = \left\{-\frac{1}{2}, \frac{\sqrt{3}}{2}\right\}
\]
and for a periodic potential we choose $m_2 = -m_1 = 1$ so that

$$\hat{k}_3 = \hat{k}_2 - \hat{k}_1 = \left\{ \frac{1}{2}, \frac{\sqrt{3}}{2} \right\}$$  \hspace{1cm} (3.11)

which is a unit vector. Therefore,

$$a_1 = \frac{4\pi}{\beta \sqrt{3}} \left\{ -\frac{\sqrt{3}}{2}, -\frac{1}{2} \right\}$$  \hspace{1cm} (3.12)

$$a_2 = \frac{4\pi}{\beta \sqrt{3}} \{0, 1\}$$  \hspace{1cm} (3.13)

To satisfy the required symmetry and asymmetries we set

$$c_1 = \frac{0.3}{\sqrt{0.3^2 + 0.8^2 + 0.8^2}} = 0.256$$  \hspace{1cm} (3.14)

$$c_2 = c_3 = \frac{0.8}{\sqrt{0.3^2 + 0.8^2 + 0.8^2}} = 0.683$$  \hspace{1cm} (3.15)

and

$$\delta_1 = \delta_2 = 0$$  \hspace{1cm} (3.16)

$$\delta_3 = 1.3 \text{ rad.}$$  \hspace{1cm} (3.17)
Kinematic Matrix Theory for Self-Propellers

4.1 Introduction

In this chapter we present the kinematic matrix (“kinematrix”) theory for self-propellers based on simple matrix algebra as an alternative to sophisticated differential-equation-based Fokker-Planck and Langevin formalisms. The contents of this chapter is published in Phys. Rev. E 89, 062304 (2014) and some passages have been quoted verbatim from it.

The key to the kinematrix approach is a body-frame description of the motion. A self-propeller, while translating, may rotate deterministically due to structural imperfection [45, 82, 83], hydrodynamic interaction with a substrate [28,31,32,84,85], or purposeful engineering [35,75,76,86–89]; they may also suffer stochastic events that influence the direction of motion such as tumbling or orientational diffusion (see Fig. 4.1). We build an empirical body frame that is anchored in dynamical (rather than geometrical) properties: the self-propeller translates at velocity $\mathbf{v} = \dot{v}\hat{v}$ while rotating at angular velocity $\mathbf{\omega} = \dot{\omega}\hat{\omega}$ at a position $\mathbf{p} = \frac{\dot{\mathbf{r}}}{\dot{\omega}}$ with respect to the center of its instantaneous circular orbit, thus yielding an orthonormal triple $[\hat{\mathbf{p}}, \hat{\mathbf{v}}, \hat{\mathbf{\omega}}]$ as a right-handed empirical body frame fixed to the self-propeller. We choose a fixed laboratory frame $[\hat{x}, \hat{y}, \hat{z}]$ that coincides with $[\hat{\mathbf{p}}, \hat{\mathbf{v}}, \hat{\mathbf{\omega}}]$ at $t = 0$. The orientation of body frame at time $t$ is related to its initial orientation.
Figure 4.1. At $t = 0$ the laboratory frame and body frame coincide. During $[0, dt)$ a self-propeller can experience small turns about $\hat{\omega}$ due to deterministic rotation, stochastic orientational diffusion, or tumbling; it can also flip about $\hat{v}$ or reverse the direction of motion. The operator $U(t)$ represents this evolution. Nourhani et al., Phys. Rev. E 89, 062304 (2014). Copyright (2014) by the American Physical Society.

by a propagator $U(t)$ such that $\hat{\xi}(t) = U(t) \hat{\xi}(0)$ for $\hat{\xi}$ being any of $\hat{p}$, $\hat{v}$ or $\hat{\omega}$. The propagator represents the net deterministic and stochastic rotation of the body frame from $0 \to t$; from its ensemble average $\langle U(t) \rangle$ we can obtain pair correlators, finite-time average displacement, finite-time mean-square displacement, and asymptotic effective diffusivity. The stochastic component of the dynamics leads to an ensemble of possible body frame orientations at time $t$, and each orientation connects to the initial orientation though an ensemble of different paths. The core of kinematrix theory is to overcome the difficulty of obtaining $\langle U(t) \rangle$ over these ensembles by turning $\langle U(t) \rangle$ into the product of ensemble averages of independent incremental rotations in the body frame, as explained below.

4.2 Theory Formulation

Divide the timeline $[0, t)$ into infinitesimal increments $dt = t/n$ (large integer $n$) with endpoints $t_i \equiv i dt$ (integer $i$). With $U_i \equiv U(t_i)$, and $R_i$ as the net rotation in the laboratory frame during the infinitesimal interval $[t_i, t_{i+1})$, the propagator takes the recursive form $U_n = R_{n-1}U_{n-1}$. Now, we transform the rotations $R_i$ in
the laboratory frame into rotations in the body frame $\tilde{R}_i = U_i^{-1} R_i U_i$, yielding, 
$U_n = R_{n-1} U_{n-1} = U_{n-1} \tilde{R}_{n-1} = \tilde{R}_0 \tilde{R}_1 \cdots \tilde{R}_{n-1}$. For processes with negligible correlation time, the $\tilde{R}_i$'s are independent and identically distributed, $\langle \tilde{R}_i \rangle = \langle \tilde{R}_0 \rangle$, resulting in

$$\langle U(t) \rangle \simeq \langle \tilde{R}_0 \rangle^{t/dt}. \quad (4.1)$$

The net rotation $\tilde{R}_0 = \tilde{R}_0^{(1)} \cdots \tilde{R}_0^{(N)}$ is the product of $N$ independent elementary processes $\tilde{R}_0^{(j)}$ (such as flipping, tumbling or orientational diffusion) involved in self-propeller’s motion during $[0, dt)$. Expanding their expectations to first order in $dt$, $\langle \tilde{R}_0^{(j)} \rangle = \mathcal{I} - \mathcal{K}^{(j)} dt + O(dt^2)$ for $j = 1, \cdots, N$, we obtain

$$\langle \tilde{R}_0 \rangle = \mathcal{I} - \mathcal{K} dt + O(dt^2). \quad (4.2)$$

We call $\mathcal{K} = \mathcal{K}^{(1)} + \cdots + \mathcal{K}^{(N)}$ the kinematrix. It is the sum of the first-order contributions $\mathcal{K}^{(i)}$ of elementary rotations and contains the kinematic effects of all such processes. In the limit $t \gg dt$, Eqs. (4.1) and (4.2) yield

$$\langle U(t) \rangle = e^{-\mathcal{K} t}. \quad (4.3)$$

Using the initial condition $[\hat{x}, \hat{y}, \hat{z}] \equiv [\hat{p}(0), \hat{v}(0), \hat{w}(0)]$ and $\hat{\xi}(t) = U(t) \hat{\xi}(0)$ for $\hat{\xi}$ any of $\hat{p}, \hat{v},$ or $\hat{w}$, we obtain the correlators for linear ($v \hat{v}$) and angular ($\omega \hat{\omega}$) velocities

$$C_{vv}(t) = \langle v(0) \cdot v(t) \rangle = \langle v(0) v(t) \rangle \left[ e^{-\mathcal{K} t} \right]_{22} \quad (4.4)$$
$$C_{\omega\omega}(t) = \langle \omega(0) \cdot \omega(t) \rangle = \langle \omega(0) \omega(t) \rangle \left[ e^{-\mathcal{K} t} \right]_{33}. \quad (4.5)$$

The subscripts on $\left[ e^{-\mathcal{K} t} \right]$ identify matrix elements. The off-diagonal elements of $e^{-\mathcal{K} t}$ give the correlators between different directions $\hat{p}, \hat{v}, \hat{w}$.

The magnitude and direction of the velocity may fluctuate as a result of random disturbances, but since the sources of these fluctuations generally differ, the fluctuations of $v$ and $\hat{v}$ are typically independent. Before discussing the effect of active speed fluctuations, we explain the formalism with a speed $v(t)$ fluctuating weakly around a mean $\langle v(t) \rangle = \bar{v}$ with negligible correlation time, so that $\langle v(0) v(t) \rangle \simeq \bar{v}^2$ (the common assumption of constant speed $[29, 45–48, 53, 90]$ is a special case).
Thus, the ensemble average and mean squared displacements are

\[ \langle \Delta r(t) \rangle = \bar{v} \int_0^t e^{-Kt} \cdot \hat{v}(0) \, dt' = \bar{v} \mathcal{K}^{-1} (\mathcal{I} - e^{-Kt}) \cdot \hat{v}(0) \]  

(4.6)

\[ \langle |\Delta r(t)|^2 \rangle = 2 \bar{v}^2 \left[ t \mathcal{K}^{-1} - \mathcal{K}^{-1} (\mathcal{I} - e^{-Kt}) \right]_{22}. \]  

(4.7)

The interplay of deterministic and stochastic dynamics creates effective diffusion at long times; the observed diffusivity of a self-propeller is the sum of its effective and passive Brownian diffusivities. The effective diffusivity \( D_{\text{eff}} \) in \( d \) dimensional space is

\[ D_{\text{eff}} = \frac{1}{2d} \lim_{t \to \infty} t^{-1} \langle |\Delta r(t)|^2 \rangle = \frac{\bar{v}^2}{d} \left[ \mathcal{K}^{-1} \right]_{22} = \frac{\bar{v}^2}{d} \frac{K_{11}K_{33} - K_{13}K_{31}}{\det \mathcal{K}}. \]  

(4.8)

If motion is strictly restricted to a plane such that \( \det \mathcal{K} = 0 \), we make the replacement \( \mathcal{K} \to \mathcal{K} + \varepsilon \mathcal{I} \), calculate Eqs. (4.4)–(4.8), and take \( \varepsilon \to 0 \) at the end.

Unsteady operation of the self-propeller’s engine leads to speed fluctuations \( \delta v(t) \). Since \( \langle v(t) v(0) \rangle = \bar{v}^2 + \langle \delta v(t) \delta v(0) \rangle \), as far as velocity correlations (4.4), mean-square displacement (5.8), and effective diffusivity (4.8) are concerned, the velocity fluctuations \( \delta v(t) \hat{v}(t) \) make an uncorrelated additive contribution. For models [51] where \( \langle \delta v(t) \delta v(0) \rangle = [\langle v^2 \rangle - \bar{v}^2] e^{-\kappa_v t} \) such contributions are equal to the corresponding properties of a self-propeller with mean speed \( \sqrt{\langle v^2 \rangle - \bar{v}^2} \) and kinematrix \( \mathcal{K}' = \mathcal{K} + \kappa_v \mathcal{I} \).

### 4.3 Elementary Processes

Equations (4.4)–(4.8) show how important physical quantities follow immediately from the kinematrix \( \mathcal{K} \). Next, we show how to build \( \mathcal{K} \) from the contributions \( \mathcal{K}^{(j)} \) of elementary processes by inspection of motion during the interval \([0, dt]\). We write \( \mathcal{K} \) in terms of a linear combination of matrices \( \mathcal{J}_k, \mathcal{P}_k \) and \( \mathcal{P}_k^\perp \). \( \mathcal{J}_k \) is the generator of infinitesimal rotation about an axis \( \hat{k} \),

\[ \mathcal{J}_x = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \quad \mathcal{J}_y = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \quad \mathcal{J}_z = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (4.9) \]
$\mathcal{P}_k$ is the orthogonal projection onto the $k$-th coordinate,

$$
\mathcal{P}_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad
\mathcal{P}_y = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad
\mathcal{P}_z = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix},
$$

(4.10)

and $\mathcal{P}_k^\perp = \mathcal{I} - \mathcal{P}_k$ is the projection onto the plane perpendicular to $\hat{k}$,

$$
\mathcal{P}_x^\perp = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad
\mathcal{P}_y^\perp = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad
\mathcal{P}_z^\perp = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}.
$$

(4.11)

We study four elementary processes: tumbles, flips, deterministic rotation, and orientational diffusion; these four processes cover a wide variety of self-propeller dynamics from artificial nanomotors to motile single-cell organisms and macroscopic movers. A tumble is a sudden rotation of angle $\theta$ with distribution $P(\theta)$ about an axis $k$, occurring at a rate $f$. We model tumbles by a Poisson process $	ilde{R}_0^\text{tumble} = \mathcal{I} + s_0 \left[ (\cos \theta - 1)\mathcal{P}_k^\perp + \sin \theta \mathcal{J}_k \right]$ where $s_0$ is 0 or 1 with probabilities $(1 - f)dt$ or $fdt$, respectively. The contribution of tumbling is then

$$
\mathcal{K}_k^\text{tumble} = f (1 - \langle \cos \theta \rangle_P) \mathcal{P}_k^\perp - f \langle \sin \theta \rangle_P \mathcal{J}_k
$$

(4.12)

where the averages $\langle \cos \theta \rangle_P$ and $\langle \sin \theta \rangle_P$ are with respect to $P(\theta)$. Flipping is tumbling by $\theta = \pi$ about an axis $k$:

$$
\mathcal{K}_k^\text{flip} = 2f \mathcal{P}_k^\perp.
$$

(4.13)

Deterministic rotation at angular speed $\omega$ about axis $k$ during $dt$ is described by $e^{\omega dt \mathcal{J}_k} = \mathcal{I} - (-\omega \mathcal{J}_k)dt + \mathcal{O}(dt^2)$, thus

$$
\mathcal{K}_k^\text{det} = -\omega \mathcal{J}_k.
$$

(4.14)

Orientational diffusion with diffusivity $D_k$ about an axis $k$ during $dt$ is described by $\tilde{R}_0^\text{ort} = e^{d\phi \mathcal{J}_k}$ where the incremental rotational angle $d\phi$ is a Wiener process of mean zero and standard deviation $\sqrt{2D_k dt}$. The contribution of $\langle \tilde{R}_0^\text{ort} \rangle = \mathcal{I} - \mathcal{O}(dt^2)$ is then

$$
\mathcal{K}_k^\text{ort} = \int_0^t \langle \tilde{R}_0^\text{ort} \rangle dt = \mathcal{I} - \mathcal{O}(dt^2).
$$

(4.15)
\[ D_k \mathcal{P}_k \mathcal{P}_k^\perp dt + \mathcal{O}(dt^2) \] to the kinematrix is

\[ \mathcal{K}_k^{\text{ort}} = D_k \mathcal{P}_k \mathcal{P}_k^\perp. \] (4.15)

### 4.4 Four Self-Propeller Scenarios

Having established the formalism, we now demonstrate how the elementary processes of Eqs. (4.12–4.15) combine to describe four different classes of self-propellers, building \( \mathcal{K} \) by inspection. We start by illustrating the application of our formalism to the previously studied classes of diffusing-and-flipping self-propellers and magnetotactic bacteria in a rotating magnetic field, calculating the asymptotic \( D_{\text{eff}} \) (4.8) as an example of ensemble properties (4.4)–(4.8). Next we study run-and-tumble motion via our continuous model – rather than traditional discrete random walks [13, 22, 23, 91, 92] – and demonstrate how to incorporate speed fluctuations. Last, we analyze a 3D swimmer and discuss the effect of rotation-translation coupling. After discussing these individual classes of self-propellers, we recast the kinematries into a form that covers all motor types; the clarity of the formalism reveals new emergent time scales with universal short and long time behavior. In building \( \mathcal{K} \) for each class, keep in mind that we inspect the motion during \([0, dt]\), hence, \( \mathcal{P}_\omega = \mathcal{P}_x \), \( \mathcal{P}_\omega = \mathcal{P}_y \), \( \mathcal{P}_z = \mathcal{P}_z \), and \( \mathcal{J}_\omega = \mathcal{J}_z \) in Eqs. (4.12)–(4.15).

**Diffusion-Flip (DF) self-propellers** include biological “circle swimmers” as well as artificial nanomotors [29, 45–48, 53]. Steric hinderance from a two dimensional (2D) planar substrate resists free orientational diffusion about any axis parallel to the substrate and forces the self-propeller to perform only sudden flips about \( \hat{v} \).

While translating and rotating in a 2D plane, the swimmer undergoes orientational diffusion with diffusivity \( D_\omega \) about \( \hat{\omega} \) perpendicular to the substrate while flipping with frequency \( f \) about \( \hat{v} \) and changing its rotation chirality. The contributions to \( \mathcal{K} \) are \(-\omega \mathcal{J}_z\) for deterministic rotation about \( \hat{\omega} \), \( D_\omega \mathcal{P}_z^\perp \) for orientational diffusion about \( \hat{\omega} \), and \( 2f \mathcal{P}_y^\perp \) for flipping about \( \hat{v} \), so that \( \mathcal{K}_{\text{2D}} = -\omega \mathcal{J}_z + D_\omega \mathcal{P}_z^\perp + 2f \mathcal{P}_y^\perp \).

Eq. (4.8) then yields (see Sec. 4.7.1)

\[ D_{\text{eff,2D}} = \frac{\hat{v}^2}{2} \frac{D_\omega + 2f}{\omega^2 + D_\omega (D_\omega + 2f)} \] (4.16)
For a fast flipping rotor \((f \gg \omega)\), the rotation rapidly averages out and the rotor acts like a linear motor \((D_{\text{eff},2D}^{\text{linear}} = \frac{\bar{v}^2}{2D_\omega})\).

**Magnetotactic bacteria (MB)** can move near a substrate and rotate in synchrony with a rotating magnetic field at angular speed \(\omega\) [63–66]. The rotation contributes \(-\omega J_z\). The trajectory is a set of U-shaped segments due to occasional reversals of \(\hat{v}\) with frequency \(f\) while preserving the chirality of the orbit (contributing \(2f P_z^\perp\)). From \(K_{\text{MB}} = (2f + D_\omega)P_z^\perp - \omega J_z\) we obtain (see Sec. 4.7.2)

\[
D_{\text{eff},\text{MB}} = \frac{\bar{v}^2}{2} \frac{D_\omega + 2f}{\omega^2 + (D_\omega + 2f)^2}.
\] (4.17)

**Run-and-tumble self-propellers (RT)** such as *E. coli* [30] and Daphnia [12, 13] undergo intermittent tumbles due to stochastic forces or switching of flagellar beating between the synchronous and asynchronous modes [33, 67]. They have been studied by *ad hoc* models of discrete random walks [13, 22, 23, 92] in quasi-2D with a distribution of turning angles. Although mathematically functional for experimental analysis, such an approach does not unfold the physical processes underlying the motion in continuous time. Here we build a continuous-time model and extend it further to include the effects of engine fluctuations. The velocity direction \(\hat{v}\) lies in the plane of motion and \(\hat{\omega}\) represents an axis perpendicular to this plane about which the self-propeller undergoes orientational diffusion (contributing \(D_\omega P_z^\perp\)) and tumbling with frequency \(f\) [contributing \(f(1 - \langle \cos \theta \rangle_p)P_z^\perp - f(\sin \theta)_p J_z\) to the kinematrix]. The kinematrix \(K_{\text{RT}} = [D_\omega + f(1 - \langle \cos \theta \rangle_p)]P_z^\perp - f(\sin \theta)_p J_z\) yields the effective diffusivity for a run-and-tumbler at mean speed \(\bar{v}\) (noted by the superscript “ms”),

\[
D_{\text{eff,RT}}^{\text{ms}} = \frac{\bar{v}^2}{2} \frac{D_\omega + f(1 - \langle \cos \theta \rangle_p)}{[f(\sin \theta)_p]^2 + [D_\omega + f(1 - \langle \cos \theta \rangle_p)]^2}.
\] (4.18)

We can extend this model to take into account speed fluctuations \(\delta v(t)\) with auto-correlation \(\langle \delta v(t) \delta v(0) \rangle = [(\bar{v}^2 - \bar{v}^2)e^{-\kappa_0 t}\) [51]. Then, the additive modification to effective diffusivity due to fluctuations (noted by the superscript “fluc”) is equal to the effective diffusivity of a self-propeller with kinematrix \(K_{\text{RT}}^{\text{fluc}} = K_{\text{RT}} + \kappa_v I\)
and mean speed $\sqrt{\langle v^2 \rangle - \bar{v}^2}$; that is,

$$D_{\text{eff,RT}}^{\text{fluc}} = \frac{(\langle v^2 \rangle - \bar{v}^2) [\kappa_v + D_\omega + f(1 - \langle \cos \theta \rangle_p)]}{2 \left[ f (\sin \theta)_p^2 + (\kappa_v + D_\omega + f(1 - \langle \cos \theta \rangle_p))^2 \right]}.$$ (4.19)

Combining these, the effective diffusivity for a run-and-tumbler with speed fluctuations is $D_{\text{eff,RT}}^{\text{ms}} + D_{\text{eff,RT}}^{\text{fluc}}$. The same procedure holds for velocity autocorrelation (4.5) and mean-square-displacement (5.8). We can advance the model further by including more elementary processes in the model, and fitting multiple models in parallel to an experimental dataset to find the best model and elucidate the underlying continuous-time motion of the run-and-tumbler.

**3D self-propeller:** The motion of biological and artificial self-propellers in three dimensions is also of interest [93–95]. In contrast to the fixed rotation plane in 2D motion, the plane of rotation for a 3D self-propeller wanders in 3D space. The kinematrix for a self-propeller moving at $\bar{v}$ while rotating at angular speed $\omega$ and suffering orientational diffusion about the three axes of the body frame is $K_{3D} = D_{\hat{p}} P_x^\perp + D_{\hat{v}} P_y^\perp + D_{\hat{\omega}} P_z^\perp - \omega J_z$. Equation (4.8) then yields

$$D_{\text{eff,3D}} = \frac{\bar{v}^2}{3} \frac{D_{\hat{\omega}} + D_{\hat{v}}}{D_{\hat{\omega}} + D_{\hat{p}} + \omega^2}.$$ (4.20)

For a 3D linear motor, setting $\omega = 0$ eliminates $D_{\hat{v}}$ from $D_{\text{eff,3D}}$, since rotation about $\hat{v}$ has no observable effect for a linear motor. In that case, $D_{\hat{p}}$ and $D_{\hat{\omega}}$’s new meanings are orientational diffusion coefficients about two perpendicular axes orthogonal to $\hat{v}$. Although the effects of rotation-translation coupling in 2D are included implicitly in the phenomenological kinematic parameters, in 3D such hydrodynamic interactions can lead to non-orthogonality of the propulsive velocity and rotation axis. Hence, the velocity has a component $\bar{v}\hat{v}$ in the instantaneous plane of rotation as well as a component $\bar{v}_\omega \hat{\omega}$ along the rotation axis, so the speed is $\sqrt{\bar{v}^2 + \bar{v}_\omega^2}$. The effective diffusivity depends on both diagonal and off-diagonal elements of $K^{-1}$ in the form

$$D_{\text{eff,3D}}^{\text{non,1}} = \frac{\bar{v}^2}{d} [K^{-1}]_{22} + \frac{\bar{v}_\omega \bar{\omega}}{d} [K^{-1}]_{23} + \frac{\bar{v}_\omega \bar{v}}{d} [K^{-1}]_{32} + \frac{\bar{v}_\omega^2}{d} [K^{-1}]_{33}.$$ (4.21)

For the 3D example here, off-diagonal terms are zero and the correction to $D_{\text{eff,3D}}$ is
an additional term \((\bar{v}_\omega^2/d)[K^{-1}]_{33} = \bar{v}_\omega^2/3(D_\beta+D_\delta)\), which is the effective diffusivity of a 3D linear motor with speed \(\bar{v}_\omega\).

### 4.5 Universalities

The clarity of kinematrix formalism facilitates further insights into universalities that previously had been hiding in the complexities required of differential-equation-based analysis. We can consolidate and recast these four scenarios into a **unified** form

\[
K_{\text{uni}} = \gamma_\omega P_z + \gamma P_z^\perp - \omega_z J_z + \delta \quad (4.22a)
\]

\[
= \begin{bmatrix}
\gamma + \delta & \omega_z & 0 \\
-\omega_z & \gamma - \delta & 0 \\
0 & 0 & \gamma_\omega
\end{bmatrix} 
\quad (4.22b)
\]

where the scenario-dependent parameters are

<table>
<thead>
<tr>
<th></th>
<th>(\gamma_\omega)</th>
<th>(\gamma)</th>
<th>(\delta)</th>
<th>(\omega_z)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D</td>
<td>(2f)</td>
<td>(D_\omega + f)</td>
<td>(f)</td>
<td>(\omega)</td>
</tr>
<tr>
<td>RT</td>
<td>0</td>
<td>(D_\omega + f(1-\langle \cos \theta \rangle))</td>
<td>(0)</td>
<td>(f \langle \sin \theta \rangle)</td>
</tr>
<tr>
<td>MB</td>
<td>0</td>
<td>(D_\omega + 2f)</td>
<td>(0)</td>
<td>(\omega)</td>
</tr>
<tr>
<td>3D</td>
<td>(D_\beta + D_\delta)</td>
<td>(D_\omega + \frac{D_\beta + D_\delta}{2})</td>
<td>(\frac{D_\omega - D_\beta}{2})</td>
<td>(\omega)</td>
</tr>
</tbody>
</table>

Defining

\[
\Omega^2 = \omega_z^2 - \delta^2,
\]

and using Eq. (4.22) and \([-\omega_z J_z + \delta(P_x - P_y)]^2 = -\Omega^2 P_z^\perp\) we obtain

\[
K^{-1} = \gamma_\omega^{-1} P_z + \left(\frac{1}{\gamma_\omega^2 + \Omega^2}\right)[\gamma P_z^\perp + \omega_z J_z - \delta(P_x - P_y)]
\quad (4.25)
\]

\[
e^{-Kt} = e^{-\gamma t} \left\{ \cos \Omega t \, P_z^\perp + \frac{\sin \Omega t}{\Omega} \left[ \omega_z J_z - \delta(P_x - P_y) \right] \right\} + e^{-\omega t} P_z.
\quad (4.26)
\]
which along with Eqs. (4.4) and (4.5) yield the autocorrelators of angular and linear velocities

\[ C_{\omega \omega}(t) = \omega^2 e^{-\gamma \omega t}, \]
\[ C_{vv}(t) = \bar{v}^2 e^{-\gamma t} \{ \cos (\Omega t) + \delta \sin \Omega t / \Omega \} \]

(4.27)

(4.28)

Five newly emergent time scales \( \gamma^{-1}, \gamma^{-1}, \delta^{-1}, \omega_z^{-1}, \) and \( \Omega^{-1} \) govern the behavior of all these self-propellers. In 3D \( C_{\omega \omega} \) measures the wandering of the orbital plane, with an exponential decay at characteristic time \( \gamma^{-1} \). In 2D it measures the loss of memory of the sense of rotation (i.e. chirality), since \( \hat{\omega} \) orients to the orbit by a right-hand rule. \( C_{vv} \) measures how fast the velocity forgets its orientation, with characteristic time \( \gamma^{-1} \). The temporal behavior is not governed by \( \omega^{-1} \), but \( \Omega^{-1} \) which can be real or imaginary depending on \( \delta \) and \( \omega_z \). For imaginary \( \Omega \), \( C_{vv} \) does not oscillate but has a longer correlation time \( (\gamma - |\Omega|)^{-1} \) as for linear nanomotors. These time scales also determine the extent to which \( \langle \Delta r(\infty) \rangle = (\gamma^2 + \Omega^2)^{-1} \bar{v} \left[ -\omega \hat{\rho}(0) + (\delta + \gamma) \hat{v}(0) \right] \) depends on the direction of initial velocity and, therefore, initial direction of rotation. This is the generalization of the “chiral diffusion” of 2D nanorotors [48], even though there is no well-defined chirality for a 3D rotary swimmer.

Equations (4.8) and (4.22) yield a unified expression for the effective diffusion coefficient in terms of the new time scales:

\[ D_{\text{eff,uni}} = \left( \frac{\bar{v}^2}{d} \right) \frac{\gamma + \delta}{\gamma^2 + \Omega^2}. \]

(4.29)

We can obtain \( D_{\text{eff}} \) for any class of self-propeller by substituting the appropriate parameters from Eq. (4.23) into Eq. (4.29). The mean square displacement (5.8) takes a unified form

\[
\langle |\Delta r(t)|^2 \rangle_{\text{uni}} = 2dD_{\text{eff}} t - 2\bar{v}^2 \left( \gamma^2 - \Omega^2 + 2\gamma \delta \right) / (\gamma^2 + \Omega^2)^2
+ \frac{2\bar{v}^2 e^{-\gamma t}}{(\gamma^2 + \Omega^2)^2} \left\{ (\gamma^2 - \Omega^2 - 2\gamma \delta) \cos \Omega t
+ (\gamma^2 - \Omega^2) \delta - 2\gamma \Omega^2 \right\} \sin \Omega t / \Omega, \]

(4.30)

It behaves ballistically (i.e. \( \bar{v}^2 t^2 \)) at short times \( t \ll \min(\Omega^{-1}, \gamma^{-1}) \) and diffusively
\((2dD_{\text{eff}}t)\) at long times. For real \(\Omega^{-1} < \gamma^{-1}\) the crossover between the two limits is oscillatory. However, for \(\Omega^{-1} > \gamma^{-1}\) the rate at which the velocity forgets its orientation is faster than the oscillation, and the oscillatory crossover is suppressed. For an imaginary \(\Omega\), on the other hand, the characteristic time of the exponential decay is \((\gamma - |\Omega|)^{-1} > \gamma^{-1}\) with no oscillatory crossover between ballistic and diffusive regimes. The special cases of 2D self-propellers with flipping [45] and without flipping [53] and magnetotactic bacteria [65] have been compared thoroughly with numerical experimental data.

### 4.6 Concluding remarks

The kinematrix formalism elegantly handles a variety of self-propellers with active fluctuations and rotation-translation coupling, and reveals universalities in self-propeller behavior. As a parsimonious means to construct models with different sets of elementary processes, the kinematrix could enable new types of analysis beyond the traditional mode of feeding forward from dynamical model to motor trajectory. For example, distinct stochastic processes that are lumped together in current treatments could be distinguished, such as local environmental noise and internal engine fluctuations which contribute towards a single distribution of turning angles within a traditional discrete model with a fixed-length random walker. In the longer term, memory effects could be disentangled from complex composite behaviors by identifying an optimal memory-free kinematix description and then extracting the residual memory-dependent phenomena. Extension of the formalism to explicitly handle memory effects is also a natural next step; the generality and intuitive clarity of this formalism provides a strong conceptual underpinning to further advances in the analysis of self-propellers.

### 4.7 Appendix: Calculating Ensemble Average Properties and Emergent Time Scales

In this appendix we provide a detailed step-by-step walk-through of the application of our theory to two scenarios: the diffusion/flip self-propeller and the
magnetotactic bacterium. We build the kinematrix by inspection and calculate the corresponding effective diffusivity using Eq. (8). We also find the emergent new time scales, $\gamma^{-1}$, $\omega^{-1}$, $\gamma^{-1}$, $\delta^{-1}$, and $\Omega^{-1}$, by comparing the scenario-specific kinematrix with the general kinematrix form (4.22). Then we can calculate the effective diffusivity and mean-square-displacement simply by plugging these parameters into Eqs. (4.29) and (4.30), respectively.

4.7.1 Diffusion-Flip self-propellers

The DF self-propeller moves with speed $\bar{v}$ and rotates with angular speed $\omega$ while diffusing orientationally about the axis of rotation $\hat{\omega}$ with diffusion coefficient $D_\hat{\omega}$ and flipping at a rate of $f$ about the direction of the velocity $\hat{v}$. The kinematrix includes contributions of three elementary processes: deterministic rotation about $\hat{\omega}$, $K_\text{det}^{\hat{\omega}} = -\omega J_\omega$, orientational diffusion about $\hat{\omega}$, $K_\text{ort}^{\hat{\omega}} = D_\hat{\omega} P_{\hat{\omega}}$, and flipping around $\hat{v}$, $K_\text{flip}^{\hat{v}} = 2f P_{\hat{v}}$. As discussed in the body of the paper, we inspect the motion during $[0, dt)$ where $P_{\hat{v}} = P_{\hat{y}}$, $P_{\hat{\omega}} = P_{\hat{z}}$, and $J_\omega = J_z$. Using the explicit forms of these matrices [Eqs. (4.9)–(4.11)], the kinematrix becomes

$$K_{2D} = K_\text{det}^{\hat{\omega}} + K_\text{ort}^{\hat{\omega}} + K_\text{flip}^{\hat{v}}$$

$$= -\omega J_\omega + D_\hat{\omega} P_{\hat{\omega}} + 2f P_{\hat{v}}$$

$$= -\omega J_z + D_\hat{\omega} P_z + 2f P_y$$

$$= \begin{bmatrix} D_\hat{\omega} + 2f & \omega & 0 \\ -\omega & D_\hat{\omega} & 0 \\ 0 & 0 & 2f \end{bmatrix}, \quad (4.31)$$

from which we obtain

$$K_{11} K_{33} - K_{13} K_{31} = (2f + D_\hat{\omega})(2f) - 0 = 2f(2f + D_\hat{\omega}) \quad (4.32)$$

and

$$\det K_{2D} = 2f \begin{vmatrix} 2f + D_\hat{\omega} & \omega \\ -\omega & D_\hat{\omega} \end{vmatrix} = 2f \left[ D_\hat{\omega}(2f + D_\hat{\omega}) + \omega^2 \right]. \quad (4.33)$$
Employing now Eq. (4.8) yields

\[ D_{\text{eff},2D} = \frac{\bar{v}^2 K_{11} K_{33} - K_{13} K_{31}}{\det \mathcal{K}} = \frac{\bar{v}^2}{2} \frac{2f + D_\omega}{D_\omega (2f + D_\omega) + \omega^2}, \]  

(4.34)

which is expression (4.16). Comparing the kinematrix (4.31) with the unified kinematrix (4.22b) immediately yields \( \gamma_\omega = 2f, \omega_z = \omega, \gamma = D_\omega + f, \delta = f, \) and \( \Omega^2 = \omega^2 - f^2, \) as tabulated in (4.23). Plugging these parameters into the unified form \( \langle |\Delta \mathbf{r}(t)|^2 \rangle_{\text{uni}} \) (4.30) gives the mean-square-displacement for diffusion/flip self-propellers,

\[ \langle |\Delta \mathbf{r}(t)|^2 \rangle_{2D} = 2\bar{v}^2 t \frac{2f + D_\omega}{D_\omega (2f + D_\omega) + \omega^2} - 2\bar{v}^2 \frac{(2f + D_\omega)^2 - \omega^2}{[D_\omega (2f + D_\omega) + \omega^2]^2} \]

\[ + 2\bar{v}^2 e^{-(D_\omega + f)t} \frac{2f + D_\omega}{[D_\omega (2f + D_\omega) + \omega^2]} \cos(t\sqrt{\omega^2 - f^2}) \]

\[ + 2\bar{v}^2 e^{-(D_\omega + f)t} \frac{f(2f + D_\omega)^2 - \omega^2 (3f + 2D_\omega)}{[D_\omega (2f + D_\omega) + \omega^2]^2} \sin(t\sqrt{\omega^2 - f^2}), \]

(4.35)

### 4.7.2 Magnetotactic Bacteria

In this scenario, motion is restricted to a plane and \( \det \mathcal{K} = 0. \) Magnetotactic bacteria move with speed \( \bar{v} \) and rotate in synchrony with a rotating magnetic field at angular speed \( \omega \) while suffering orientational diffusion about \( \hat{\omega} \) and occasional chirality-preserving reversals of \( \hat{v} \) with frequency \( f. \) Three elementary processes contribute to the kinematrix: deterministic rotation about \( \hat{\omega}, \mathcal{K}_\omega^{\text{det}} = -\omega \mathcal{J}_\omega, \) orientational diffusion about \( \hat{\omega}, \mathcal{K}_\omega^{\text{ort}} = D_\omega \mathcal{P}_\omega \), and reversals of \( \hat{v} \) with frequency \( f \) while preserving the chirality which is equivalent to \( 180^\circ \) rotation of \( \hat{v} \) about \( \hat{\omega}, \) so that \( \mathcal{K}_\omega^{\text{flip}} = 2f \mathcal{P}_\omega \). Summing up these contributions and keeping in mind that \( \mathcal{P}_\omega = \mathcal{P}_z \) and \( \mathcal{J}_\omega = \mathcal{J}_z, \) we obtain the kinematrix for the magnetotactic bacteria,

\[ \mathcal{K}_{\text{MB}} = \mathcal{K}_\omega^{\text{det}} + \mathcal{K}_\omega^{\text{ort}} + \mathcal{K}_\omega^{\text{flip}} \]

\[ = -\omega \mathcal{J}_\omega + D_\omega \mathcal{P}_\omega + 2f \mathcal{P}_\omega \]

\[ = -\omega \mathcal{J}_z + D_\omega \mathcal{P}_z + 2f \mathcal{P}_z \]
In this example, the motion is strictly in the $xy$ plane and $\det K_{MB} = 0$, such that Eq. (4.8) for effective diffusivity gives the indeterminate form $0/0$. To resolve this problem, as discussed following Eq. (4.8), we replace $K \rightarrow K^{(\varepsilon)} \equiv K + \varepsilon I$, perform the calculations, and then take the limit $\varepsilon \rightarrow 0$. Therefore, we write

$$K^{(\varepsilon)}_{MB} = K_{MB} + \varepsilon I = \begin{bmatrix} D\dot{\omega} + 2f + \varepsilon & \omega & 0 \\ -\omega & D\dot{\omega} + 2f + \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{bmatrix},$$

(4.37)

from which we obtain

$$K_{11}^{(\varepsilon)}K_{33}^{(\varepsilon)} - K_{13}^{(\varepsilon)}K_{31}^{(\varepsilon)} = \varepsilon(D\dot{\omega} + 2f + \varepsilon) - 0 = \varepsilon(D\dot{\omega} + 2f + \varepsilon)$$

(4.38)

and

$$\det K^{(\varepsilon)}_{MB} = \varepsilon \left| \begin{array}{ccc} D\dot{\omega} + 2f + \varepsilon & \omega \\ -\omega & D\dot{\omega} + 2f + \varepsilon \\ 0 & 0 & \varepsilon \end{array} \right|$$

$$= \varepsilon \left[ (D\dot{\omega} + 2f + \varepsilon)^2 + \omega^2 \right].$$

(4.39)

Now, using Eqs. (4.8), (4.38), and (4.39) we can calculate the effective diffusivity in the limit $\varepsilon \rightarrow 0$,

$$D_{eff,MB} = \lim_{\varepsilon \rightarrow 0} \frac{\bar{v}}{2\varepsilon} \frac{\varepsilon(D\dot{\omega} + 2f + \varepsilon)}{(D\dot{\omega} + 2f + \varepsilon)^2 + \omega^2}$$

$$= \frac{\bar{v}^2}{2} \frac{D\dot{\omega} + 2f}{(D\dot{\omega} + 2f)^2 + \omega^2}.$$

(4.40)

which is Eq. (4.17). An alternative approach is to compare the kinematrix (4.36) with the unified form (4.22b) which yields $\omega_z = \omega$, $\gamma = D\dot{\omega} + 2f$, $\delta = \gamma \omega = 0$ and $\Omega = \omega$. Plugging these parameters into Eq. (4.29) directly gives Eq. (4.17) without need for the substitution $K \rightarrow K + \varepsilon I$. Moreover, similar to diffusion-flip self-propellers, by plugging these parameters into Eq. (4.30) we obtain the
mean-square displacement of magnetotactic bacteria.
Chapter 5

Gaussian Memory in Kinematic Matrix Theory

5.1 Introduction

In this chapter, first in section 5.2 we advance the kinematrix approach to include Gaussian noise with finite correlation time, yielding Eqs. (5.3) – (5.9). This extended kinematrix formalism again circumvents the need for probability distributions; it also makes the calculations significantly easier by extracting the necessary information solely from the autocorrelation of the correlated noise. Section 5.3 then provides an application of the theory, to rectilinear self-propellers with fluctuating engines to study the effects of orientational Gaussian memory (modeled by an Ornstein-Uhlenbeck process) in producing a variety of ensemble regimes. The contents of this chapter is published in Phy. Rev. E, 90, 062304 (2014) and some passages have been quoted verbatim from it.

5.2 Theory Formulation

The kinematrix formalism is based on an examination of elementary dynamical processes in a self-propeller’s body frame. The tail-to-head vector $\chi$ of the swimmer which has a fixed orientation $\hat{\chi}$ in the body frame of the self-propeller evolves with time in the laboratory frame such that, for a given realization of noise, we have at
time $t$ the updated value $\hat{\chi}(t) = U(0, t)\hat{\chi}(0)$. The propagator $U(0, t)$ represents the net rotation of the body frame from time 0 to time $t$; its ensemble average gives the velocity pair correlator of Eq. (5.6) and the ensemble-average spatial displacement quantities of Eqs. (5.7)–(5.9).

To obtain $\langle U(0, t) \rangle$ we work on a discrete timeline $T = \{0, dt, 2dt, 3dt, \ldots\}$ with infinitesimal time steps $dt \ll t$. We write $U_n$ for $U(0, ndt)$ and $R_n$ for the net rotation between $ndt$ and $(n+1)dt$ in the laboratory frame; in the body frame, the same rotation is expressed as $\tilde{R}_n = U^{-1}_nR_nU_n$. Rewriting the recursive expression $U_n = R_n - 1U_{n-1}$ in terms of the body frame thus yields

$$\langle U_n \rangle = \langle \tilde{R}_0\tilde{R}_1\cdots\tilde{R}_{n-1} \rangle$$  \hspace{1cm} (5.1)

where the brackets average over all possible realization of noises. If the body-frame rotations $\tilde{R}_n$ are independent (the white-noise limit) then the average of their product in Eq. (5.1) is equal to the product of their averages. Then the expansion $\langle \tilde{R}_n \rangle = I - \mathcal{K} dt + \mathcal{O}(dt^2)$ yields $\langle U(0, t) \rangle = \exp(-\mathcal{K}t)$ where the kinematrix $\mathcal{K}$ captures the kinematic properties of the elementary motile processes [62].

However, for correlated noise the $\tilde{R}_n$'s are not independent. Assuming physically distinct and independent correlated and uncorrelated noises, we write the rotation $R_n = \tilde{R}_n^{\text{corr}}\tilde{R}_n^{\text{un}}$ as the product of correlated $\tilde{R}_n^{\text{corr}}$ and uncorrelated $\tilde{R}_n^{\text{un}}$ rotations (these being for an infinitesimal interval, the ordering of the rotations makes a negligible difference). Thus, $\langle U_{n+1} \rangle = \langle U_n, \tilde{R}_n^{\text{corr}} \rangle \langle \tilde{R}_n^{\text{un}} \rangle$. The incremental correlated rotation can be written in the form $\tilde{R}_n^{\text{corr}} = \exp(\xi_n dt \cdot \mathcal{J})$, where the $\mathcal{J}_\alpha$ are the generators of rotations in $SO(3)$ (Greek subscripts or superscripts denote Cartesian components $x$, $y$ and $z$). $\{\xi_n\}$ is assumed to comprise a stationary centered Gaussian process with a continuous covariance: $\langle \xi_n \rangle = 0$ and $\langle \xi_n \xi_m \rangle$ is a continuous function of $(n - m)dt$. Expanding the exponential $\exp(\xi_n dt \cdot \mathcal{J})$ and expanding uncorrelated rotations to $\mathcal{O}(dt)$ as $\langle \tilde{R}_n^{\text{un}} \rangle \simeq I - \mathcal{K}^{\text{un}} dt$ ($\mathcal{K}^{\text{un}}$ is the kinematrix of the uncorrelated elementary processes), we obtain

$$\langle U_{n+1} \rangle = \langle U_n \rangle - \langle U_n \rangle \mathcal{K}^{\text{un}} dt + \langle U_n (\xi_n \cdot \mathcal{J}) \rangle dt + \mathcal{O}(dt^2).$$  \hspace{1cm} (5.2)

Large rotations are possible, but exceedingly rare. Their contribution to the expectation is negligible and we can work up to linear terms in $dt$. Now, for a centered
Gaussian-distributed vector $\mathbf{x}$ of any dimension, the integration-by-parts identity
\[ \langle f(x)x^\alpha \rangle = \sum_\beta \langle \partial f / \partial x^\beta \rangle \langle x^\beta x^\alpha \rangle \] holds [96]. Applying this identity and noting that $U_n$ depends only on $\xi_j$ for $j < n$ yields
\[ \langle U_n \xi_n \rangle \cdot \mathbf{J} = \sum_{j<n} \left[ \sum_{\alpha,\beta} \langle \xi_n^\alpha \xi_j^\beta \rangle \langle \tilde{R}_0 \cdots [\mathbf{J}_\beta \tilde{R}_j] \cdots \tilde{R}_n \rangle \mathbf{J}_\alpha \right] dt. \]

Substituting into Eq. (5.2) and reinterpreting the difference $((U_{n+1}) - \langle U_n \rangle)/dt$ as a derivative leads to
\[ \frac{d}{dt} \langle U(0, t) \rangle = \sum_{\alpha,\beta} \int_0^t \langle U(0, t') \mathbf{J}_\beta U(t', t) \mathbf{J}_\alpha \rangle \langle \xi^\alpha(t) \xi^\beta(t') \rangle dt' - \langle U(0, t) \rangle K_{\text{uncr}}. \] (5.3)

The change of $\langle U(0, t) \rangle$ with time is due to the noise at time $t$. Noise uncorrelated with what has gone before tends to degrade memory of the past in a simple indiscriminate manner. But noise which is correlated with the past, as $\xi$ is, has a more complicated effect. Since a Gaussian distribution is determined by its mean and covariance, the appearance of a simple covariance function in the governing equation (5.3) is a natural consequence.

Pretty as Eq. (5.3) is, it becomes difficult to work with in three or more dimensions since the matrices do not necessarily commute. However, the two-dimensional case is already very rich and many experimental studies involve self-propellers with an essentially two-dimensional motion due to a confining planar substrate. We therefore confine ourselves to the planar motion in the remainder of this paper. All rotations are about the $z$ axis and the only matrices involved are
\[ \mathbf{J}_z = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathcal{P}_z^\perp = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \] (5.4)

where $\mathbf{J}_z$ is the generator of infinitesimal rotation about the $z$-axis and $\mathcal{P}_z^\perp$ projects into the $xy$-plane. Since $\langle U(0, t) \rangle$ is written in terms of $\mathcal{P}_z^\perp$ and $\mathbf{J}_z$, and $[\mathcal{P}_z^\perp, \mathbf{J}_z] = \mathcal{P}_z^\perp \mathbf{J}_z - \mathbf{J}_z \mathcal{P}_z^\perp = 0$, the commutation $[\mathbf{J}_z(t', t), \mathbf{J}_z] = 0$ holds, and Eq. (5.3) yields
an exact solution in terms of the autocorrelation of the Gaussian noise:

\[
\langle U(0, t) \rangle = \exp \left[ -K^{\text{uncr}} t - F_\xi(t) P_z^\perp \right] \tag{5.5a}
\]

\[
F_\xi(t) = \frac{1}{2} \int_0^t \int_0^t \langle \xi(t')\xi(t'') \rangle \, dt'' \, dt' \tag{5.5b}
\]

By capturing the essential physics in the noise autocorrelation integral \( F_\xi(t) \), the kinematrix treatment avoids the complication of dealing explicitly with probability distributions by extracting the necessary information solely from the noise autocorrelation function.

A swimmer’s tail-to-head direction \( \hat{\chi} \) coincides with its instantaneous direction of deterministic velocity \( \hat{v} \) in a rectilinear motion. While such a swimmer usually moves forward along tail-to-head axis (\( \hat{v} = \hat{\chi} \)), it can also occasionally swim backward along the same axis (\( \hat{v} = -\hat{\chi} \)). We reference the instantaneous velocity to the tail-to-head direction by writing \( v \equiv \hat{v} := v_s \hat{\chi} \). It is important to distinguish between \( v \) and \( v_s \) since the former is the speed (magnitude of the velocity) while the latter is a one dimensional velocity along the \( \hat{\chi} \) axis such that for forward motion \( v_s = v \) and for backward motion \( v_s = -v \). As such, hereafter we refer to \( v_s \) as “signed-speed”.

Now, choosing the laboratory frame such that \( \hat{y} \equiv \hat{\chi}(0) \), the velocity pair correlator \( \langle \mathbf{v}(0) \cdot \mathbf{v}(t) \rangle \), the ensemble average of displacement \( \langle \Delta \mathbf{r}(t) \rangle \), the mean square displacement \( \langle |\Delta \mathbf{r}(t)|^2 \rangle \), and effective diffusivity \( D_{\text{eff}} \) of the self-propeller can be obtained from

\[
\langle \mathbf{v}(0) \cdot \mathbf{v}(t) \rangle = \langle v_s(0)v_s(t) \rangle \langle U(0, t) \rangle_{22}, \tag{5.6}
\]

\[
\langle \Delta \mathbf{r}(t) \rangle = \bar{v}_s \left[ \int_0^t \langle U(0, t') \rangle dt' \right] \cdot \hat{\chi}(0), \tag{5.7}
\]

\[
\langle |\Delta \mathbf{r}(t)|^2 \rangle = 2 \int_0^t (t - t') \langle v_s(0)v_s(t) \rangle \langle U(0, t') \rangle_{22} dt', \tag{5.8}
\]

and

\[
D_{\text{eff}} = \frac{1}{2} \int_0^\infty \langle v_s(0)v_s(t) \rangle \langle U(0, t') \rangle_{22} dt', \tag{5.9}
\]

where the subscript “22” denotes a matrix element. If there is no backwards motion (for example, the commonly-studied case of constant speed), then the propagator
can monitor the time evolution of the dynamical velocity vector rather than the structural tail-to-head vector. For such systems we make the modifications \( v_s \mapsto v \) and \( \dot{\chi} \mapsto \dot{v} \) in Eqs. (5.6)–(5.9).

The main contribution of this paper is extending the kinematic matrix theory to include Gaussian memory, as expressed by Eqs. (5.3)–(5.9). In the next section, as an example, we employ the formalism to discuss the physics of a rectilinear self-propeller with signed-speed fluctuation and Gaussian memory.

### 5.3 Linear motion with fluctuating speed and Gaussian Memory

The interplay of multiple time scales of the elementary processes of motion determines different regimes of swimmer ensemble behavior, quantified by asymptotic effective diffusivity and mean-square-displacement. In this section we study a self-propeller subjected to velocity fluctuations and orientational inertia, such as appears in the upper left of Fig. 1.1. Velocity fluctuations lead to stochastic variation of speed, which may also have inertial memory. The direction of motion may be influenced by stochastic noises arising from environmental fluctuations (e.g., Brownian kicks from fluid particles to a micron-sized self-propeller [45,48,53], spatially scattered food supply [52], or interaction with a substrate [79]) or internal fluctuations such as stochastic internal engine torque or decision-making processes of an organism.

Using a Fokker-Planck formalism, Peruani and Morelli [51] studied a self-propeller with speed fluctuation and Brownian orientational diffusion, which can account for internal engine fluctuations of biological systems. However, the lack of orientational inertia cannot capture the essential physics of self-propeller dynamics in many cases. For instance, Gautrais et al. [10] analyzed trajectories of *Kuhlia mugil* fish swimming in a tank, observing constant speed motion with persistent turns that cannot be modeled by a white noise. Rather, there was an inertia associated with the angular velocity leading to a decaying exponential autocorrelation. Correcting the white noise model with a finite inertial time leads to an Ornstein-Uhlenbeck process (OUP) for the angular velocity. Correspondingly, Gegond and
Motsch [11] used a Fokker-Planck formalism to obtain the effective diffusivity of the fish with constant speed and OUP orientational dynamics. Their model [10,11] matches experimental data well, setting a solid ground for the presence of OUP dynamics in self-propeller dynamics. By adding a finite inertial time to a white noise, the OUP [97] serves as the simplest colored noise that not only shows success in self-propellers [10,11,47,98–102], but also applies to other fields of physics such as quantum processes [103–106], network dynamics [107] and genetics [108–110].

We analyze a more general model including both velocity fluctuations and orientational inertia, subsuming the results of [11,51], yet with less complexity and more intuitive connection to the self-propeller physics. The self-propeller moves in a plane at fluctuating velocity \( \mathbf{v}(t) = v_s \mathbf{\hat{\chi}} \) and with an orientation \( \theta \), defined by \( \cos \theta = \mathbf{\hat{x}} \cdot \mathbf{\hat{\chi}} \). The self-propeller’s orientation changes according to

\[
\frac{d\theta}{dt} = \xi, \tag{5.10}
\]

in which \( \xi \) is a stationary OUP and \( \eta \) is Gaussian white noise of intensity \( \tau^{-2}D_o \):

\[
d\xi/dt = -\tau^{-1}\xi(t) + \eta(t) \tag{5.11a}
\]

\[
\langle \eta(t)\eta(t') \rangle = 2\tau^{-2}D_o\delta(t-t') \tag{5.11b}
\]

\[
\langle \xi(t)\xi(0) \rangle = \tau^{-1}D_\omega e^{-|t|/\tau\xi}. \tag{5.11c}
\]

Understanding the orientational wandering as being due to random torques, this model takes into account the self-propeller’s rotational inertia. The variance of the angular velocity, which may be a more convenient quantity for applications than \( D_o \), is simply \( D_o/\tau\xi \). In the limit \( \tau\xi \to 0 \), \( \xi \) acts as a white noise, recovering the simpler model of orientational Brownian motion diffusing at \( D_o \) with no inertia [51]. The autocorrelation integral [Eq. (5.5b)] for the OUP angular velocity \( \xi \) is monotonically increasing:

\[
F_{\xi^{\text{OUP}}}^\theta(t) = D_o t + D_o t \left[ \frac{e^{-t/\tau\xi} - 1}{t/\tau\xi} \right]. \tag{5.12}
\]

The first term is the white-noise contribution and the second term is the modification due to inertia. Equations. (5.5b), (5.10), and (5.12) yield the mean square
Figure 5.1. The disorientation time for a self-propeller to forget its initial orientation depends on the ratio of inertial $\tau_\xi$ and orientational diffusion $D_o^{-1}$ time scales. If the $\tau_\xi \ll D_o$ we are close to the white noise limit and the self-propeller disorients over an orientational diffusion time scale $\tau_\theta \sim D_o^{-1}$. On the other hand, when the inertial time is much larger than the orientational time scale, the disorientation time is the geometric average of inertial and orientational diffusion time scales, $\tau_\theta \sim (\tau_\xi D_o^{-1})^{1/2}$. Nourhani et al., Phys. Rev. E, 90, 062304 (2014). Copyright (2014) by the American Physical Society.

angular displacement

$$\langle |\Delta \theta(t) |^2 \rangle = 2F^\text{cup}_\xi(t) \approx \begin{cases} 2D_o t & t \gg \tau_\xi \\ (t/\tau_\xi)D_o t & t \ll \tau_\xi. \end{cases} \quad (5.13)$$

Here, $\tau_\xi$ is the crossover time from ballistic to diffusive angular dynamics. However, we shall see below that the physical regime of the ensemble behavior is governed not only by $\tau_\xi$, but also the disorientation time $\tau_\theta$ over which the orientation changes significantly: $\langle |\Delta \theta(\tau_\theta) |^2 \rangle \sim 1$. As illustrated in Fig. (5.1), $\tau_\theta$ can be distinct from both the orientational diffusion time $D_o^{-1}$ and the inertial time $\tau_\xi$.

If the inertial timescale is very short ($\tau_\xi \ll D_o^{-1}$), then the self-propeller “forgets” its prior orientation through pure diffusion and $\tau_\theta \sim D_o^{-1}$. If the inertial time is large ($D_o^{-1} \ll \tau_\xi$), then $\langle |\Delta \theta |^2 \rangle$ becomes order one already in the ballistic regime and $\tau_\theta \sim (D_o^{-1} \tau_\xi)^{1/2}$. Altogether, $D_o \tau_\theta \sim \max (1, \sqrt{D_o \tau_\xi})$. For example, the fish of [10] have $D_o \tau_\xi \sim 1/2$. 
Figure 5.2. Effective diffusion coefficient $D_{\text{eff}}$ of the linear self-propeller with orientational Gaussian noise characterized by correlation time $\tau_\xi$ and speed fluctuations characterized by correlation time $\tau_v$ and asymptotic orientational diffusion coefficient $D_o$. (a) the mean-speed and fluctuation speed make contributions to $D_{\text{eff}}$ proportional to $\Phi(D_o\tau_\xi, \infty)$ and $\Phi(D_o\tau_\xi, D_o\tau_v)$ respectively. (b) $\Phi$ shows two major regimes depending upon whether the speed correlation time is smaller or larger than the disorientation time $\tau_\theta$. In the former case, the diffusion is essentially determined by speed fluctuations and in the latter by orientational wandering. The disorientation time $\tau_\theta$ is proportional to $(D_o^{-1}\tau_\xi)^{1/2}$ when $D_o \ll \tau_\xi$, and saturates to $\sim 1$ as $D_o\tau_\xi \to 0$. (c) $D_{\text{eff}}$ may contain several crossovers as a result of the relative sizes and individual crossovers of the mean-speed and fluctuation-speed components. Note that for $D_o\tau_\xi \gg [\text{var}(v_s)/\bar{v}_s^2](D_o\tau_v)^2$, the mean-speed component always dominates. (d) Slices through $D_{\text{eff}}$ in the other direction, normalized to the $D_o\tau_\xi = 0$ value. Nourhani et al., Phys. Rev. E, 90, 062304 (2014). Copyright (2014) by the American Physical Society.

Getting back to velocity fluctuations, a signed-speed autocorrelation function

$$\langle v_s(t)v_s(0) \rangle = \bar{v}_s^2 + \text{var}(v_s)e^{-t/\tau_v}$$

appears naturally in many physical systems. It may arise from a self-propeller’s interactions with the environment, varying terrain or fuel availability, and $\tau_v$ reflects the inertia associated with signed-speed relaxation. The use of signed-speed
subsumes the ordinary speed (velocity magnitude) case where the motion is always directed along the tail-to-head direction, but also situations where the motion can sometimes be “backward”. That might apply to crowded environments, such as for an individual cell in a cell monolayer [19–24]. If the dominance of forward over backward motion is slight, the dimensionless measure \( \frac{\text{var}(v_s)}{\bar{v}_s^2} \) of signed-speed fluctuations can be very large. In that case, we observe multiple crossovers in the mean-square-displacement curves, as will be discussed later. The form (5.14) may represent a biased OUP processes with mean \( \bar{v}_s \). Alternatively, it may arise from internal engine fluctuations where the signed-speed jumps between discrete values. Such a case can be modeled by a Poisson distribution (at rate \( 1/\tau_v \)) of “reset times” at each of which a new signed-speed is chosen independently from a fixed distribution with mean \( \bar{v}_s \) and variance \( \text{var}(v_s) \). The path length between signed-speed resets has a mean \( \bar{v}_s \tau_v \) and variance \( \text{var}(v_s) \tau_v^2 \). For a self-propeller, a simple origin for such behavior might be a bistable engine, giving two possible values for \( v_s \).

With the OUP autocorrelation integral (5.12) for persistent turning and the signed-speed autocorrelation function (5.14) thus motivated, we proceed to calculate the effective diffusivity \( D_{\text{eff}} \) of the self-propeller using Eqs. (5.5) and (5.9) as

\[
D_{\text{eff}} = \frac{\bar{v}_s^2}{2D_o} \Phi(D_o \tau_\xi, \infty) + \frac{\text{var}(v_s)}{2D_o} \Phi(D_o \tau_\xi, D_o \tau_v),
\]

where we have defined the dimensionless function \( \Phi \) with the following physical limits:

\[
\Phi(x, y) := \int_0^\infty \exp\{-x [e^{-z/x} - 1] - z\} e^{-z/y} \, dz
\]

\[
= e^x \sum_{k=0}^{\infty} (-x)^k / [k! (1 + 1/y + k/x)]
\]

\[
\approx \begin{cases} 
  e^x (1 + 1/y)^{-1}, & x \ll 1 \\
  (\pi x)^{1/2}, & 1 \ll x \ll y^2 \\
  y, & x \gg \max(1, y^2).
\end{cases}
\]

The first term in the right-hand side of Eq. (5.15) describes the effective diffusion that would arise in the absence of signed-speed fluctuations, and the second
term describes the unique contribution of signed-speed fluctuations to the effective diffusion. The reason for this clean separation is given below.

Figure 5.2 plots $D_{\text{eff}}$ and $\Phi$ across a range of correlation times for orientation and speed. The diagram below facilitates an intuitive account of this behavior:

The self-propeller’s signed-speed can be split into a mean and a fluctuation:

$$v_s(t) = \bar{v}_s + \sqrt{\text{var}(v_s)} \nu(t),$$  \hspace{1cm} (5.17)

where the noise $\nu$ obeys

$$\langle \nu(t) \rangle = 0, \quad \langle |\nu(t)|^2 \rangle = 1. \hspace{1cm} (5.18)$$

The displacement can be similarly split as $\Delta r(t) = \Delta r^{\text{mean}}(t) + \Delta r^{\text{flct}}(t)$. The diagram depicts the independent random inputs $\eta$ and $\nu$. Strictly speaking, $\Delta r^{\text{mean}}(t)$ and $\Delta r^{\text{flct}}(t)$ are not independent since they are driven by the same orientation process $\theta(t)$. But, they are probabilistically orthogonal, because the mean-speed and fluctuation-speed are: $\langle \nu(t) \rangle = 0$. As a result, $\Delta r^{\text{mean}}(t)$ and $\Delta r^{\text{flct}}(t)$ (and through them the mean signed-speed and signed-speed fluctuation) contribute to $D_{\text{eff}}$ in a simple additive way.

Three major features of $\Phi(D_o\tau_\xi, D_o\tau_v)$ in Fig. 5.2(a) leap to the eye. First, $\Phi(D_o\tau_\xi, \infty)$, the curve for infinite $D_o\tau_v$ exhibits a crossover from a constant 1 to $\sim \sqrt{D_o\tau_\xi}$ at $D_o\tau_\xi \sim 1$. Second, for smaller values $1 \ll D_o\tau_v < \infty$, the curves follow that for $D_o\tau_v = \infty$ up to $D_o\tau_\xi \sim (D_o\tau_v)^2$, at which point they saturate to a value approximately $D_o\tau_v$. Finally, for very small speed correlation time $D_o\tau_v \ll 1$, $\Phi(D_o\tau_\xi, D_o\tau_v) \approx D_o\tau_v$ depends only weakly on $D_o\tau_\xi$. An intuitive physical interpretation of these observations and the asymptotics in Eq. (5.16c) follows from a comparison of the disorientation time $\tau_\theta$ and speed correlation time
τ_v. Henceforth, we use a more precise definition for the disorientation time:

\[ D_0 \tau_\theta := \left[ \max \left( 1, \frac{\pi}{2} D_0 \tau_\xi \right) \right]^{1/2}, \]  
\[ (5.19) \]

to recast Eq.(5.16c) into

\[ \Phi(D_0 \tau_\xi, D_0 \tau_v) \approx \begin{cases} 
D_0 \tau_v, & \tau_v \ll \tau_\theta \\
D_0 \tau_\theta, & \tau_v \gg \tau_\theta.
\end{cases} \]  
\[ (5.20) \]

Figure 5.2(b) reveals two regimes of this equation, showing \( \tau_\theta \sim D_0^{-1} \) is independent of \( \tau_\xi \) for \( D_0 \tau_\xi \ll 1 \). A straightforward understanding of Eq. (5.20) is at hand. To better understand this behavior, we rewrite

\[ \Gamma := \Delta r_{\text{fluc}} / [2D_0^{-1} \text{var}(v_s)]^{1/2} \]  
\[ (5.21a) \]

\[ \Phi(D_0 \tau_\xi, D_0 \tau_v) = \lim_{t \to \infty} \frac{1}{t} \langle |\Gamma(t)|^2 \rangle \]  
\[ (5.21b) \]

and analyze \( \Phi(D_0 \tau_\xi, D_0 \tau_v) \) as the diffusive behavior of \( \Gamma \). In the limit \( \tau_v \ll \tau_\theta \) where signed-speed changes very rapidly compared to orientation, the fluctuation part resembles a one-dimensional random walk along a slowly changing direction with step-duration \( \Delta t = \tau_v \) and step-length-squared \( \langle |\Delta r_{\text{fluc}}|^2 \rangle \approx \langle |\nu(t)|^2 \rangle \text{var}(v_s) \tau_v^2 \). By Eq. (5.18), \( \Phi \approx \langle |\Delta \Gamma|^2 \rangle / \tau_v \approx D_0 \tau_v \). In the opposite limit, \( \tau_v \gg \tau_\theta \), the fluctuation part has speed of order \( \sqrt{\langle |\nu(t)|^2 \rangle \text{var}(v_s)} \) which remains nearly constant during the time \( \tau_\theta \), and resembles a two-dimensional random walker with step-duration \( \tau_\theta \) and step-length-squared \( \langle |\Delta r_{\text{fluc}}|^2 \rangle = \text{var}(v_s) \tau_\theta^2 \). This leads to a \( \nu \)-averaged diffusivity \( \Phi \approx \langle |\Gamma|^2 \rangle / \tau_\theta \approx D_0 \tau_\theta \). Figure 5.2(a) now stands rationalized via Fig. 5.2(b) and Eq. (5.20).

Turning now to the interpretation of the more complicated behavior of the effective diffusivity (5.15) depicted in Fig. 5.2(c), we note that the various asymptotic regimes can be collected into

\[ 2D_{\text{eff}} \sim \bar{v}_s^2 \tau_\theta + \text{var}(v_s) \min (\tau_v, \tau_\theta). \]  
\[ (5.22) \]

The critical parameter determining the number of crossovers is \( D_0 \tau_v \).

If the orientational diffusion time scale greatly exceeds the speed correlation
time ($\tau_v \ll D_o^{-1}$), we have $\min(\tau_v, \tau_\theta) = \tau_v$; the fluctuation-speed contribution $\text{var}(v_s)\tau_v$ is independent of $D_o\tau_\theta$ and the only question is when this dominates the mean-speed contribution. In case $[\text{var}(v_s)/\bar{v}_s^2]D_o\tau_v \ll 1$, the answer is never. This is exemplified by the solid green hockey-stick shaped curve in Fig. 5.2(c). Otherwise, there is a crossover from fluctuation-speed domination to mean-speed domination at $D_o\tau_\theta \approx [\text{var}(v_s)/\bar{v}_s^2]^{1/2}$, as shown in the blue dashed curve.

On the other hand, if the time required for changing signed-speed is much longer than the orientational diffusion time scale ($\tau_v \gg D_o^{-1}$), the story starts off similarly with a roughly constant value $2D_{\text{eff}} \approx \bar{v}_s^2 + \text{var}(v_s)$ up to about $\tau_\theta \sim D_o^{-1}$, at which point it shifts into the arm of the hockey stick with $2D_{\text{eff}} \approx [\bar{v}_s^2 + \text{var}(v_s)](D_o^{-1}\tau_\theta)^{1/2}$. But, when $D_o\tau_\theta$ exceeds $(D_o\tau_v)^2$, the mean-speed contribution continues to increase, while the fluctuation-speed contribution plateaus. If $\text{var}(v_s)/\bar{v}_s^2 \gg 1$, this appears as a clear plateau, as seen in the dotted red curve of Fig. 5.2(c), until the mean-speed contribution becomes dominant at $\tau_\theta \sim D_o[\text{var}(v_s)/\bar{v}_s^2]^{1/2}$ and the $\sqrt{D_o\tau_\theta}$ behavior of the hockey stick returns.

Figure 5.2(d) gives another perspective on $D_{\text{eff}}$ by slicing in the other direction and taking a ratio to the white noise limit ($D_o\tau_\theta \rightarrow 0$)

$$D_{\text{eff}}^{\text{white}} = \frac{\bar{v}_s^2}{2D_o} + \frac{\text{var}(v_s)}{2D_o} \frac{1}{1 + 1/D_o\tau_v}. \quad (5.23)$$

In the limit $D_o\tau_v \rightarrow 0$ of rapid speed fluctuations the effective diffusivity depends only on average speed $D_{\text{eff}} \sim \bar{v}_s^2\tau_\theta$, and as $D_o\tau_v \rightarrow \infty$, $D_{\text{eff}} \sim [\bar{v}_s^2 + \text{var}(v_s)]\tau_\theta$. In either extreme, $D_{\text{eff}}$ is simply proportional to $\tau_\theta$, which is $D_o^{-1}$ in the white noise limit. So, for both very large and very small $D_o\tau_v$, $D_{\text{eff}}/D_{\text{eff}}^{\text{white}} \approx D_o\tau_\theta$, independently of the signed-speed parameters $\bar{v}_s$ and $\text{var}(v_s)$. In between, if $\text{var}(v_s)/\bar{v}_s^2$ is large enough, there is a region where $D_{\text{eff}}$ is insensitive to $D_o\tau_\theta$ up to a large value. This corresponds to the long dashed blue plateau shown at $D_o\tau_v = 0.1$ in Fig. 5.2(c).

The effective diffusivity characterizes only the asymptotic behavior of the mean-square displacement. The full time dependence exhibits additional complexity. Using Eq. (5.8) we obtain the mean square displacement

$$\langle |\Delta \mathbf{r}(t)|^2 \rangle := 4tD_{\text{eff}} + 4t \frac{\bar{v}_s^2}{2D_o} \hat{\Phi}(D_o\tau_\theta, \infty, D_o t)$$
Figure 5.3. Mean-squared displacement of the linear self-propeller with Gaussian orientational noise of correlation time $\tau_\xi$, signed-speed fluctuations with correlation time $\tau_v$, and asymptotic orientational diffusion coefficient $D_o$. If the self-propeller disorients faster than signed-speed changes value, $\tau_\theta < \tau_v$, (upper curves) we observe a single crossover from ballistic to diffusive regimes at $\tau_\theta$; with increase in inertial time $\tau_\xi$ the crossover happens later. In the opposite regime $\tau_\theta \gg \tau_v$ (lower curves) for large signed-speed fluctuations $\text{var}(v_s)/\bar{v}_s^2 \gg 1$ the signed-speed fluctuation contribution shows a one-dimensional ballistic to diffusive crossover about $\tau_v$. Combined with mean signed-speed part (behaving like the $\tau_\theta \ll \tau_v$ case), this produces three crossovers. Nourhani et al., Phys. Rev. E, 90, 062304 (2014). Copyright (2014) by the American Physical Society.

\[ + 4t \frac{\text{var}(v_s)}{2D_o} \tilde{\Phi}(D_o \tau_\xi, D_o \tau_v, D_o t), \]

(5.24)

where

\[ \tilde{\Phi}(x, y, z) = \frac{e^x}{z} \sum_{k=0}^{\infty} \frac{(-x)^k}{k!(1 + 1/y + k/x)^2} \left[ e^{-(1+1/y+k/x)z} - 1 \right] \]

(5.25a)

\[ \approx \begin{cases} \frac{1}{2} z - \Phi(x, y), & z \ll \min(1, x, y) \\ 0, & z \to \infty. \end{cases} \]

(5.25b)

For times much shorter than all the characteristic time scales, $t \ll \min(D_o^{-1}, \tau_\xi, \tau_v)$, we have ballistic motion $\langle |\Delta r(t)|^2 \rangle \approx [\bar{v}_s^2 + \text{var}(v_s)]t^2$, independently of orientational, inertial and signed-speed correlation time scales. At very long times the self-propeller behaves diffusively; $\langle |\Delta r(t \to \infty)|^2 \rangle$ is $4tD_{\text{eff}}$ and depends on all
three time scales $D_0^{-1}$, $\tau_\xi$ and $\tau_v$. Figure 5.3 shows the behavior of Eq. (5.24) in the limit of large speed fluctuations for a variety of time scales. Since $\langle|\Delta r_{\text{mean}}(t)|^2\rangle$ and $\langle|\Delta r_{\text{flct}}(t)|^2\rangle$ each has its own ballistic-to-diffusive crossover, in the limit of rapid, large signed-speed fluctuations, i.e. $D_0\tau_v \ll 1$ and $\text{var}(v_s)/\bar{v}_s^2 \gg 1$, three clear crossovers are observed. We analyze the two limiting regimes $\tau_v \ll \tau_\theta$ and $\tau_\theta \ll \tau_v$. The mean-speed contribution $\langle|\Delta r_{\text{mean}}(t)|^2\rangle$ is invariably in the latter limit. Suppose first that the self-propeller disorients much faster than its signed-speed changes, i.e., $\tau_\theta \ll \tau_v$. Then, an individual self-propeller has a ballistic-to-diffusive crossover at time $\tau_\theta$. Its speed is stable over much longer times, so it behaves as though its diffusion coefficient were fluctuating on the time scale $\tau_v$. On the other hand, if $\tau_v \ll \tau_\theta$, the fluctuation part of the displacement $[\Delta r_{\text{flct}}(t)]$ of an individual self-propeller has a ballistic-to-diffusive crossover at $\tau_v$, but to a nearly one-dimensional diffusive motion since much before the self-propeller disorients, the signed-speed has changed many times. There is a second crossover, to genuinely two-dimensional diffusion, at $\tau_\theta$ when the self-propeller starts to disorient. In either case, however, the ensemble average $\langle|\Delta r_{\text{flct}}(t)|^2\rangle$ will evidence only the primary crossover at $\min(\tau_\theta, \tau_v)$. When $\tau_\theta \ll \tau_v$ (the upper set of curves in Fig. 5.3), the full mean-square displacement exhibits just a single ballistic-to-diffusive crossover at $\tau_\theta$. In case $\tau_v \ll \tau_\theta$, the speed-fluctuation contribution $\Delta r_{\text{flct}}$ becomes diffusive earlier. If $\langle|\Delta r_{\text{mean}}(\tau_\theta)|^2\rangle/\tau_\theta \sim \bar{v}_s^2\tau_\theta \gg \text{var}(v_s)\tau_v \sim \langle|\Delta r_{\text{flct}}(\tau_\theta)|^2\rangle/\tau_\theta$, the total motion can re-enter a ballistic regime when $\Delta r_{\text{mean}}$ comes to dominate somewhere between $\tau_v$ and $\tau_\theta$. Later, at $\tau_\theta$, this component, too, becomes diffusive. This is exemplified by the lower set of curves in Fig. 5.3.

5.4 Concluding Remarks

The extension of kinematic matrix theory to incorporate correlated Gaussian noises expands its applicability to real-world systems with significant inertia. The ability to work straightforwardly from just the noise autocorrelation simplifies calculations significantly and helps one to focus more on the physics of the problem. Our streamlined and close-to-the-physics treatment of the rectilinear self-propeller with velocity fluctuations and persistent turning — a model with real-world interest [11, 51] — exemplifies this. This simplicity of kinematic matrix theory enables the
study of more complicated systems with less mathematical sophistication, and provides a useful tool for experimentalists to develop models for analyzing their data.
Future Research

In this dissertation, I discussed the interplay between the deterministic and stochastic in self-propellers and developed methodologies to analyze them. The phenomena of chiral diffusion in rotary self-propellers is studied in the white-noise limit of the orientational diffusion. The next question that arises is the effect of orientational inertia on the chiral diffusion. Neither a purely deterministic rotation nor a purely orientational diffusion leads to diffusion, but their combination results in chiral displacement. The orientational inertia should diminish the effect of rapid orientational changes in the white-noise limit, so it would be a natural expectation to have less chiral effect as the inertial time scale increases.

Another chiral phenomenon studied here was guiding and sorting rotary self-propeller through interaction with a soft periodic potential. The problem opens many further questions for which answering can lead to at least another Ph.D. dissertation. The main focus of chapter 3 was controlled drift of rotary self-propellers, where I did not discuss the variations of potential parameters. The studied potential has a hexagonal symmetry with one local minima in each unit cell. Adjusting $k_i$’s we can have different lattice structures with multiple local minima in a unit cell. Moreover, I briefly mentioned the possibility of chaotic dynamics in the white region of the drift phase diagram in Fig. 3.1c. In this region we observed sensitivities to initial condition and trajectory periodicity of multiple rotation period with high sensitivity to potential strength (see Fig. 6.1a). The nonlinear dynamics in this region is rich and need to be studied throughly. Finally, for some value of $(\alpha, \beta)$ we observed more than one trajectory attractor (see Fig. 6.1b). The mech-
anism for the formation of these trajectory attractors and the transition between
them induced by stochastic noise is an open question.

The last half of the dissertation dealt with the kinematic matrix theory. I
extended the white noise limit to Gaussian memory. The natural next step is to
include the non-Gaussian memory effects. The ensemble average propagator in the
kinematic matrix theory consists of rotations is SO(3). Using the same formalism,
we can extend the theory to study stochastic processes on Lie group. Also, the
theory can be extended to discuss the evolution of quantum vectors, such as spin.
These developments are in progress.
Bibliography


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