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Dynamics of Chiral Particles in Viscous Fluids

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Doctor of Philosophy
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August 2022
Abstract

Colloidal suspensions — micron sized particles in a molecular solvent, typically water — are found everywhere in nature, e.g. milk, and in artificial materials, e.g. paint. The dynamics of colloidal particles are therefore of interest to both academia and industry. The sedimentation of particles in suspensions is relevant in multiple fields, such as its application to the transport and separation of biological particles (viruses, bacteria, etc.). Many classical fluid mechanics studies have looked at the sedimentation, and/or tumbling due to shear, of a single particle, either using analytic methods or, more recently, numerical techniques. By now it is well understood that the particle shape uniquely determines its dynamics, but the precise trajectory and orientational dynamics are only known for a limited set of shapes. This is because, barring the simplest of shapes, the analytic calculations are challenging and often involve reducing approximations. The way chiral particles sediment and behave under shear are still unknown, and in the process of being studied and understood. This is true, in particular, for conditions under which the trajectories of such particles are chiral. In this thesis, therefore, the focus will be on the behaviour of chiral particles suspended in fluids at low Reynolds number — where the viscosity dominates over the inertia.

The dynamics of chiral objects is studied using Resistive Force Theory, which assumes that the body can be partitioned into segments but ignores the hydrodynamic couplings between the parts of the particle. These studies are then compared to a numerical calculation [Palanisamy and Otter, J. Chem. Phys. 148, 194112 (2018)] that accounts for the hydrodynamic interactions using the Rotne-Prager-Yamakawa approximation. For a sedimenting helix, great agreement is found between the analytic and numerical results. Helices, for most initial conditions, sediment performing a superhelical trajectory — a helical path with the symmetry axis parallel to the direction of gravity — for which the handedness is opposite to that of the helix. It is also observed that a helix, in an almost
horizontal configuration, is either attracted to the horizontal orientation, in which it sediments in a straight line in the direction of gravity, or to trajectories that form an unstable helical-like path. Alternatively, when a helix is in a simple shear flow it travels performing Jeffery-like orbits with a lateral drift perpendicular to the plane of shear.

To better understand the result for the helix sedimentation, the settling of L- and C-shapes is also considered. Here it shown that an object does not need to be chiral for its sedimentation trajectory to possess chirality, in agreement with the findings by Krapf et al. [Phys. Rev. E 79, 056307 (2008)]. Counter-intuitively, it was observed that the result, by Taylor, of a sedimenting rod — the rod does not reorient — is not obtained by taking the limit of an L-shape with a vanishing short leg. This is because any minute perturbation away from the rod limit leads to the emergence of a fixed point to the dynamics at infinite time due to orientational couplings in the Grand Mobility Matrix that persist for all perturbations.

Thanks to this understanding of simple (chiral) objects, insight was gained into the sedimentation behaviour of a complicated shape: a Möbius strip. This object has a rich state diagram for its settling behaviour, which is strongly dependent on its initial orientation. This diagram, for a single Möbius strip, is portrayed and insight into the identified trends is given.

Overall, it was shown that the sedimentation of anisotropic or chiral particles is chiral and future work could include finding analytic expressions to describe these trajectories. Whereas, for a helix in a shear flow, the properties and dependencies of the lateral drift observed can be further studied.
Lay Summary

Colloidal suspensions are composed of micron-sized particles suspended in a liquid, typically water, and are found in a wide range of natural and artificial materials such as milk and paint. Understanding the dynamics of these particles is crucial for many applications in fields such as biology, chemistry, and materials science and because of how common the systems are these studies are interesting to both academic scientists and industry.

While previous studies have investigated the motion of individual particles, it is often challenging to predict the behaviour of more complex shapes accurately. This thesis focuses on the behaviour of chiral particles, which have a distinct handedness, and how they move when suspended in fluids where viscosity dominates over inertia, which is common for very small particles or in very viscous fluids.

Both theoretical models and numerical simulations are used to investigate the sedimentation behaviour of chiral particles. The results showed that chiral and anisotropic (asymmetric) objects, such as helices, L-shapes, and C-shapes, sediment in a manner that depends on their shape and orientation. For instance, a helix often follows a curved path that is opposite to its own handedness when it falls through a fluid. Moreover, the study revealed that a particle does not have to be chiral to produce a similar sedimentation path.

The thesis also explored the behaviour of a complex shape, a Möbius strip, and presented a diagram showing many different types of sedimentation behaviour. The findings showed that the sedimentation of anisotropic or chiral particles is chiral, and there is potential for future work to describe these trajectories.
Declaration

I declare that this thesis was composed by myself, that the work contained herein is my own except where explicitly stated otherwise in the text, and that this work has not been submitted for any other degree or professional qualification except as specified.

Parts of this work have been published in [3].

(Martina Palusa, August 2022)
Acknowledgements

I would like to sincerely thank my supervisor Alexander Morozov for his help, support and kindness over the past few years. Thank you also to our collaborator Joost de Graaf whose work and ideas have significantly helped me, I am also incredibly grateful for his taking his time to give me invaluable feedback as I was working on this thesis.

I would also like to thank all my colleagues in the Physics department who have been great companions during my four years in the Physics building and have been of great support through all the ups and downs of life as a PhD student. It is unfortunate that the time spent together was cut short due to Covid-19 lock-downs that occurred during 2 of my 4 years of PhD.

Thank you to my friends and family for all their support, interest and company all these years. In particular thank you to my parents whose love and support has shaped me into who I am today and helped me get to where I am.

Finally, I would like to acknowledge the Higgs Centre for funding during my PhD.

Mille grazie e un grande abbraccio ai miei genitori e alla mia famiglia.
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Chapter 1

Introduction

This thesis concerns itself with the dynamics of chiral, slender objects in viscous Newtonian fluids. In particular, the microhydrodynamics of helices is emerging as an important research topic across many disciplines. Motivated by their abundance in microscopic organisms [5-7], helical shapes were recently studied in the context of self-propulsion [7], swimming driven by a helical flagellum [8-9], sedimentation [2-10], and their dynamics in a shear flow [11-18]. In a more general context, recent experimental and theoretical work suggests that chiral objects often follow chiral trajectories when sedimenting in viscous fluids due to gravity [2-19-20], while both chiral and non-chiral objects exhibit spatial drift under shear flow [12-14-21]. The underlying physics of the latter was presented as a way to separate chiral objects in viscous media by external electric fields or shear [22-23]. Additionally, the sedimentation of complex shaped particle can be important as it applies to the transport and separation of biological particles (viruses, bacteria, etc.) [24]. Sedimentation is an important process employed in many industrial processes and applied to processes where the density and size distributions of suspended particles can be used for phase separation [25].

What is meant by viscous fluid in the context of this thesis is now defined. The equations that macroscopically describe the rheological behaviour of a fluid are obtained from the conservation of mass and of momentum imposed on the fluid
itself and are given by,

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0, \quad (1.1) \]

\[ \frac{\partial}{\partial t} \rho \mathbf{u} + \nabla \cdot \rho \mathbf{u} \mathbf{u} = -\nabla p + \nabla \cdot \sigma + \rho \mathbf{g}, \quad (1.2) \]

where \( \rho \) is the density of the fluid, \( \mathbf{u} \) is the flow field, \( p \) is the pressure in the surrounding fluid, and \( \sigma \) is the stress tensor. Note that Eqs. (1.1) and (1.2) are valid for any type of fluid, as only (basic) conservation laws have been used in their derivation \[26\]. When it comes to colloidal suspensions and microswimmers, however, only incompressible fluids are considered and Eq. (1.1), known as the \textit{continuity equation}, reduces to

\[ \nabla \cdot \mathbf{u} = 0. \quad (1.3) \]

In this thesis, only Newtonian fluids are considered. These are fluids, such as water and oil, that have a viscosity independent of the shear rate. For such fluids, viscosity is assumed to be constant and the stress tensor \( \sigma \) can be expressed as

\[ \sigma = \mu \left( \nabla \mathbf{u} + \left( \nabla \mathbf{u} \right)^T \right), \quad (1.4) \]

Therefore, for an incompressible Newtonian fluid, Eq. (1.2) can be simplified and expressed in a form known as the Navier-Stokes equation

\[ \rho \left( \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u}. \quad (1.5) \]

When de-dimensionalised, the Navier-Stokes equation gives rise to the Reynolds number, a dimensionless quantity that is often encountered and used and is defined as,

\[ Re = \frac{\rho UL}{\mu}, \quad (1.6) \]

where \( U \) and \( L \) are the characteristic velocity and length scale respectively, \( \rho \) is the fluid density and \( \mu \) is the viscosity of the fluid. The Reynolds number represents the ratio between the inertial forces and the viscous forces. This number,
therefore, gives rise to two distinct regimes: the high Reynolds number regime, in which the inertial forces are dominant, and the low Reynolds number regime where the viscous forces dominate over the inertial ones. A person swimming and fish are examples of swimmers with a high Reynolds number and fluid dynamics in this regime is well studied and intuitively understood [27]. Bacteria and other microorganisms, on the other hand, belong to the world of low Reynolds number where the swimming methods used by larger organisms, such as fish, birds and insects, no longer work. A theorem formulated by Purcell, and known in literature as the Scallop Theorem [28], shows the importance of the swimming ‘style’ of a swimmer. The theorem states that, in order to achieve propulsion in a Newtonian fluid at low Reynolds number, a swimmer has to exhibit a motion that is not time symmetric. The name of this theorem is attributed to scallops that, in opening and closing a single hinge, would not be able to move in highly viscous environments.

The motion of a particle suspended in a Newtonian fluid becomes quite complex (e.g. chiral, unstable, highly dependent on initial conditions) if the particle shape is not simple like a sphere or a straight rod [11, 29, 30]. For example, propeller-like particles settle under the influence of gravity, changing their orientation and velocity periodically [12, 31, 32]. In shear flow such propellers can even move with a velocity that is different from the velocity of the fluid. How a particle, placed in a Newtonian fluid, settles down under gravity is an important problem in colloid science and particle technology due to, amongst other things, its application to the chemical and petroleum industries. Systems that could benefit from a deeper knowledge of sedimentation include activities such as hydro-transport of particles [33] or the transport of micro-sensors to fractures in rock formations that report back information on rock structure, fluid viscosity, and other properties [34]. Multiple studies for the sedimentation of simple particles (sphere [35, 37], rod [37-39]) have been done and are well documented in literature [11, 30, 35]. Not many studies, however, have been done for complex shaped particle such as helices, L-shapes and Möbius strips. The latter being a shape that has recently seen applications in chemistry [40, 41]. Considering the interest in dynamics of (rigid) slender bodies in viscous fluids, the sedimentation of particles, such as the helix and the Möbius strip, and the effect of shear flow on rigid helical filaments are studied.

From here on, the focus will be on particles with irregular shapes were two (or one) dimension is much smaller than the others. These constitute slender
bodies, examples are rods, helices, Möbius strip and more. Elongated slender particles are of great interest due to most biological swimmers exploiting the motion of slender appendages (“flagella”) for locomotion \[42-46\]. Reasons for the locomotion include bacteria, such as \textit{E. coli} using chemotaxis to detect gradients in nutrients and move to regions of higher concentration \[6\], and the swimming to the ovum of the spermatozoa of many organisms \[47\]. This chapter will introduce some of the theories, developed to try to solve for and approximate the forces acting on a slender anisotropic body in the Stokes regime.

First, Slender Body Theory (SBT) is introduced; this theory considers the flow around a long slender solid body, which can possess curvature. This theory is chosen as such a body is a suitable model for a fibre or thread-like particle which may be either rigid (i.e. the Kirchhoff rod, assumed to be inextensible and unshearable) or flexible (i.e. the Cosserat, which in addition to bending and twisting, also allows stretching and shearing \[48-49\]); in this thesis, only rigid objects are considered. In SBT the solution to the problem of Stokes flow resulting from the motion of a slender body is constructed using the singularity method of using Stokeslets \[50-56\]. Alternatively, the translation of any rigid slender body through a viscous fluid can be analysed by so-called Resistive-Force Theory (RFT) \[57\], provided the radius of curvature is large compared with the body radius. The underlying assumption of Resistive-Force Theory is that the hydrodynamic forces are proportional to the local body velocity, with the constant of proportionality being defined as the force (or drag) coefficient. As pointed out by Lighthill \[5\], this assumption is inconsistent with the true hydrodynamic situation, in which viscous effects dominate and produce long-range hydrodynamic interactions. Whilst both methods can be applied to a similar category of particle shapes, RFTs are more computationally efficient. However, RFTs can, at best, produce semi-quantitative approximations of actual drag forces on extended objects \[9, 58, 59\] and, at worst, fail even qualitatively there where the inclusion of hydrodynamic interactions is crucial \[60\]. SBTs, on the other hand, are accurate, but are computationally more inefficient as they require a large dimension matrix inversion \[61\].

Going beyond filaments, slender ribbons are considered, as their added property of having sides, unlike the filaments, gives them more features and can create new configurations. This theory was first introduced by Koens and Lauga \[62\] and called Slender Ribbon Theory (SRT). It is covered here as the results, obtained for the mobility coefficients of a stadium-shaped particle by Koens and Lauga \[4\],
Finally, an efficient and more general method to calculate, in the Stokes regime, the coupled translational and rotational dynamics of arbitrarily shaped particles based is introduced. The sedimenting objects are approximated as a rigid collection of spheres and the dynamics are solved for by using a method developed by Palanisamy and Den Otter [1]. This proposed method gives way to computational studies of dynamics of bodies that have, so far, only been theoretically approximated. This was independently implemented in the C++ programming language by Joost de Graaf.

1.1 Thesis Outline

The remainder of this thesis is organised as follows.

Chapter 2 provides the theoretical background for the methods used throughout by introducing some of the theories developed to try to solve for, and approximate, the forces acting on a slender anisotropic body in the Stokes regime. These include Slender Body Theory, Resistive Force Theory, Slender Ribbon Theory and a Rotne-Prager-Yamakawa level numerical approximation method [1]. The latter was implemented in C++ by Joost de Graaf, and the author benchmarked it against literature results for a sphere and sedimenting rod.

In Chapters 3 and 4 the sedimentation of a rigid helix in the Stokes regime is studied. In Chapter 3 RFT is employed in order to establish the sedimentation dynamics of a helix subjected to gravity. It is found that, for most initial orientations, the helix sediments performing a superhelical trajectory with a chirality that depends on the chirality of the helix itself. For near-horizontal initial orientations, however, a regime of unstable sedimentation is found. These results are then numerically verified in Chapter 4 using the Rotner-Prager-Yamakawa (RPY) bead method. Here good qualitative and semi-quantitative agreement with the approximations for the trajectory obtained using Resistive-Force Theory and the Rotne-Prager-Yamakawa method for a sedimenting helix is observed.

Chapter 5 focuses on the sedimentation of the achiral, anisotropic L- and C-shapes. First, the sedimentation of an L-shape, parallel to the plane of gravity, is studied using both RFT and the RPY-bead method. Here, a discrepancy between the RFT and RPY predictions was found. This indicates that, for an L-shape, the
hydrodynamic coupling between the various parts could be an important factor in determining the dynamics. An L-shape, when sedimenting, re-orientates itself to a preferred orientation that depends on the ratio of the two legs and is independent of its initial orientation. The approach to the ideal limit of a rod (short leg tends to zero) is also analysed. In the second part of Chapter 5, the dynamics of the sedimentation of a C-shaped particle that is at an angle to the plane of gravity is evaluated. It is found that the C-shape sediments with a chiral trajectory that is more complex than the superhelical trajectory recovered for the sedimenting helix. The properties of this trajectory, including its chirality, are found to be dependent on the initial conditions imposed on the system.

The focus is shifted back to the sedimentation of a chiral particle in Chapter 6. Here, results for the mobility coefficients of a stadium shaped particle, which can be considered an achiral version of the Möbius strip, obtained by employing Slender Ribbon Theory and the RPY-bead method are compared. In the following section, the dynamics of a Möbius strip are then studied. Here, a state diagram is presented in order to show the range of behaviours exhibited by the Möbius strip. A Möbius strip, when sedimenting, is found to have a chiral trajectory with an opposite handedness to the handedness of the strip itself. Additionally, the properties of the chiral trajectory are dependent on the initial conditions imposed on the orientation of the strip.

In Chapter 7, finally, the dynamics of a rigid helix in a shear flow are evaluated. It is found that a helix placed in a shear flow, with its major axis of symmetry in the shear plane, performs Jeffery-like orbits and experiences a lateral drift in the positive (or negative) $z$-direction. The sign of the drift depends on the chirality of the helix, as well as on the parity of its number of turns ($N$ even or odd). Examining then a helix where its major axis is at an angle with the plane of shear, a kayaking motion is observed. A critical value, of the initial angle of the helix with respect to the shear plane, that delimits the two regions of behaviour, kayaking and Jeffery orbits, is found.

Overall, it was shown that the sedimentation of anisotropic or chiral particles is chiral and with a handedness dependent on the handedness of the particle (if the particle is chiral) or the initial orientation (if the particle is achiral). Future work could involve finding analytic expressions to describe these trajectories, as well as correcting the discrepancies between SRT and the RPY method. For a helix in a shear flow, in agreement with multiple observations [11–18], a lateral drift perpendicular to the shear plane is found. Better understanding
the dependence of this drift on the helix’s properties could help progress in fields such as enantiomer separation [63]. This is summarised in a brief concluding chapter, Chapter 8.
Chapter 2

Methods

In this thesis, the dynamics of slender particles suspended in a viscous fluid are studied. These will sediment due to gravity or be subjected to shear flow. The theoretical framework used throughout this thesis to study slender objects is laid out in the following sections.

2.1 Properties of the Fluid

In Chapter 1, the Navier-Stokes equations for an incompressible Newtonian fluid were introduced in Eqs. (1.3) and (1.5). These are reported again in the following.

\[ \nabla \cdot \mathbf{u} = 0, \]
\[ \rho \left( \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u}, \]

where \( \rho \) is the density of the fluid, \( \mathbf{u} \) is the flow field, and \( p \) is the pressure in the surrounding fluid. Typically, a particle is a boundary condition to the flow and, considering this, there are two roughly equivalent viewpoints in tackling hydrodynamics problems. The first involves solving for the entire flow field and computing forces on the boundary, this includes methods such as the Lattice Boltzmann Method (LBM) \[64\], Multi-Particle Collision Dynamics (MPCD) \[65\], Smoothed Particle Dynamics \[66, 67\], Dissipative Particle Dynamics (DPD) \[68\] and other numerical methods \[69, 70\]. The second method, described and used
in this thesis, employs a boundary-only description (Boundary Element Method (BEM) [71], Oseen [72], RPY [73, 74], etc.). Before describing the methods used, however, the equation system introduced is further analysed.

To solve for the force distribution on a particle, the Navier-Stokes equations, Eqs. (1.3) and (1.5), need to be solved for the flow field \( \mathbf{u} \) and pressure \( p \) in the surrounding fluid. Eq. (1.5) can then be further generalised by de-dimensionalling it,

\[
Re \left( \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} = -\nabla \hat{p} + \nabla^2 \mathbf{u},
\]

(2.3)

where \( \hat{\cdot} \) is used to denote dimensionless quantities, and \( \mathbf{u} = U\hat{\mathbf{u}}, \nabla = \frac{1}{L} \nabla, \frac{\partial}{\partial t} = \frac{U}{L} \frac{\partial}{\partial \hat{t}}, \) and \( p = \frac{1}{U^2} \hat{p}. \) Here the dimensionless factor, \( Re, \) called the Reynolds number, also introduced in Chapter 1 in Eq. (1.6), is given by

\[
Re = \frac{\rho U L}{\mu} = \frac{F_{\text{inertial}}}{F_{\text{viscous}}},
\]

(2.4)

where \( L \) and \( U \) are the length and speed of the body in the fluid respectively. The Reynolds number can be interpreted as the ratio between the inertial and viscous forces; for \( Re \to \infty, \) viscous forces are negligible, and the system is dominated by the inertial forces; for \( Re \ll 1, \) instead, viscous forces dominate and the term on the left-hand side of Eq. (2.3) can be neglected, giving the Stokes equation:

\[
-\nabla \hat{p} + \nabla^2 \mathbf{u} = 0.
\]

(2.5)

The incompressible Stokes equations, Eqs. (1.3) and (2.5), are linear and independent of time.

### 2.2 Dynamics of a Suspended Particle

Considering the second viewpoint in tackling hydrodynamic problems mentioned above, and turning to a boundary description, the net hydrodynamic force and torque on the body is linearly related to its velocity and angular velocity by

\[
\mathbf{F} = -K_{\mathbf{xU}} \mathbf{U}.
\]

(2.6)
where $F$ is a six-component vector containing the hydrodynamic forces and torques and $\tilde{U}$ is a six-component vector containing the velocity and angular velocity of the body. The $6 \times 6$ resistance matrix $K_{FU}$, in Eq. (2.6), is proportional to the viscosity and only depends on the size and shape of the body. For most problems, the geometry of the body makes this matrix not possible to calculate analytically and the solution is, therefore, typically obtained numerically through the use of flow singularities. Singularities are obtained by determining the Green’s function for Stokes equation’s \cite{72}, which is given by

$$8\pi \mu U^s(R; f) = \frac{1}{|R|} + \hat{R}\hat{R} \cdot f,$$

where $R$ is the vector to the singularity, $\hat{R}$ is the unit vector in the direction of $R$, and $\mathbb{1}$ is the identity tensor. This fundamental solution is called the Stokeslet \cite{75} and represents the flow created by a point force in the fluid of strength $f$.

Most colloidal particles and biological organisms cannot be accurately described by a point. Because of the finite size and irregular shape of most particles, there are only relatively few problems in which it is possible to find closed-form analytic expressions for the equations of motion in the Stokes regime for flow around a single isolated solid body. Stokes \cite{76} has calculated the flow around a solid sphere undergoing uniform translation through a viscous fluid, Oberbeck \cite{77} considered an analogous problem for a spheroid, Payne and Pell \cite{78} found general solutions for the case of axisymmetric flow relative to lens-shaped bodies, and Brenner \cite{29} calculated the flow around a slightly deformed sphere, the velocity field being obtained as an expansion in terms of the deformation. However, many particles encountered in nature possess an irregular shape, and it is, therefore, of interest to investigate the flow around a class of bodies of irregular shape for which one may solve the Stokes equations.

### 2.3 Slender-Body Theory

The objective of Slender-Body Theory is to make use of the slenderness in order to obtain simplifications when finding approximate solutions for the flow around such particles. The development of low Reynolds number SBT evolved through the work of Burgers \cite{50} and Tuck \cite{51}; late works \cite{52,56} concentrated on construction of slender-body solutions by distributions of
fundamental singularities along an axis of the body. Note that, with the exception of Batchelor’s work for arbitrary cross-section, researchers have concentrated on bodies of circular cross-section.

SBT aims to capture the hydrodynamics of a long thin body by placing Stokeslets and source dipoles along its centreline. The SBT equations derived by Johnson for a slender filament of length 2l, and thickness 2rb, give the velocity $U(s)$ at a specific arc length $s$ along the filament as an integral

$$
8\pi \mu U(s) = \int_{-l}^{l} \left[ \frac{1}{|R_0|} \cdot f(s') - \frac{1 + \hat{t} \hat{t}}{|s' - s|} \cdot f(s) \right] ds' 
+ \ln \left( \frac{4l^2(1 - s^2)}{r^2 b^2 g(s) e} \right) (1 + \hat{t} \hat{t}) \cdot f(s) + 2(1 - \hat{t} \hat{t}) \cdot f(s).
$$

With $-l \leq s \leq l$ parametrising the centreline of length 2l, $U(s)$ being the velocity field at $s$, $g(s)$ is the dimensionless radial surface distribution, $2rbg(s)$ is the diameter of the body at $s$, and $R_0 = r(s) - r(s')$ the vector pointing from $s'$ to $s$, and $\hat{t}$ being the unit tangent to the centreline at $s$. Note that, in the first term of the above equation, there is a cancellation of singular functions as $s' \to s$, therefore avoiding a singularity. What Eq. (2.8) shows is that the velocity field at $s$ produced by the distribution of singularities, has to be equal to the velocity of the surface with respect to the fluid at that point, so that the flow vanishes.

Johnson’s SBT has been very successful in capturing the hydrodynamics of slender filaments in a variety of scenarios. Combined with experimental measurement, slender-body theory has helped to improve the understanding of the motion of swimming microorganisms. This improved understanding has then led to the creation and study of artificial microswimmers.

### 2.4 Resistive Force Theory

#### 2.4.1 Drag Forces and Torques on an Object in the Body Frame

To describe the kinematics, two Cartesian coordinate systems are introduced: the lab frame $\{X,Y,Z\}$ and the body frame $\{1,2,3\}$.

The body frame is related to the lab frame via the Euler angles $(\theta, \phi, \psi)$: first,
Figure 2.1 Definitions of coordinate systems \{X,Y,Z\} and \{1,2,3\} and of Euler angles used.

\{X,Y,Z\} is rotated by \(\phi\) around its \(Z\) axis; second, there is a rotation by an angle \(\theta\) around the new \(y\)-axis; and finally, there is a rotation about the new \(z\)-axis by an angle \(\psi\).

These rotations, when combined, give the transformation matrix \(D(\phi, \theta, \psi)\):

\[
D(\phi, \theta, \psi) = \\
\begin{pmatrix}
\cos \phi \cos \theta \cos \psi - \sin \phi \sin \psi & \sin \phi \cos \theta \cos \psi + \cos \phi \sin \psi & -\sin \theta \cos \psi \\
-\cos \phi \cos \theta \sin \psi - \sin \phi \cos \psi & -\sin \phi \cos \theta \sin \psi + \cos \phi \cos \psi & \sin \theta \sin \psi \\
\cos \phi \sin \theta & \sin \phi \sin \theta & \cos \theta
\end{pmatrix}
\]

(2.9)

So that a vector \(a\) can be related in the body and lab frames by:

\[
(a_1, a_2, a_3)^T = D(\phi, \theta, \psi)(a_X, a_Y, a_Z)^T,
\]

(2.10)
where $T$ denotes the transpose of a matrix. The angular velocities in both frames can then be related through the Euler angles by,

\[ \Omega_x' = -\dot{\theta} \sin \phi + \dot{\psi} \cos \phi \sin \theta, \]  
\[ \Omega_y' = \dot{\theta} \cos \phi + \dot{\psi} \sin \phi \sin \theta, \]  
\[ \Omega_z' = \dot{\phi} + \dot{\psi} \cos \theta, \]

and

\[ \Omega_1 = \dot{\theta} \sin \psi - \dot{\phi} \cos \psi \sin \theta, \]  
\[ \Omega_2 = \dot{\theta} \cos \psi + \dot{\phi} \sin \psi \sin \theta, \]  
\[ \Omega_3 = \dot{\phi} \cos \theta + \dot{\psi}, \]

where the dot denotes the time derivative.

Considering an object made up of many small rods joined together and employing resistive-force theory, the drag force acting on a small element $ds$ can be expressed as,

\[ dF = -\left[ K_\parallel (V \cdot t) t + K_\perp \{ V - (V \cdot t) t \} \right] ds, \]

where $K_\parallel$ and $K_\perp$ are the parallel and perpendicular friction coefficients respectively, $V$ is the velocity of the object element with respect to its surrounding fluid and $t$ is the unit vector in the direction of the element at the given point, as shown in Figure 2.2. The total drag force acting on the body is then given by

\[ F = \int dF. \]  
\[ (2.18) \]

And similarly, the total torque acting on the body by the drag forces is:

\[ T = \int r \times dF. \]  
\[ (2.19) \]

where $r$ is the position vector of any point on the given object.

It is assumed that the centre of the body frame moves with velocity $U$ and rotates with angular velocity $\Omega$ so that the velocity of the body can be expressed as $V = U + \Omega \times r$. Final expressions for the three components of the total drag force and torque can then be found by substituting the expression for the velocity into Eqs. (2.18) and (2.19) and performing the integration over the elements of the body.
2.4.2 Solving for the Dynamics

In the Stokes limit, the motion of the body is determined by the condition that the total forces and torques acting on it are equal to zero,

\[ F_{\text{drag}}(\mathbf{U}, \Omega) + F_{\text{ext}}(\theta, \phi, \psi) = 0, \]
\[ T_{\text{drag}}(\mathbf{U}, \Omega) + T_{\text{ext}}(\theta, \phi, \psi) = 0, \]

(2.20) \hspace{1cm} (2.21)

Transforming the force and torque balance to the body frame, the solution methodology used in solid body mechanics [90] can be adopted. First, the equations of motion are solved in order to find the velocity and angular velocity components in the body frame, and these are then used to solve for the dynamics of the Euler angles. The time-dependent Euler angles are then used to relate the body-frame kinematics to the lab-frame trajectories.

2.4.3 Resistance Matrix

\begin{figure}[h]
\centering
\includegraphics[scale=0.5]{figure2.2.png}
\caption{Diagram showing the tangent vector \( \mathbf{t} \) for a small filament \( ds \).}
\end{figure}

In addition to directly solving for the dynamics of the Euler angles, it is also possible to derive analytical expression for the resistive matrix of a slender body as put forward by Di Leonardo et al. in [91]. Using Resistive Force Theory [5], an element of the body will act on the fluid with a force given by:

\[ dF = K \cdot V \, ds \]

(2.22)

where \( ds \) is the length of the element and \( \mathbf{V} \) is its velocity. The newly introduced matrix \( K \) is the anisotropic resistance tensor per unit length of an element,

\[ K = K_{\perp} \mathbf{1} + (K_{\parallel} - K_{\perp}) \hat{\mathbf{t}} \hat{\mathbf{t}}, \]

(2.23)
with \( \hat{t} \) the local tangent vector, as shown in Figure 2.2 and \( K_\parallel \) and \( K_\perp \) the parallel and perpendicular drag coefficients per unit length, respectively. The net force \( \mathbf{F} \) and torque \( \mathbf{T} \) applied on the fluid by a rigid slender body moving a velocity \( \mathbf{U} \) and angular velocity \( \Omega \) can then be related by three resistance tensors \( \Gamma, R \) and \( C \) by,

\[
\mathbf{F} = \Gamma \cdot \mathbf{U} + C \cdot \Omega, \tag{2.24}
\]
\[
\mathbf{T} = C^T \cdot \mathbf{U} + R \cdot \Omega, \tag{2.25}
\]

and each element of the rigid body has a velocity

\[
\mathbf{V} = \mathbf{U} + \Omega \times \mathbf{r} \tag{2.26}
\]

and the net force and torque applied on the fluid are given by:

\[
\mathbf{F} = \int K \cdot \mathbf{V} \, ds, \tag{2.27}
\]
\[
\mathbf{T} = \int \mathbf{r} \times K \cdot \mathbf{V} \, ds. \tag{2.28}
\]

Substituting Eqs. (2.23) and (2.26) in Eqs. (2.27) and (2.28), the following expressions for the three resistance tensors can be obtained:

\[
\Gamma = \int K \, ds, \tag{2.29}
\]
\[
R = -\int \mathbf{r} \times K \times \mathbf{r} \, ds, \tag{2.30}
\]
\[
C = -\int K \times \mathbf{r} \, ds. \tag{2.31}
\]

## 2.5 Slender Ribbon Theory

As an extension to Slender Body Theory, Koens and Lauga [62] investigated the flow around a long slender body with a width that is much larger than its thickness, which they called a ribbon. The added property of having sides, unlike the filaments, gives ribbons more features and can create new configurations making them relevant to many fields of research [87, 92, 100]; for example when a ribbon has half a twist and is bent into a circle it produces a Möbius strip. There have been studies to determine the structural shapes of ribbons, both theoretically [101, 102] and experimentally [103], but less is known about
Figure 2.3 Sketch of a slender ribbon of length $2l$, width $2b$, and thickness $2a$: $\hat{t}$ is the tangent vector to the ribbon’s centreline, $\hat{T}$ is a unit vector pointing in the direction of the ribbon’s width, $\rho(s_1)$ is the cross-sectional shape of the ribbon width, and $s_1$ and $s_2$ are the arc lengths along the ribbon’s centreline and width, respectively. Figure taken from [4].

their behaviour in viscous fluids. For this reason, Koens and Lauga [62] have recently determined, asymptotically, the leading-order hydrodynamic behaviour of a slender ribbon in Stokes flows using what they called Slender-Ribbon Theory (SRT).

Similarly to SBT, the derivation assumes that the length of the ribbon is much larger than its width, which itself is much larger than its thickness. The final result is an integral equation for the force density on a ruled surface, called a ribbon plane, located inside the ribbon. Their asymptotic results provide a useful framework that can be used to predict the behaviour of slender ribbons at low Reynolds numbers in a variety of biological and engineering problems.

Consider a slender ribbon defined by its centreline, $r(s_1)$, and a unit vector $\hat{T}(s_1)$ which is perpendicular to the centreline’s tangent vector, $\hat{t}(s_1)$, and points in the direction of the ribbon’s width (see sketch in Figure 2.3). The centreline length of the ribbon, $2l$, is then assumed to be much larger than the width, $2b$, which in turn is much larger than the thickness $2a$ (i.e. $l \gg b \gg a$). This assumption enforces the slenderness of the ribbon.

Stokeslet singularities (point forces) are subsequently placed over the ribbon plane to determine the hydrodynamics of the ribbon, and the resulting velocity on the ribbon surface is expanded in orders of $b_l \equiv b/l \ll 1$ and $a_l \equiv a/l \ll 1$ [62]. This derivation, by Koens and Lauga, then generates an integral equation, valid to
\[ O(b_l), \text{ with the form} \]

\[
8\pi U(s_1, s_2) = \int_{-1}^{1} ds_1' \left[ \frac{1 + \hat{R}_0 \hat{R}_0}{|\hat{R}_0|} \cdot \langle f(s_1') \rangle - \frac{1 + \hat{t} \hat{t}}{|s_1' - s_1|} \cdot \langle f(s_1) \rangle \right] \\
+ \int_{-1}^{1} ds_2' \left\{ \ln \left( \frac{4(1 - s_1^2)}{b_l^2 \rho(s_1)^2(s_2 - s_2')^2} \right) (1 + \hat{t} \hat{t}) \cdot f(s_1, s_2') \right\} + 2(\hat{T} \hat{T} - \hat{t} \hat{t}) \cdot \langle f \rangle(s_1), \tag{2.32}
\]

where \( U(s_1, s_2) \) is the velocity on the surface of the ribbon at arc lengths \((s_1, s_2)\), \( \rho(s_1) \) is the cross-sectional shape of the ribbon width, \( f(s_1, s_2) \) is the force distribution over the Stokeslet plane, \( s_1 \) is the arc length along the centreline, \( s_2 \) is the arc length along the ribbon’s width, \( R_0 = r(s_1) - r(s_1') \), and \( \langle \cdot \rangle \equiv \int_{-1}^{1} ds_2 \) denotes the total across the width of the ribbon. Eq. (2.32) is dimensionless; lengths have been scaled by \( l \), velocities by a typical ribbon velocity \( U \), forces by \( \mu l U \), and torques by \( \mu l^2 U \). Furthermore, in order to obtain this equation, \( \rho(s_1) \) is assumed to be locally ellipsoidal near the ends of the ribbon.

The total force and torque on the fluid from the ribbon are given by

\[
F_h = \int_{-1}^{1} ds_1 \int_{-1}^{1} ds_2 f(s_1, s_2), \tag{2.33}
\]

\[
T_h = \int_{-1}^{1} ds_1 \int_{-1}^{1} ds_2 Y(s_1, s_2) \times f(s_1, s_2), \tag{2.34}
\]

where \( Y(s_1, s_2) = r(s_1) + b_l s_2 \rho(s_1) \hat{T}(s_1) \) is the scaled ribbon plane. This integral equation, Eq. (2.32) from [62], was significantly simplified by the Koens and Lauga in a later work [4]. In their later work [4], Koens and Lauga reduce the equations for an arbitrary isolated slender ribbon to

\[
8\pi U(s_1, s_2) = \pi \int_{-1}^{1} dq \left[ \frac{(1 + \hat{R}_0 \hat{R}_0) \cdot f_1(s_1 + q)}{|\hat{R}_0|} - \frac{(1 + \hat{t} \hat{t}) \cdot f_1(s_1)}{\langle q \rangle} \right] \\
+ \pi [L_{SRT}(1 + \hat{t} \hat{t}) - 2\hat{t} \hat{t} + 2\hat{T} \hat{T}] \cdot f_1(s_1) \\
+ 2\pi(1 + \hat{t} \hat{t}) \cdot [\ln(2)f_1(s_1) + s_2 f_2(s_1)], \tag{2.35}
\]

for looped bodies (where the two ends are attached to each other). In this equation, \( L_{SRT} = \ln(4/b_l^2) \).
2.6 Grand Mobility Matrix

Using results for the flow field generated by a point force in the Stokes limit, by Oseen [72] and Burgers [50], Riseman and Kirkwood [104] derived expressions for the translational and rotational tensors for a rigid group of particles. This framework was then expanded on [105, 106] by including the hydrodynamics interactions between two spheres. Rotne and Prager [73] and Yamakawa [74], when looking at the hydrodynamic interactions between two spheres, derived a \((6 \times 6)\) mobility matrix relating the translational and rotational velocities of a body to the total force and torque acting on that body, whilst considering the hydrodynamic interaction between the parts of the body and solving for the constraints that make the body rigid.

Following this approach, an \(11 \times 11\) grand mobility matrix (GMM), which relates the force \(F\), torque \(T\), and stress \(S\), acting on the centre of mass of the body, to the velocity \(V\), angular velocity \(\Omega\), and strain rate \(E\) respectively can be computed and used to efficiently simulate the dynamics of the body. For the case of a rigid body, the mobility matrix in the body frame remains constant, thus needing to be evaluated only once. Quaternions are used to describe the orientation of the body, relative to its hydrodynamic centre. This is due to the fact that the use of four quaternion coordinates removes the degeneracy encountered with three rotational coordinates (i.e. Euler angles). The derivation of the GMM proposed by Palanisamy and Den Otter [1] is now outlined.

In the mobility representation, for an object made up of \(N\) unconnected spherical particles, the translational velocity \(V_i\) and rotational velocity \(\Omega_i\) of the \(i^{th}\) particle, with position \(x_i\), are related to the potential-based forces \(F_j\) and torques \(T_j\) on all particles \(j\), via the mobility tensor,

\[
\begin{pmatrix}
V_i \\
\Omega_i \\
E^\infty
\end{pmatrix} = \sum_{j=1}^{N} \begin{pmatrix}
\mu_{V,i} & \mu_{V,j} & \mu_{V,j} \\
\mu_{\Omega,i} & \mu_{\Omega,j} & \mu_{\Omega,j} \\
\mu_{E,i} & \mu_{E,j} & \mu_{E,j}
\end{pmatrix} \begin{pmatrix}
F_j \\
T_j \\
S_j
\end{pmatrix},
\]

where the strain rate \(E^\infty\) is uniform throughout the system. The approximate analytical expressions for the mobility matrix of two interacting spherical particles are summarised in Appendix A [1, 11].

The objective is to derive, starting from Eq. (2.36), a mobility matrix relating the translation and rotation of a rigid cluster of \(N\) spherical particles to the total
potential force and torque. Note that the stress and strain rate, \( S \) and \( E^\infty \), are rank-2 tensors and consequently the \( \mu^E \) and \( \mu_S \) elements of the matrix in Eq. (2.36) are tensors of the rank-3 or 4. The combination of various ranks in the grand mobility tensor disallows the use of standard routines for square matrices. The stress and strain rate, \( S \) and \( E \), are therefore converted from tensors to five-vectors, \( \mathcal{S} \) and \( \mathcal{E} \) using the method outlined in Appendix B. Having performed these conversions, Eq. (2.36) can be rewritten as

\[
\begin{pmatrix}
V_i \\
\Omega_i \\
-\mathcal{E}^\infty
\end{pmatrix} = \sum_{j=1}^{N} \begin{pmatrix}
\mu_{V,i} & \mu_{V,i} & \mu_{V,i} \\
\mu_{T,j} & \mu_{T,j} & \mu_{T,j} \\
\mu_{S,j} & \mu_{S,j} & \mu_{S,j}
\end{pmatrix} \begin{pmatrix}
F_j \\
T_j \\
S_j
\end{pmatrix}.
\] (2.37)

Note that the matrix in the above equation is now an \( 11N \times 11N \) matrix. Given the forces, torques, and stresses on the individual particles in a rigid cluster, the total force, torque, and stress on the cluster are given by,

\[
F = \sum_{i=1}^{N} F_i,
\] (2.38)

\[
T = \sum_{i=1}^{N} (T_i + \mathbf{r}_i \times F_i),
\] (2.39)

\[
S = \sum_{i=1}^{N} (S_i + \mathbf{r}_i \otimes F_i).
\] (2.40)

Applying these addition rules to the \( 11N \times 11N \) resistance matrix, found by inverting the \( 11N \times 11N \) mobility matrix, yields the \( 11 \times 11 \) grand resistance matrix of the cluster,

\[
\begin{pmatrix}
F \\
T \\
S
\end{pmatrix} = \begin{pmatrix}
\xi^F_V & \xi^F_{\Omega} & \xi^F_{\mathcal{E}} \\
\xi^T_V & \xi^T_{\Omega} & \xi^T_{\mathcal{E}} \\
\xi^S_V & \xi^S_{\Omega} & \xi^S_{\mathcal{E}}
\end{pmatrix} \begin{pmatrix}
V \\
\Omega \\
-\mathcal{E}^\infty
\end{pmatrix}.
\] (2.41)

Explicit expressions for the nine sub-matrices are provided in Appendix C. The velocities, for given generalised forces and a given background flow field, are then to be evaluated in order to simulate the dynamics of the cluster. This is done by partial inversion of Eq. (2.41) to arrive at the Grand Mobility Matrix of the
cluster,  
\[
\begin{pmatrix}
V \\
\Omega \\
\mathbf{S}
\end{pmatrix} = 
\begin{pmatrix}
\mu_V & \mu_V & \mu_V \\
\mu_V & \mu_V & \mu_V \\
\mu_V & \mu_V & \mu_V
\end{pmatrix} 
\begin{pmatrix}
F \\
T \\
-\mathbf{E}^\infty
\end{pmatrix},
\tag{2.42}
\]

where \(\mu_i^j\) are the sub-matrices containing the mobility coefficients. For the case of a rigid object, the mobility matrix in the body frame remains constant, thus needing to be evaluated only once. The algorithm, to compute the GMM for a rigid object made up of an arrangement of spheres, put forward by Palanisamy and Den Otter [1] was implemented independently in the \texttt{C++} programming language by Joost de Graaf; tensor operations were handled using the \texttt{Armadillo} library [107], which makes use of \texttt{LAPACK} [108] to improve computational efficiency. Here the composite objects were constructed with a sphere separation of 2.001\(a\), where \(a\) is the bead radius and is set to \(a = 1\) throughout the project.

For the specific problem of sedimentation, which is considered in this thesis, only the 6 \(\times\) 6 sub-block relating the force and torque to the velocity and angular velocity is required. Therefore, from now the thesis will consider only the 6 \(\times\) 6 block of the GMM.

### 2.6.1 The Dynamics

As previously mentioned, to solve for the dynamics using the GMM, and to remove the degeneracy given by three rotational coordinates, quaternions are used and introduced in the following.

A rotation matrix in 3-dimensional space can be expressed in terms of the unit quaternion four-vector, \(\mathbf{q} = (q_0, q_1, q_2, q_3)\), with \(|\mathbf{q}| = 1\), where the conversion from the body frame \((\cdot)_{(b)}\) to the lab frame \((\cdot)_{(l)}\) used is given by,

\[
A_{(b)}^{(l)} = 
\begin{pmatrix}
q_0^2 + q_1^2 - q_2^2 - q_3^2 & 2q_1q_2 - 2q_0q_3 & 2q_1q_3 - 2q_0q_2 \\
2q_1q_2 + 2q_0q_3 & q_0^2 - q_1^2 + q_2^2 - q_3^2 & 2q_2q_3 - 2q_0q_1 \\
2q_1q_3 - 2q_0q_2 & 2q_2q_3 + 2q_0q_1 & q_0^2 - q_1^2 - q_2^2 + q_3^2
\end{pmatrix},
\tag{2.43}
\]

In the simulation algorithm the conversion of angular velocities in the lab frame
to quaternion velocities is realised by

\[ B^{\dot{q}}_{(l)} = \frac{\partial \dot{q}}{\partial \omega^{(l)}} = \frac{1}{2q^4} \begin{pmatrix}
-q_1 & -q_2 & -q_3 \\
q_0 & q_3 & -q_2 \\
-q_3 & q_0 & q_1 \\
q_2 & -q_1 & q_0
\end{pmatrix} \]  \hspace{1cm} (2.44)

and the conversion of angular velocities in the body frame to quaternion velocities is realised by

\[ B^{\dot{q}}_{(b)} = \frac{\partial \dot{q}}{\partial \omega^{(b)}} = \frac{1}{2q^4} \begin{pmatrix}
-q_1 & -q_2 & -q_3 \\
q_0 & q_3 & q_2 \\
q_3 & q_0 & -q_1 \\
-q_2 & q_1 & q_0
\end{pmatrix} \]  \hspace{1cm} (2.45)

The latter two matrices can then be related by \( B^{\dot{q}}_{(b)} = B^{\dot{q}}_{(l)} A^{(l)}_{(b)} \).

For a \((6 \times 6)\) mobility matrix, the equations of motion for translation and rotation are

\[ \begin{pmatrix} \Delta x \\ \Delta q \end{pmatrix} = \begin{pmatrix} A^{(l)}_{(b)} & 0 \\ 0 & B^{\dot{q}}_{(b)} \end{pmatrix} \begin{pmatrix} \mu^V_F & \mu^V_T \\ \mu^\Omega_F & \mu^\Omega_T \end{pmatrix}^{(b)} \begin{pmatrix} A^{(b)}_{(l)} F^{(l)} \\ A^{(b)}_{(l)} T^{(l)} \end{pmatrix} \Delta t + \begin{pmatrix} 0 \\ \lambda q \end{pmatrix} \]  \hspace{1cm} (2.46)

In the first term, the forces and torques in the space frame are converted to the body frame by a single rotation, and the generalized velocities are solved from a force balance in the body frame, converted back to the lab frame and multiplied by the time step, \( \Delta t \), to obtain a displacement. The final term then represents the constraint to keep the quaternion of unit length. The laboratory-based grand mobility matrix will vary with the orientation of the object, but the body-based matrix remains constant. Hence the GMM has to be evaluated only once in order to simulate the dynamics of the cluster.

At every \( n^{th} \) time-step a new set of \( x = (x, y, z) \) coordinates and an updated quaternion four vector, \( q = (q_0, q_1, q_2, q_3) \), is printed onto the output file, where \( x \) is located at the centre of the helix.
2.6.2 Simple Benchmarks: Composite Spheres and Rods

The implementation of the GMM algorithm was benchmarked against two well-known systems, spheres and rods, for which analytic results are available. Starting with the results for spheres, various composite spheres were created to check the accuracy and behaviour of the numerically obtained GMM. The radius, $R$, scales with the square root of the number of unit spheres which make up the composite sphere; this computationally limits the composite sphere to have a maximum size of $R = 30.7$ (corresponding to 2401 unit spheres). It was verified that the composite spheres were approximately symmetrical: the diagonal elements $\mu_i^i$ were nearly identical for the rotational and translational sub-blocks, respectively, see Figure 2.4(a), which shows the relevant mobility ratios. As the sphere surface was refined (larger $R$), the agreement between the diagonal elements improved, see Figure 2.4(a), as expected. Additionally, Figure 2.4(b) shows that, in the limit of a composite sphere with a smooth surface, the composite sphere has the expected mobility prefactors for a solid sphere.

![Figure 2.4](image)

**Figure 2.4** Quality of the RPY approximation in capturing the behaviour of a solid sphere. (a) The ratio of mobility coefficients (symbols) as a function of the inverse sphere radius $1/R$. The value of these ratios approaches 1, as expected, and therefore only the departure away from this value (black dashed line) for the translational $\mu_i^i/\mu_1^1$ ($i = 2, 3$) and rotational $\mu_i^i/\mu_4^4$ ($i = 5, 6$) component are shown. (b) The approach to the prefactors for the translational $\mu_t$ and rotational $\mu_r$ mobility of a solid sphere with radius $a = 1$. The ratios $\mu_t^1/(\mu_t R)$ (blue symbols) and $\mu_r^4/(\mu_r R^3)$ (orange symbols) approach unity (dashed black line) from below as expected. This is further visualized using the interpolated trends (solid curves).

Next, a rod of length $L$ with an initial orientation given by the angle, $\theta$, which is measured with respect to the vertical, see Figure 2.5, was considered. The rod sediments due to the gravitational force acting along the $z$-axis in the negative direction. The well-known result by Taylor [52] states that the rod’s orientation
does not change during the sedimentation \( \theta(t) = \theta(t = 0) = \theta_0 \) for all times \( t \). In addition, the rod does not sediment vertically, instead, its velocity vector makes an angle \( \alpha \) with the \( z \)-direction that depends on \( \theta_0 \) and is given by

\[
\cos \alpha = \frac{\sin^2 \theta_0 + \gamma \cos^2 \theta_0}{\sqrt{\sin^2 \theta_0 + \gamma^2 \cos^2 \theta_0}},
\]  

(2.47)

where \( \gamma = \frac{K_\perp}{K_\parallel} \) is the ratio between the rod’s perpendicular and parallel friction coefficient, which are given by

\[
K_\parallel = \frac{2 \pi L \eta}{\ln \frac{L}{a} - \frac{1}{2}},
\]  

(2.48)

\[
K_\perp = \frac{4 \pi L \eta}{\ln \frac{L}{a} + \frac{1}{2}},
\]  

(2.49)

respectively [57]. Here, \( L \) is the length of the rod, and \( a \) its radius. Note that the value of \( \alpha \) is also constant in time.

The grand mobility matrix, \( \mu \), was then computed for a rod, approximated by a line of \( 2N + 1 \) spheres of radius \( a = 1 \), with a separation of 2.01, and the associated translational mobility ratio \( \gamma = \mu_3^3/\mu_1^1 \), where \( \mu_a^b \) represents the element in the \( a \)th row and \( b \)th column of the mobility tensor \( \mu \) was determined. Sedimentation trajectories using these GMMs for several values of \( \theta_0 = \left[ \frac{\pi}{20}, \frac{\pi}{10}, \frac{3\pi}{20}, \frac{\pi}{4}, \frac{3\pi}{10}, \frac{\pi}{2}, \frac{\pi}{5}, \frac{3\pi}{20}, \frac{2\pi}{5}, \frac{9\pi}{20}, \frac{\pi}{2} \right] \) were obtained and the corresponding value of \( \alpha \) was computed using

\[
\alpha = \arctan \frac{x(t_2) - x(t_1)}{z(t_2) - z(t_1)},
\]  

(2.50)

where \( x(t) \) and \( z(t) \) are the \( x \) and \( z \) positions of the rod’s centre of mass at time \( t \). Note that the linearity of the sedimentation trajectory is used here for some appropriate choices of \( t_1 \) and \( t_2 \). It is found that the trajectory is a straight line from time \( t = 0 \) onward, as expected.

Figure 2.5(a) shows the dependence of \( \alpha \) on \( \theta_0 \) for a rod of length \( L = 400 \). The blue symbols indicate the numerical RPY result, the black dashed line shows the prediction of Eq. (2.47) using the mobility coefficients \( K_\parallel \) and \( K_\perp \) obtained using Eqs. (2.48) and (2.49), respectively. The solid orange line shows the prediction of Eq. (2.47) using a value of \( \gamma = \frac{K_\perp}{K_\parallel} \) obtained using the relevant coefficients of the RPY-based GMM. Overall, the agreement is excellent. Lastly, the effect of the finite size of the rod was explored in the result in Figure 2.5(b), which shows the
Figure 2.5  (a) The trajectory’s angle with respect to the vertical $\alpha$ as a function of the rod’s initial angle with respect to the vertical $\theta_0$, for a rod of length $L = 400$ (200 beads). The blue symbols indicate the numerical RPY result, the black dashed line shows the prediction of Eq. (2.47) using Eqs. (2.48) and (2.49), respectively. The solid orange line shows the RPY-fitted prediction of Eq. (2.47), see main text. Inset shows diagram of rod and defines parameters.  (b) Plot of $\alpha$ as a function of $\theta$ for different rod lengths as indicated in the legend. The inset shows the approach to a limit value of $\alpha$, as $L \to \infty$, as a function of $1/L$ for $\theta_0 = 3\pi/10$.

$\alpha$ as a function of $\theta_0$ for several values of $L = 80, 160, 240, 320, 400, 480$, and $600$. Note that these numerical results converge on the prediction of Eqs. (2.47), (2.48), and (2.49) for an infinite rod, indicating that the slender-body result holds well in the limit.

2.7 Concluding Remarks

The main focus of this thesis is to study the motion of anisotropic particles which perform a chiral trajectory when sedimenting. Krapf and Witten [2, 10] found that, while all chiral particles sediment with a chiral trajectory, chiral trajectories can also be performed by non-chiral particles with an asymmetry which is reflected in the particle’s mobility matrix. Consequently, the following chapters will examine the sedimentation dynamics of chiral particles (helix and Möbius strip) and non-chiral particles (C-shape and L-shape).

In this chapter, four methods by which it is possible to study this hydrodynamic problem were introduced. Additionally, the accuracy of the RPY-based calculation of the Grand Mobility Matrix and its dynamics was confirmed by testing the simulation against the well-known results for a sphere and a sedimenting rod. While there are other hydrodynamic methods available, such as explicitly solving
the flow around the body using numerical simulations (i.e. lattice Boltzmann simulations) used, for example, by Barbera Droste (whose masters’ thesis was mentioned in the introduction), these can be more computationally demanding and become difficult at low Reynolds numbers [109, 110]. For this project, the interest is in bulk fluids. Most simulation methods, however, have periodic boundary conditions and, for this case, the poor scaling of the hydrodynamic finite-size effects means that approaching bulk using LBM, MPCD, etc. is not useful. The specific interest here is in particles that can be drawn as slender filaments or as looped ribbons, hence SBT, RFT and SRT are chosen as efficient theories to describe these dynamics. Furthermore, all these particles can be drawn as a collection of unit spheres and their GMM can be calculated by considering hydrodynamic interactions between each of the spheres.

The following chapter will study the sedimentation of a rigid helix using Resistive-Force Theory.
Chapter 3

Sedimentation of a Rigid Helix

In this chapter, the microhydrodynamics of helices sedimenting due to gravity are considered. At this length scale, the dynamics enter the low Reynolds number regime, where viscous forces prevail over the inertial forces and therefore the latter become negligible. This regime of helix motion is of wide interest, due to their prevalence in micro-organisms (e.g. *E. coli* have helical flagella) and consequently, helical shapes have been studied in the areas of self-propulsion (in order to study the swimming of microorganisms) [7, 111–113], construction of artificial bacteria and micro-robots [97, 114–116] and micro-flow sensors and the deformation of flexible helices in the micro-scale [117, 118]. Solving the equations of motion in the Stokes regime, for irregular shaped particles, is computationally and analytically difficult. Various theories have been developed to approximate the forces acting on a body (see Chapter 2) in this regime, but the focus of this Chapter will be on RFT [57]. As previously mentioned, this approach has the advantage of being computationally efficient, but produces semi-quantitative approximations at best. RFT is employed in order to establish the sedimentation dynamics of a helix subjected to gravity and the drag forces and torques are computed. It is found that, for most initial orientations, the helix sediments performing a *superhelical* trajectory with a chirality that depends on the chirality of the helix itself; for near-horizontal initial orientations, however, a regime of unstable sedimentation is found. These results will be numerically verified in Chapter 4 where, unlike RFT, hydrodynamics couplings are taken into account. The results shown in this Chapter were published in [3].
3.1 Forces and Torques on Helix in Body Frame

The body-frame forces and torques acting on a helix in a viscous fluid are calculated in this Section, where the helical filament is assumed to be rigid and slender; such helical filament is a valid approximation for helical flagella [119] and robotic microhelices [114–116]. Additionally, it is assumed that the helix is sufficiently long so that Resistive-Force Theory, introduced in Section 2.4, can be used to approximate the local hydrodynamic forces acting on infinitesimal sections of the filament.

The position vector of any given point on the helix is parametrised by an angle $\alpha$ such that:

$$\mathbf{r}_h(\lambda, R, \alpha) = \left( R \cos \alpha, R \sin \alpha, \frac{\lambda}{2\pi} \alpha \right), \quad (3.1)$$

where $R$ is the radius of the helix, $\lambda$ is its pitch and the helical axis is chosen to be oriented along the 3-direction of the body frame, as seen in Figure 3.1. The angle $\alpha$ has values in the interval $\alpha \in [-\pi N + \alpha_0, \pi N - \alpha_0]$, where $\alpha_0$ represents how much the helix deviates from having an integer number of turns $N$, and can take values in the range of $\alpha_0 \in \left[ -\frac{\pi}{2}, \frac{\pi}{2} \right)$. The total length of the helix, $L$, can then be calculated from Eq. (3.1) to be $L = \lambda (N - \alpha_0/\pi)$.

It will prove convenient to introduce a new parameter $\chi$, which is the angle that the filament of the helix makes with the vertical (i.e. the 3-direction), and express the radius of the helix as $R = \frac{\lambda}{2\pi} \tan \chi$. Recall the expression for the drag force acting on a small element, $ds$, introduced in Section 2.4.1

$$d\mathbf{F} = -\left[ K_\parallel (\mathbf{V} \cdot \mathbf{t}) \mathbf{t} + K_\perp \{ \mathbf{V} - (\mathbf{V} \cdot \mathbf{t}) \mathbf{t} \} \right] ds. \quad (3.2)$$

To first approximation, the drag coefficients of a straight rod [30] can be used as the friction coefficients $K_\parallel$ and $K_\perp$. This approach, however, does not take into account the interactions between adjacent elements of the filament. To incorporate these interactions, Lighthill [5] put forward the following expressions for the friction coefficients

$$K_\parallel = \frac{4\pi \mu}{2 \log(c_L \lambda/r) - 1}, \quad (3.3)$$

$$K_\perp = \frac{8\pi \mu}{2 \log(c_L \lambda/r) + 1}, \quad (3.4)$$

where $\mu$ is the viscosity of the fluid, $r$ is the radius of the filament, and $c_L =$
Figure 3.1 Geometry of the helix: $R$ and $\lambda$ are the radius and the pitch, correspondingly, while $L$ is the total length of the helix along its symmetry axis; $\alpha_0$ is defined as the angle between the shortest distance between the end-point of the helix and its axis of symmetry, and the line obtained by rotation of the former in the 12-plane until it is parallel to the 1-direction. It serves as a measure of how much the number of helical turns, $L/\lambda$, deviates from an integer. (a) Side view. (b) Top view.

0.18 is the Lighthill constant; additionally, $\gamma = K_\perp/K_\parallel$ is introduced. In the following, $\gamma = 2$ is considered when comparing analytical and numerical results in their dimensionless form in order to avoid the additional parameter $r$, the radius of the filament. When looking at the prediction in physical units, instead, Eqs. (3.3) and (3.4) are used for the friction coefficients.

For the helical filament $\mathbf{r}_h(\alpha)$, the unit vector $\mathbf{t}$ is along the direction of the tangent $\partial \mathbf{r}_h/\partial \alpha$ so that:

$$
\mathbf{t} = (-\sin \chi \sin \alpha, \sin \chi \cos \alpha, \cos \chi), \quad \text{and} \quad ds = \frac{\lambda}{2\pi} \sec \chi \ d\alpha, \quad (3.5)
$$

where $\chi$ is the angle that the helical filament makes with the helix’s major axis. The total drag force acting on the helix is then given by

$$
\mathbf{F} = \int_{-\pi N + \alpha_0}^{\pi N - \alpha_0} d\mathbf{F}(\alpha). \quad (3.6)
$$
Similarly, the total torque acting on the helix by the drag forces is:

\[
T = \int_{\alpha_0}^{\pi - \alpha_0} \mathbf{r}_h(\alpha) \times d\mathbf{F}(\alpha).
\]  

(3.7)

Final expressions for the three components of the total drag force and torque are found, by substituting the expression for the velocity, \( \mathbf{V}(\alpha) = \mathbf{U} + \Omega \times \mathbf{r}(\alpha) \), first introduced in Section 2.4.1 into Eqs. (3.6) and (3.7). Performing the integration over \( \alpha \) then gives,

\[
F_1 = \frac{K_{||}L}{\cos \chi} \left[ - \gamma U_1 
+ \frac{\gamma - 1}{2} \left\{ (1 + \Delta_1)U_1 \sin^2 \chi - \left( \frac{1}{2} \cos 2\alpha_0 + 1 + \frac{3}{2} \Delta_1 \right) \frac{\lambda}{2\pi} \Omega_1 \sin^2 \chi \right\} \right],
\]  

(3.8)

\[
F_2 = \frac{K_{||}L}{\cos \chi} \left[ - \gamma \left( U_2 - \Delta_2 \frac{\lambda}{2\pi} \Omega_3 \tan \chi \right) + \frac{\gamma - 1}{2} \left\{ (1 - \Delta_1)U_2 \sin^2 \chi - \Delta_2 U_3 \sin 2\chi 
+ \left( \frac{1}{2} \cos 2\alpha_0 - 1 + \frac{3}{2} \Delta_1 \right) \frac{\lambda}{2\pi} \Omega_2 \sin^2 \chi - 2\Delta_2 \frac{\lambda}{2\pi} \Omega_3 \sin^2 \chi \tan \chi \right\} \right],
\]  

(3.9)

\[
F_3 = \frac{K_{||}L}{\cos \chi} \left[ - \gamma \left( U_3 + \Delta_2 \frac{\lambda}{2\pi} \Omega_2 \tan \chi \right) + (\gamma - 1) \left\{ - \Delta_2 U_2 \sin \chi \cos \chi + U_3 \cos^2 \chi 
+ \left( (-1)^N \cos \alpha_0 + 2\Delta_2 \right) \frac{\lambda}{2\pi} \Omega_2 \sin \chi \cos \chi + \frac{\lambda}{2\pi} \Omega_3 \sin^2 \chi \right\} \right],
\]  

(3.10)
where the following were introduced

\[ \Delta_1 = \frac{\lambda}{2\pi L} \sin 2\alpha_0, \]  
\[ \Delta_2 = \frac{(-1)^N \lambda}{\pi L} \sin \alpha_0. \]  

Taking the limit of \( \lambda \to \infty \) and \( \chi \to 0 \) (for a rod-like limit), Eqs. (3.8)-(3.13)
reduce to

\[ F_1 = - K L \gamma U_1, \quad (3.16) \]
\[ F_2 = - K L \gamma U_2, \quad (3.17) \]
\[ F_3 = - K L U_3, \quad (3.18) \]
\[ T_1 = - \frac{1}{12} K L^3 \gamma \Omega_1, \quad (3.19) \]
\[ T_2 = - \frac{1}{12} K L^3 \gamma \Omega_2, \quad (3.20) \]
\[ T_3 = 0. \quad (3.21) \]

When solving the equations of motion using the above equations for the drag force and torque, the expected results for the rod sedimentation, outlined in Section 2.6.2 are recovered.

### 3.2 Equation of Motion

In the low-Reynolds number regime, the equations of motion of a helix sedimenting due to gravity can be found by imposing the requirement that there is no net force or torques acting on the helix, i.e.:

\[ \mathbf{F} + \mathbf{F}_g = 0, \quad (3.22) \]
\[ \mathbf{T} = 0, \quad (3.23) \]

where \( \mathbf{F}_g \) is the force due to gravity and is given by

\[ \mathbf{F}_g = - \left( 1 - \frac{\rho_f}{\rho_h} \right) M g \hat{Z} \equiv - P \hat{Z}, \quad (3.24) \]

where \( M \) is the mass of the helix, \( \rho_f \) and \( \rho_h \) are the densities of the suspending fluid and the helix respectively and \( \hat{Z} \) is the unit vector along the Z-direction of the lab frame.

Transforming the forces and torques into the body frame, the equations of motion
for each component are:

\[
\begin{align*}
F_1 + P \cos \psi \sin \theta &= 0, \\
F_2 - P \sin \psi \sin \theta &= 0, \\
F_3 - P \cos \theta &= 0, \\
T_1 &= T_2 = T_3 = 0.
\end{align*}
\] (3.25, 3.26, 3.27, 3.28)

The above equations of motions are solved to find expressions for the components of the velocity and the angular velocity in the body frame. These expressions are then used to solve for the dynamics of the Euler angles and the velocities in the lab frame in order to then analyse the trajectories of the helix in the lab frame.

### 3.3 Approximate Solution for Long Helices

The solution strategy outlined is straightforward since the equations of motion, given by Eqs. (3.25)-(3.28), are linear in the components of the velocity and angular velocity and can, therefore, be easily solved. Due to the results having a large number of terms, the limit of long helices is considered instead. Furthermore, it will be demonstrated that the approximate solution developed is considerably accurate even when looking at relatively short helices. First of all, the equations of motion, Eqs. (3.25)-(3.28), are put in a dimensionless form by scaling all lengths with \( L \) and time with a timescale defined as

\[
\tau = \frac{K_2 \lambda^2}{P} \frac{\pi c_0^2}{6(\gamma - 1) \sin^2 \chi \cos \chi},
\] (3.29)

where \( \lambda \) is the pitch of the helix, \( P \) is the magnitude of the gravitation force, introduced in Eq. (3.24), and \( c_0 = \gamma + \gamma \cos^2 \chi + \sin^2 \chi \). Dimensionless variables are denoted by a tilde. Next, \( \epsilon = \lambda / L \) is introduced and used a small parameter. Analysis of the equations of motion shows that, to the lowest order, all dimensionless velocity components are \( \mathcal{O}(\epsilon^2) \), \( \tilde{\Omega}_1 \) and \( \tilde{\Omega}_2 \) are \( \mathcal{O}(\epsilon^3) \), while \( \tilde{\Omega}_3 \) is \( \mathcal{O}(\epsilon) \). So, up to \( \mathcal{O}(\epsilon^3) \), the angular velocities are given by
\[ \tilde{\Omega}_1 = -\epsilon^3 (2 + \cos 2\alpha_0) \cos \psi \sin \theta, \]  
(3.30)

\[ \tilde{\Omega}_2 = \epsilon^3 (2 - \cos 2\alpha_0) \sin \psi \sin \theta, \]  
(3.31)

\[ \tilde{\Omega}_3 = -\epsilon \frac{\pi^2}{3\gamma \tan^2 \chi} \cos \theta - \epsilon^2 \frac{2(-1)^N \pi c_0 \sin \alpha_0 \cos \chi}{3(\gamma - 1) \sin^3 \chi} \sin \psi \sin \theta 
- \epsilon^3 \frac{(-1)^N}{3 \tan \chi} (4 \cos \alpha_0 - \cos 3\alpha_0) \sin \psi \sin \theta. \]  
(3.32)

Using Eqs. (2.14)-(2.16) the differential equations for the Euler angles obtained are

\[ \frac{\partial \theta}{\partial \tilde{t}} = -\epsilon^3 \cos 2\alpha_0 \sin 2\psi \sin \theta, \]  
(3.33)

\[ \frac{\partial \phi}{\partial \tilde{t}} = \epsilon^3 (2 + \cos 2\alpha_0 \cos 2\psi), \]  
(3.34)

\[ \frac{\partial \psi}{\partial \tilde{t}} = -\epsilon \frac{\pi^2}{3\gamma \tan^2 \chi} \cos \theta - \epsilon^2 \frac{2(-1)^N \pi c_0 \sin \alpha_0 \cos \chi}{3(\gamma - 1) \sin^3 \chi} \sin \psi \sin \theta 
- \epsilon^3 \frac{(-1)^N}{3 \tan \chi} (4 \cos \alpha_0 - \cos 3\alpha_0) \sin \psi \sin \theta - \epsilon^3 (2 + \cos 2\alpha_0 \cos 2\psi) \cos \theta. \]  
(3.35)

Keeping the lowest-order terms and the next order corrections, the solutions of these equations are

\[ \theta (\tilde{t}) = \theta_0 - \frac{\epsilon^2}{\omega} \cos 2\alpha_0 \sin \theta_0 \sin \epsilon \omega \tilde{t} \sin (2\psi_0 - \epsilon \omega \tilde{t}), \]  
(3.36)

\[ \phi (\tilde{t}) = \phi_0 + 2\epsilon^3 \tilde{t} + \frac{\epsilon^2}{\omega} \cos 2\alpha_0 \sin \epsilon \omega \tilde{t} \cos (2\psi_0 - \epsilon \omega \tilde{t}), \]  
(3.37)

\[ \psi (\tilde{t}) = \psi_0 - \epsilon \omega \tilde{t} - \frac{\epsilon}{\omega} \frac{2(-1)^N \pi c_0 \sin \alpha_0 \cos \chi}{3(\gamma - 1) \sin^3 \chi} \sin \theta_0 \sin (\psi_0 - \epsilon \omega \tilde{t}) - \epsilon^3 (4 \cos \alpha_0 - \cos 3\alpha_0) \sin \psi \sin \theta_0, \]  
(3.38)

where \( \omega = \pi^2 c_0^2 \cos \theta_0 / (3\gamma \tan^2 \chi) \), and \( \theta_0, \phi_0 \) and \( \psi_0 \) are the initial values of the corresponding Euler angles. The above equations show that \( \phi \) and \( \psi \) grow linearly in time with small oscillations superimposed on top, while \( \theta \) oscillates around \( \theta_0 + (\epsilon^2 / \omega) \cos 2\alpha_0 \sin \theta_0 \cos 2\psi_0 \) with the amplitude \( (\epsilon^2 / 2\omega) \cos 2\alpha_0 \sin \theta_0 \).

To verify these predictions, the dimensionless equations of motion are solved numerically following the same methodology as above but keeping all the terms in Eqs. (3.25)-(3.28). The resulting equations for the Euler angles are solved numerically using Scientific Python [120] by employing the fourth-order Runge-
Kutta time-stepping method [121].

### 3.3.1 Validation of the Approximation

In Figures 3.2 and 3.3 the truncated approximations in Eqs. (3.36)-(3.38) are compared to the results obtained by numerically solving the differential equations, for the Euler angles and the velocities, obtained by rearranging Eqs. (3.25)-(3.28). In Figure 3.2 the Euler angle dynamics is shown for a relatively long helix with \( N = 4, \alpha_0 = 0, \) and \( \chi = 0.733 \) (approximately 42 degrees) with initial conditions \( \theta_0 = 1.0, \phi_0 = 0.2, \) and \( \psi_0 = 0.5; \) the solid lines are the exact dynamics, while the dashed lines correspond to Eqs. (3.36)-(3.38). For this geometry \( \epsilon = 0.25, \) and the numerical solution and the large-\( L \) approximation show very good agreement. In Figure 3.3 the Euler angle dynamics is shown for a relatively short helix with \( N = 2, \alpha_0 = -1.34 \) (approximately \(-77\) degrees), and the same \( \chi = 0.733, \) starting from \( \theta_0 = 1.0, \phi_0 = 0.0, \) and \( \psi_0 = 0.0. \) This case corresponds to \( \epsilon = 0.41, \) and exhibits deviations between the exact numerical solution and the large-\( L \) limit. However, even in this case the leading-order prediction of Eqs. (3.36)-(3.38) is relatively good: \( \theta(\hat{t}) \) is well-approximated by a constant value \( \theta_0 + (\epsilon^2/2\omega) \cos 2\alpha_0 \sin \theta_0 \cos 2\psi_0 \) (note the scale on the vertical axis of Figure 3.3(a), while the slopes of linear increase/decrease of \( \phi(\hat{t}) \) and \( \psi(\hat{t}) \) are in reasonable agreement with Eqs. (3.37) and (3.38). The main reason why the large-\( L \) approximation works relatively well even for short helices is that the leading term in Eq. (3.36) is \( O(\epsilon^3) \), which is sufficiently small even for helices with approximately two turns (\( \epsilon \sim 0.5 \)). This approximation clearly fails for shorter chiral objects that comprise parts of a single helical turn, which are not considered here.

The implications of Eqs. (3.36)-(3.38) for the spatial trajectories of the helix in the lab frame are now studied. To leading order, the dimensionless equations of motion give for the velocity components
\begin{align*}
\ddot{U}_1 &= \frac{\epsilon^2 \pi c_0}{3(\gamma - 1) \sin^2 \chi} \cos \psi \sin \theta, \\
\ddot{U}_2 &= -\frac{\epsilon^2 \pi c_0}{3(\gamma - 1) \sin^2 \chi} \sin \psi \sin \theta, \\
\ddot{U}_3 &= \frac{\epsilon^2 \pi c_0^2 (\gamma - c_0)}{6\gamma(\gamma - 1) \sin^2 \chi} \cos \theta.
\end{align*}

Using Eqs. (2.9) and (2.10), these velocity components are transformed into the shifted lab frame \{x', y', z'\}.

**Figure 3.2** Comparison between the predictions of Eqs. (3.36)-(3.38) (dashed lines) and the exact numerical solutions (solid lines) of the full equations of motion for a helix with $N = 4$, $\alpha_0 = 0$, and $\chi = 0.733$ ($\epsilon = 0.25$): a) $\theta(\tilde{t})$, b) $\phi(\tilde{t})$, and c) $\psi(\tilde{t})$. The initial conditions are $\theta_0 = 1.0$, $\phi_0 = 0.2$, and $\psi_0 = 0.5$. 

\[\tilde{U}_1 = \frac{\epsilon^2 \pi c_0}{3(\gamma - 1) \sin^2 \chi} \cos \psi \sin \theta,\]  
\[\tilde{U}_2 = -\frac{\epsilon^2 \pi c_0}{3(\gamma - 1) \sin^2 \chi} \sin \psi \sin \theta,\]  
\[\tilde{U}_3 = \frac{\epsilon^2 \pi c_0^2 (\gamma - c_0)}{6\gamma(\gamma - 1) \sin^2 \chi} \cos \theta.\]
Figure 3.3 Same as Figure 3.2 for a helix with $N = 2$, $\alpha_0 = -1.34$, and $\chi = 0.733$ ($\epsilon = 0.41$). The initial conditions are $\theta_0 = 1.0$, $\phi_0 = 0.0$, $\psi_0 = 0.0$.

\begin{align*}
\dot{U}_x &= \frac{1}{2} \left( \frac{\epsilon^2 \pi c_0}{3(\gamma - 1) \sin^2 \chi} - \frac{\epsilon^2 \pi c_0^2 (c_0 - \gamma)}{6\gamma (\gamma - 1) \sin^2 \chi} \right) \cos \phi \sin 2\theta, \\
\dot{U}_y &= \frac{1}{2} \left( \frac{\epsilon^2 \pi c_0}{3(\gamma - 1) \sin^2 \chi} - \frac{\epsilon^2 \pi c_0^2 (c_0 - \gamma)}{6\gamma (\gamma - 1) \sin^2 \chi} \right) \sin \phi \sin 2\theta, \\
\dot{U}_z &= -\frac{\epsilon^2 \pi c_0^2 (c_0 - \gamma)}{6\gamma (\gamma - 1) \sin^2 \chi} \cos^2 \theta - \frac{\epsilon^2 \pi c_0}{3(\gamma - 1) \sin^2 \chi} \sin^2 \theta.
\end{align*}

where the dimensionless factor $\frac{\epsilon^2 \pi c_0}{3(\gamma - 1) \sin^2 \chi}$, in Eqs. (3.39)-(3.44), has a magnitude of order $O(10^{-1})$. These components coincide with their values in the $\{X, Y, Z\}$ frame. Using the leading order prediction for the Euler angle dynamics, i.e. $\theta (\tilde{t}) \approx \theta_0$, $\phi (\tilde{t}) \approx \phi_0 + 2\epsilon \tilde{t}$, and $\psi (\tilde{t}) \approx \psi_0 - \epsilon \omega \tilde{t}$, the position of the origin of the body frame in the lab frame is given by
\[ X(\tilde{t}) = \tilde{X}_0 + \tilde{\rho} \sin \phi_0 - \tilde{\rho} \sin \left( \phi_0 + 2\pi \frac{\tilde{t}}{\tilde{T}} \right), \quad (3.45) \]
\[ Y(\tilde{t}) = \tilde{Y}_0 - \tilde{\rho} \cos \phi_0 + \tilde{\rho} \cos \left( \phi_0 + 2\pi \frac{\tilde{t}}{\tilde{T}} \right), \quad (3.46) \]
\[ Z(\tilde{t}) = \tilde{Z}_0 - \tilde{\Lambda} \frac{\tilde{t}}{\tilde{T}}, \quad (3.47) \]

where

\[ \tilde{\rho} = \frac{\pi c_0 \sin 2\theta_0}{12\epsilon (\gamma - 1) \sin^2 \chi} \left[ \frac{c_0 (c_0 - \gamma)}{2\gamma} - 1 \right], \quad (3.48) \]
\[ \tilde{\Lambda} = \frac{\pi^2 c_0}{3 \epsilon (\gamma - 1) \sin^2 \chi} \left[ \frac{c_0 (c_0 - \gamma)}{2\gamma} \cos^2 \theta_0 + \sin^2 \theta_0 \right], \quad (3.49) \]

and the period \( \tilde{T} = \pi/\epsilon^3 \); \( (\tilde{X}_0, \tilde{Y}_0, \tilde{Z}_0) \) is its initial position at \( \tilde{t} = 0 \). According to Eqs. (3.45)-(3.47), the origin of the body frame moves downwards, along the direction of gravity, with the sedimentation speed given by \( \tilde{\Lambda}/\tilde{T} \). In the process, it traces a helical trajectory in the lab frame with a dimensionless radius \( |\tilde{\rho}| \) (note that \( \tilde{\rho} \) can be negative) and pitch \( \tilde{\Lambda} \), and in what follows, this trajectory will be referred to as a superhelix.

To illustrate the main features of such superhelical trajectories, in Figure 3.4 the analytical predictions for the path traced by the origin of the body frame and the instantaneous orientation for a helix with \( N = 4, \alpha_0 = 0, \) and \( \chi = 0.733 \) are plotted. The initial values of the Euler angles are \( \theta_0 = 1.0, \phi_0 = 0.2, \) and \( \psi_0 = 0.5, \) while the origin of the body frame is initially at \((0,0,0)\) in the lab frame. The dashed line represents the trajectory of the centre of the helix, given by Eqs. (3.45)-(3.47), while colours correspond to the instantaneous orientation of the helix at various times: \( \tilde{t} = 0 \) (orange), \( \tilde{t} = \tilde{T}/4 \) (red), \( \tilde{t} = \tilde{T}/2 \) (green), \( \tilde{t} = 3\tilde{T}/4 \) (violet), and \( \tilde{t} = \tilde{T} \) (brown). For each time, the orientation of the helix is constructed by applying the rotation matrix, Eq. (2.9), to the spatial positions of the material points of the helix, Eq. (3.1), where the Euler angles are given by Eqs. (3.36)-(3.38). For visualisation purposes the radius of the helix is made 5 times larger than its actual value and \( \tilde{Z} \)-axis is scaled by 50, since the pitch of the superhelix is much larger than its radius.

Both the pitch and the radius of the superhelical trajectory are large, \( O(\epsilon^{-1}) \), and thus significantly exceed the length of the helix, which is set to unity in the
Figure 3.4 Example of a superhelical trajectory traced by the origin of the body frame for a helix with \( N = 4 \), \( \alpha_0 = 0 \), and \( \chi = 0.733 \). The initial values of the Euler angles are \( \theta_0 = 1.0 \), \( \phi_0 = 0.2 \), and \( \psi_0 = 0.5 \), while centre of the helix is at \((0,0,0)\) at time \( \tilde{t} = 0 \). The dashed line represents the trajectory of the origin of the body frame, given by Eqs. (3.45)-(3.47), while colours correspond to the instantaneous orientation of the helix at various times: \( \tilde{t} = 0 \) (orange), \( \tilde{t} = \tilde{T}/4 \) (green), \( \tilde{t} = \tilde{T}/2 \) (red), \( \tilde{t} = 3\tilde{T}/4 \) (violet), and \( \tilde{t} = \tilde{T} \) (brown). The radius of the helix is increased by a factor of 5 compared to its actual value for visualisation purposes. a) Side view. b) Top view.

Dimensionless units. Also, the pitch is at least ten times larger than the radius of the superhelix (note the difference in scales of the axes) for all helices and initial values of \( \theta_0 \), see Eqs. (3.48) and (3.49). While the origin of the body frame is moving along the superhelical trajectory, the symmetry axis of the helix, given by \( e_3 = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta) \) in the \( \{x', y', z'\} \) frame, rotates around \( Z \) with the frequency \( 2\pi/\tilde{T} \), thus performing exactly one full rotation while travelling down a single pitch \( \tilde{\Lambda} \) of the superhelix. At all times the angle between the symmetry axis of the helix and the tangent to the superhelical trajectory is constant. Finally, the helix is rotating around its axis of symmetry with \( \tilde{\Omega}_3 \), which is much faster than \( 2\pi/\tilde{T} \), thus completing \( O(\epsilon^{-2}) \) turns in one period \( \tilde{T} \). Additionally, Eqs. (3.45)-(3.47) show that the handedness of the superhelical trajectory is opposite to the handedness of the helix: for right-handed helices defined through Eq. (3.1), trajectories are left-handed helices, while for left-handed helices, defined through Eq. (3.1) with \( \lambda \rightarrow -\lambda \), implying \( \epsilon \rightarrow -\epsilon \) in the analysis above, Eqs. (3.45)-(3.47) predict right-handed trajectories. It is possible that the opposite chirality observed is due to a ‘conservation of chirality’ effect. When a helix is subjected to a torque in low-Reynolds conditions, it translates in a straight line; but when a force is applied, the helix experiences a torque. The trajectory could, therefore, be influenced by the fact that gravity is a force without
torque; however a deeper physical understanding of how the resulting handedness is determined is currently lacking. Chirality, and therefore handedness, however, is not necessary to produce handed trajectories as will be seen in Chapter 5.

In Figure 3.5 the superhelical trajectories predicted by Eqs. (3.45)-(3.47) are compared to the numerical solution of the full equations. As above, two cases are considered: a relatively long helix with \( N = 4 \), \( \alpha_0 = 0 \), and \( \chi = 0.733 \) starting from \( \theta_0 = 1.0, \phi_0 = 0.2, \) and \( \psi_0 = 0.5 \), shown in Figure 3.5(a), and a short helix with \( N = 2 \), \( \alpha_0 = -1.34 \), and \( \chi = 0.733 \), starting from \( \theta_0 = 1.0, \phi_0 = 0.0, \) and \( \psi_0 = 0.0 \), shown in Figure 3.5(b). The dashed lines are the large-\( L \) predictions, while the open circles are the numerical solution. As with the dynamics of the Euler angles, the large-\( L \) prediction is only qualitatively correct for the short helix \( (N = 2) \), but shows excellent agreement for the longer one \( (N = 4) \). Given that the large-\( L \) approximation loses its quantitative accuracy for a short helix consisting of only two turns \( (N = 2) \), it is improbable for this method to yield reliable results when applied to a helix comprising only one turn, \( (N = 1) \).

![Figure 3.5](image)

**Figure 3.5** Comparison between the superhelical trajectories predicted by Eqs. (3.45)-(3.47) (dashed lines) and the numerical solutions of the full equations (circles and solid lines). a) Long helix: \( N = 4, \alpha_0 = 0, \) and \( \chi = 0.733 \) with \( \theta_0 = 1.0, \phi_0 = 0.2, \) and \( \psi_0 = 0.5 \). b) Short helix: \( N = 2, \alpha_0 = -1.34, \) and \( \chi = 0.733, \) with \( \theta_0 = 1.0, \phi_0 = 0.0, \) and \( \psi_0 = 0.0 \).

Finally, there are two special orientations, corresponding to the vertical and horizontal sedimentation, that are discussed separately. The former is given by the \( \theta_0 \to 0 \) limit of Eqs. (3.45)-(3.47), and requires no special treatment. The latter, however, requires additional analysis, as is shown in the next section.
3.4 Sedimentation in Almost-Horizontal Orientations

The large-\(L\) approximation for the dynamics of the Euler angles, Eqs. (3.36)-(3.38), developed in the previous Section, relies on the assumption that the first term on the right-hand side of Eq. (3.35), \(O(\epsilon)\), is the dominant one. In an almost-horizontal orientation, when the initial condition \(\theta_0\) is close to \(\pi/2\), the first term on the right-hand side of Eq. (3.35) becomes small compared to the second term, even though it is \(O(\epsilon)\), while the second term is \(O(\epsilon^2)\). Comparing the two terms yields the following estimate for the transitional value of \(\theta_0\), where the \(O(\epsilon^2)\)-contribution in Eq. (3.38) becomes the dominant term

\[
\theta_0^{(tr)} \approx \frac{\pi}{2} - \frac{4\epsilon \gamma}{\pi \epsilon_0 (\gamma - 1) \sin 2\chi}. \tag{3.50}
\]

For \(\theta_0 > \theta_0^{(tr)}\), the solution to Eqs. (3.33)-(3.35) changes significantly. Before discussing the dynamics of the Euler angles and the corresponding spatial trajectories for this regime, the linear stability of the strictly horizontal orientation is analysed. When \(\theta_0 = \pi/2\), the right-hand side of Eq. (3.33) vanishes, implying

\[
\theta(\tilde{t}) = \theta_0, \quad \text{while the evolution of } \psi \text{ is given by the leading term in Eq. (3.35)}
\]

\[
\frac{\partial \psi}{\partial \tilde{t}} = -A \sin \psi, \tag{3.51}
\]

Figure 3.6 Examples of stable horizontal configurations for a helix with \(N = 4\):

a) \(\alpha_0 = 0.24\), the stable configuration is given by \(\psi = 0\).

b) \(\alpha_0 = -0.24\), the stable configuration is given by \(\psi = \pm\pi\) (both configurations look the same). The relative orientation in the \(\tilde{X}\tilde{Y}\)-plane is chosen arbitrarily as the helix is rotating around the \(\tilde{Z}\) axis.
where
\[ A = \epsilon^2 \frac{2(-1)^N \pi c_0 \sin \alpha_0 \cos \chi}{3(\gamma - 1) \sin^3 \chi}. \] (3.52)

The solution to this equation,
\[ \tan \left( \frac{\psi(t)}{2} \right) = \tan \left( \frac{\psi_0}{2} \right) e^{-At}, \] (3.53)
demonstrates that \( \psi \) asymptotically approaches a constant value, determined by the sign of the constant \( A \), which, in turn, is set by the sign of \((-1)^N \sin \alpha_0\). Based on the parametrisation of the helix introduced in this Chapter, this can be translated into a simple geometrical interpretation: helices with a number of turns smaller than the closest integer \( N \) (i.e. helices with \( \alpha_0 > 0 \)) sediment with their free ends pointing downwards, while helices with the number of turns larger than the closest integer (\( \alpha_0 < 0 \)) sediment with their free ends pointing upwards, see Figure 3.6 for example. As can be seen from Eqs. (3.33)-(3.35), \( \theta = \pi/2 \) and \( \psi = 0 \) or \( \psi = \pm \pi \) are stationary points of those equations, while \( \phi \) increases linearly in time, \( \phi(t) = \phi_0 + 2\epsilon^3 t \). This implies that horizontally oriented helices move in a straight line along the direction of gravity with the velocity \( \dot{U}_z \) given by Eq. (3.44) with \( \theta = \pi/2 \), while rotating around the vertical axis with the dimensionless angular velocity \( 2\epsilon^3 \).

To now study the linear stability of the horizontal orientation, a small perturbation to the Euler angles is considered: \( \theta(t) = \theta_0 + \delta\theta(t) \) and \( \psi(t) = \psi_0 + \delta\psi(t) \), where \( \psi_0 \) is either 0 or \( \pm \pi \), see above. Assuming that \( \delta\theta \) and \( \delta\psi \) are infinitesimal, Eqs. (3.33) and (3.35) are linearised and the following equation for the perturbation is obtained,
\[ \frac{\partial^2 \delta\theta}{\partial t^2} = -\epsilon^4 \frac{\pi^2 c_0^2 \cos 2\alpha_0}{3\gamma \tan^2 \chi} \delta\theta. \] (3.54)

This equation has exponentially growing solutions for \( |\alpha_0| > \pi/4 \), and it is, therefore, possible to conclude that the horizontal orientation is stable with respect to small perturbations for helices with \( |\alpha_0| < \pi/4 \), and is unstable, otherwise. As a result, the dynamics of the Euler angles for \( \theta_0 > \theta_0^{(tr)} \) depend strongly on the value of \( \alpha_0 \), as is now demonstrated.

In Figure 3.7, the \( \theta(t) \) and \( \psi(t) \) obtained by numerically solving the full equations of motion for a helix with \( N = 4 \) and \( \chi = 0.733 \), with \( \theta_0 = \pi/2 - 0.07 \), \( \phi_0 = 0.2 \), and \( \psi_0 = 0.2 \) are plotted; the solid lines in Figure 3.7 correspond to \( \alpha_0 = -0.5 \), while the dashed lines correspond to \( \alpha_0 = 0.5 \). This combination of the helix
Figure 3.7  Numerical solution of the full equations of motion for a) $\theta(\tilde{t})$ and b) $\psi(\tilde{t})$. The parameters of the helix are $N = 4$ and $\chi = 0.733$, and the initial conditions are given by $\theta_0 = \pi/2 - 0.07$, $\phi_0 = 0.2$, and $\psi_0 = 0.2$. The solid and dashed lines correspond to $\alpha_0 = -0.5$ and $\alpha_0 = 0.5$, respectively. In a) the dotted line is at $\theta = \pi/2$. In b) the dotted lines are at $\psi = 0$ and $\psi = -\pi$.

parameters and the initial values corresponds to the regime $\theta_0 > \theta_0^{(tr)}$, discussed above ($\theta_0^{(tr)} \approx 0.083$ for this case). As Figure 3.7 indicates, in this regime the dynamics are attracted towards the horizontal orientation, $\theta = \pi/2$, which is linearly stable for $\alpha_0 = \pm 0.5$. When $\alpha_0 = -0.5$, $\psi$ approaches $-\pi$, while for $\alpha_0 = 0.5$, $\psi$ goes to zero, in line with the discussion of stable horizontal orientations above.

Figure 3.8  a) Spatial trajectory obtained by numerical integration of the exact equations of motion (solid line) for a helix with $N = 4$, $\alpha_0 = -1.3$ and $\chi = 0.733$ ($c = 0.226562$) for $\theta_0 = \pi/2 - 0.05$, $\phi_0 = 0.2$, and $\psi_0 = 0.2$. The analytical superhelical trajectory predicted by Eqs. (3.45)-(3.47), dashed line, is given for reference. b) Power spectrum of $\tilde{X}(\tilde{t})$ corresponding to the trajectory in a)(black line). The red dashed line shows the power spectrum of $\tilde{X}(\tilde{t})$ corresponding to a stable superhelical trajectory.

This behaviour changes significantly when $|\alpha| > \pi/4$. In this regime, a
trajectory starting from $\theta_0 > \theta_0^{(tr)}$ is still being attracted towards the horizontal configuration, but the latter is now linearly unstable, the trajectory is pushed away from the horizontal orientation, and the whole process repeats itself, leading to (quasi-)periodic oscillations of $\theta(t)$. These oscillations are similar to the oscillations of $\theta(t)$ in the superhelical regime but with a significantly larger amplitude. Figure 3.8(a) shows the plot of the spatial trajectory traced by the origin of the body frame in the lab frame (solid lines) obtained by numerical integration of the full equations of motion for a helix with $N = 4$, $\alpha_0 = -1.3$, $\chi = 0.733$, where the initial conditions are $\theta_0 = \pi/2 - 0.05$, $\phi_0 = 0.2$, and $\psi_0 = 0.2$. For reference, the superhelical trajectory (dashed line), Eqs. (3.45)-(3.47), for the same values of the parameters is also plotted. As can be seen from Figure 3.8(a), the oscillations in $\theta$ result in a superhelical-like spatial trajectory, although its characteristics are no longer given by Eqs. (3.45)-(3.47). The observed radius and the pitch of the trajectory are significantly larger than their superhelical counterparts, Eqs. (3.48) and (3.49), and the trajectory appears to be less regular. To assess this irregularity, in Figure 3.8(b) the power spectrum of $\tilde{X}(\tilde{t})$ for the trajectory in Figure 3.8(a) is plotted. As can be seen by the red dashed line in Figure 3.8(b), the power spectrum of $\tilde{X}(\tilde{t})$ for a stable superhelical trajectory, such as the one shown in Figure 3.4, is characterised by a single main peak, representing the radius of the superhelix. For a helix with $|\alpha_0| > \pi/4$, in an unstable superhelical-like regime, the power spectrum of $\tilde{X}(\tilde{t})$ is given by the black line in Figure 3.8(b) instead. While the main peak, associated with the superhelical component of the trajectory, is still prominent in this power spectrum, there are many other frequencies involved, although the dynamics do not seem to be chaotic.

3.5 Concluding Remarks

In summary, in this Chapter, RFT [5, 57] was employed to compute the sedimentation of a helical filament. It is found that for most initial orientations the helix performs a superhelical trajectory when sedimenting. The superhelical trajectories that are predicted for a wide range of parameters can be understood in a rather intuitive way. Since the helix is an elongated object, it is expected to sediment with an instantaneous velocity lying in the plane spanned by its axis of symmetry and the direction of gravity and forming a non-zero angle to both directions [30]. The chirality of the helix ensures that this motion then causes the
helix to rotate around the direction of gravity and around its axis of symmetry, due to the translational-rotational coupling \[30\], leading to a steady rotation of the sedimentation plane mentioned above. The resulting path traced by the origin of the body frame in the lab frame is a superhelix.

These calculations also predict the dynamics of a helix in two limiting cases: sedimentation in the vertical and horizontal orientations. In both cases, the helix moves in a straight path along the direction of gravity and simultaneously rotates around it. For helices with \(|\alpha_0| < \pi/4\), the stable horizontal orientation corresponds to its free ends pointing downwards (along the direction of gravity) when \(\alpha_0 > 0\), and to its ends pointing upwards, for \(\alpha_0 < 0\); no stable horizontal orientation for helices with \(|\alpha_0| > \pi/4\) is predicted.

\[\begin{align*}
\text{Figure 3.9} & \quad \text{State diagram for a helix with } N = 4 \text{ and } \chi = 0.733. \text{ For a given combination of } \alpha_0 \text{ and } \theta_0, \text{ the exact equations of motion are numerically integrated with } \phi_0 = \psi_0 = 0. \text{ The colour indicates the amplitude of oscillations of } \theta(\tilde{t}) \text{ in a steady state or at long times, if the steady state is not reached, see the main text. a) The dashed line gives the analytical prediction for the boundary between the superhelical and horizontal orientations } \theta_0^{(tr)} \text{, Eq. } (3.50). \text{ The solid lines are the analytical predictions, } \alpha_0 = \pm \pi/4, \text{ for the threshold between the linearly stable horizontal orientations and quasi-superhelical trajectories with large oscillations of } \theta(\tilde{t}). \text{ b) Zoom-in for } \theta_0 \lesssim \theta_0^{(tr)}. 
\end{align*}\]

Figure 3.9 shows a representative example of a helix with \(N = 4\) and \(\chi = 0.733\) to summarise these findings. As discussed in the previous sections, the type of spatial trajectory can be inferred from the dynamics of the Euler angle \(\theta\), and this property is used to delineate the parameter space. The full equations of motion for the Euler angles starting from \(\phi_0 = \psi_0 = 0\), while \(\theta_0\) is varied in the range \([0, \pi/2]\) are numerically solved. The geometric parameter \(\alpha_0\), which controls how close is the number of pitches in the helix to an integer, see Eq. (3.1), is varied within the range \([-\pi/2, \pi/2]\). For each set of parameters, the amplitude of oscillations of \(\theta\) when the dynamics have reached a steady state, or after three full periods of oscillation when a true steady state is not achieved (as in Figure 3.8), is measured.
The results are then plotted in Figure 3.9 as a function of $\alpha_0$ and the initial value $\theta_0$.

The largest region in Figure 3.9 is occupied by weak oscillations in $\theta$ close to the initial $\theta_0$, associated with the superhelical solution, Eqs. (3.36)-(3.38) and (3.45)-(3.47). This behaviour changes above some critical value $\theta_0^{(tr)}$, and the estimate of $\theta_0^{(tr)}$, Eq. (3.50), (dashed line in Figure 3.9), is in good agreement with the numerical data as long as $\alpha_0$ is not too small, where it underestimates the critical value. For $\theta_0 > \theta_0^{(tr)}$, the helix either ends up in a linearly stable horizontal orientation, when $|\alpha_0| < \pi/4$, or follows an irregular superhelix-like spatial trajectory with a very large radius and pitch, when $|\alpha_0| > \pi/4$, and the horizontal orientation is predicted to be linearly unstable. The transition thresholds, $|\alpha_0| = \pi/4$, are given by solid lines in Figure 3.9.

It is rather unlikely that the superhelical trajectories can be observed experimentally with macroscopic helices in confined geometries, like a fluid in a tank. According to Eq. (3.48), the radius of the superhelical trajectory in physical units, $L\tilde\Lambda$, scales as $L^2/\lambda$, which implies a very wide trajectory. In turn, the size of the tank used in such an experiment should be significantly larger than $L\tilde\Lambda$, implying rather wide geometries. Worse still, the pitch of the superhelical trajectory is significantly larger than its radius, implying not only wide, but also very tall fluid tanks. For instance, consider a helix with $L = 10$ cm, $\chi = 0.733$ and four full turns, $N = 4$ and $\alpha_0 = 0$. If the radius of the helical filament is $r = 0.5$ mm, the ratio of the friction coefficients becomes $\gamma \approx 1.26$ (using Eqs. (3.3) and (3.4) for $K_{\parallel}$ and $K_{\perp}$). With these parameters, and selecting $\theta_0 = \pi/4$, $\rho \approx 2L = 20$ cm and $\Lambda \approx 285L = 28.5$ m is obtained.

Recent advances in manufacturing [117, 122, 123] and manipulation of microhelices under flow conditions [117, 118] suggest that it could be more appropriate to look for microfluidic realisations of superhelical trajectories. Due to the linear nature of the Stokes equation and the absence of a length-scale in the problem besides the dimensions of the helix, all lengths in the estimates above will still be correct when scaled by a common factor. Therefore, for 50 $\mu$m-long helices, which is within the range used by Pham et al. [118], for instance, one would need a 1 cm-long microfluidic channel to detect superhelical trajectories.

As mentioned previously, RFT can, at best, produce semi-quantitative approximations of actual drag forces on extended objects [9, 58, 59]. At worst, it would fail even qualitatively there where the inclusion of hydrodynamic interactions is
crucial [60]. Therefore, to verify the applicability of these results, the following Chapter will look at the sedimentation of a helix using the numerical computation of a Grand Mobility Matrix [1] introduced in Chapter 2.6.
Chapter 4

Rotne-Prager-Yamakawa (RPY) Modelling of Helix Sedimentation

Figure 4.1  Diagram of a helix made up of collection of spheres. Here the helix is parametrised as Eq. (3.1) and is described by the same geometry as in Figure 3.1.

In Chapter 3 the sedimentation of a helix within the framework of RFT was considered. This theory has its limitations, primarily it neglects hydrodynamic interactions between different parts of the rigid body. Thus, the results obtained there are seen as indicative of the real dynamics. Therefore, in this chapter, a more exact algorithm based on the RPY approximation is made use of. This accounts for (some of the effects of) hydrodynamic coupling between elements of
the helix, by approximating the object as a collection of spheres, see Figure 4.1. Specifically, an implementation of the algorithm by Palanisamy and Den Otter [1], which is described in greater detail in Section 2.6, is used. Helices, made up of beads, of various lengths \( L \) and \( \alpha_0 = 0 \) are considered at first. It is found, using the implemented algorithm, that the GMM for a helix has a general form given by,

\[
M = \begin{pmatrix}
\mu^1_1 & 0 & 0 & \mu^4_1 & 0 & 0 \\
0 & \mu^2_2 & \mu^3_2 & 0 & \mu^5_2 & \mu^6_2 \\
0 & \mu^2_3 & \mu^3_3 & 0 & \mu^5_3 & \mu^6_3 \\
\mu^1_4 & 0 & 0 & \mu^4_4 & 0 & 0 \\
0 & \mu^2_5 & \mu^3_5 & 0 & \mu^5_5 & \mu^6_5 \\
0 & \mu^2_6 & \mu^3_6 & 0 & \mu^5_6 & \mu^6_6
\end{pmatrix}.
\] (4.1)

In the matrix in Eq. (4.1), the presence of cross-coupling terms gives indication that the dynamics of the helix is non-trivial. In this chapter, the GMM of helices with different lengths, \( L \), and different \( \alpha_0 \)'s, will be evaluated and used to study the translational and orientational dynamics of sedimenting helices.

The RFT solution for the sedimentation of long helices constructed in Chapter 3 and 3, indicates that the origin of the body frame of the helix moves downwards tracing a superhelical trajectory in the lab frame. The superhelical path has a dimensionless radius \( \tilde{\rho} \) and pitch \( \tilde{\Lambda} \) given by,

\[
\tilde{\rho} = \frac{\pi c_0 \sin 2\theta_0}{12\epsilon (\gamma - 1) \sin^2 \chi} \left[ \frac{c_0 (c_0 - \gamma)}{2\gamma} - 1 \right],
\] (4.2)

\[
\tilde{\Lambda} = \frac{\pi^2 c_0}{3\epsilon (\gamma - 1) \sin^2 \chi} \left[ \frac{c_0 (c_0 - \gamma)}{2\gamma} \cos^2 \theta_0 + \sin^2 \theta_0 \right],
\] (4.3)

and period \( \tilde{T} = \pi/\epsilon^3 \). Here, \( c_0 = \gamma + \gamma \cos^2 \chi + \sin^2 \chi \), \( \gamma = K_\perp/K_\parallel \) and \( \epsilon = \lambda/L \); with \( K_\perp \) and \( K_\parallel \) defined in Eqs. (3.3) and (3.4). The dimensionless form is obtained by scaling all lengths with \( L \) and time with the timescale \( \tau \) defined in Eq. (3.29). Both equations for the radius and pitch of the superhelix depend on the parameter \( \gamma \), which is the ratio between the perpendicular and parallel drag coefficients. Due to this dependence, the theoretical approximation for \( \gamma \) and the ratio of the perpendicular and parallel drag coefficients, obtained by computing the Grand Mobility Matrix, are compared and analysed in the following Section.
4.1 The Friction Ratio $\gamma$

The properties of the superhelical trajectory, in Eqs. (4.2) and (4.3), depend on the ratio of the perpendicular and parallel drag coefficients of a helical filament $\gamma_{\text{fil}} = K_\perp/K_\parallel$; where $K_\parallel$ and $K_\perp$ are given by Eqs. (3.3) and (3.4) respectively. It is, therefore, of interest to start the comparison between the RPY algorithm and RFT by looking at the drag coefficients obtained from each theory. For the RPY theory, the parallel friction coefficient will be given by the translational couplings in the radial plane of the helix ($x - x$ or $y - y$), while the perpendicular friction coefficients will be given by the translational coupling along the major axis direction ($z - z$); i.e. the first three diagonal components of the GMM. Note that, $\gamma_{\text{fil}}$ is the ratio of the drag coefficients for a helical filament, and does not consider the length of the full helix, while the ratio of the coefficients from the GMM is evaluated by consider the entire helix. Hence, an RFT ratio that considers the full length of the helix, $\gamma_{\text{hel}}$, is introduced. This is found by taking the ratio of the coefficients of the $U_1$ and $U_3$ velocity component in the expression for the force component $F_1$ (in Eq. (3.8)) and $F_3$ (in Eq. (3.10)) respectively, and is given by,

$$\gamma_{\text{hel}} = \frac{-\gamma_{\text{fil}} + \frac{\gamma_{\text{mol}} - 1}{2} \sin^2 \chi}{-\gamma_{\text{fil}} + (\gamma_{\text{mol}} - 1) \cos^2 \chi},$$

(4.4)

where $\Delta_{1,2} = 0$ as only helices with $\alpha_0 = 0$ are currently considered.

The $11 \times 11$ Grand Mobility Matrices for a helix with an $N = 4$ number of turns, $\alpha_0 = 0$, $\chi = 0.733$ and various lengths ($L = 200, 300, 400, 500, 600, 700, 800$) are then computed and the ratio of the friction coefficients for each helix is found by taking $\mu_i^3/\mu_i^1$; where $\mu_i^l$ is an element of the mobility matrix (introduced in Eq. (2.42)) and $i, j \in [1, 6]$. The values $N = 4$ and $\chi = 0.733$ are chosen as such to match the parameters for the helix mainly considered throughout Chapter [3]. The dependence of $\mu_1^3/\mu_1^1$, $\mu_2^3/\mu_2^1$, $\gamma_{\text{hel}}$, and $\gamma_{\text{fil}}$ with respect to $1/L$ is plotted and shown in Figure [4.2].

Note that, due to the radial symmetry of the helix, both $\mu_1^1$ and $\mu_2^1$ can be taken as the parallel friction coefficients. The ratios of $\mu_2^3/\mu_1^1$ and $\mu_2^3/\mu_2^1$ are, therefore, compared in order to check this holds. It can in fact be seen, in Figure [4.2] that choosing either of the parallel friction coefficients from the grand mobility matrix ($\mu_1^1$ and $\mu_2^1$) makes no significant difference. Therefore, from here on, the GMM friction
Figure 4.2  Plot showing the dependence on the length of the helix for: $\mu_3/\mu_1$ (blue dots), $\mu_3/\mu_2$ (orange ×), $\gamma_{\text{hel}}$ (green +), and $\gamma_{\text{fil}}$ (red down-pointing triangles) for a helix with $N = 4$, $\chi = 0.733$ and $\alpha_0 = 0$. The lines going through the points are obtained from the interpolation of the data.

ratio considered will be the one obtained using $\mu_1$: $\gamma_{\text{GMM}} = \mu_3/\mu_1$.

It can be seen, in Figure 4.2, that the ratio of the coefficients from the GMM and $\gamma_{\text{hel}}$ do not show a strong dependence on the length of the helix, unlike $\gamma_{\text{fil}}$.

### 4.2 Spatial Trajectory

In this Section the predictions of the trajectory obtained using Resistive-Force Theory are compared to the results from the dynamics simulation using the dynamics implementation. It is found that for most initial orientations the helix performs a superhelical trajectory when sedimenting, with the superhelix having a pitch and radius in agreement with the RFT approximation. The handedness of the superhelix is also found to be dependent on the handedness of the sedimenting helix, as is shown in Figure 4.3. Here Figure 4.3(a) shows the sedimentation trajectory for a right-handed helix with $N = 4$, $\chi = 0.733$, $\alpha_0$ and initial orientation $\theta_0 = 0.35\pi$, $\phi_0 = 0$, and $\psi_0 = 0$; whilst Figure 4.3(b) shows the trajectory for a left-handed helix with the same conditions.
4.2.1 Radius of the Superhelix

To calculate the radius of the superhelical trajectory drawn by the helix in the simulation, the minimum value of the \( x \)-coordinate is subtracted by the maximum value and that difference is divided by 2 \( (\rho_{\text{sim}} = \frac{\max(x) - \min(x)}{2}) \). This value is then divided by the length, \( L \), of the given helix in order to obtain the dimensionless result \( \tilde{\rho}_{\text{sim}} \).

The plot showing dependence of the radius of the superhelical trajectory with the initial orientation \( \theta_0 \), for both the theoretical prediction and the simulation for helices of different lengths, \( L \), is shown in Figure 4.4. It can be seen that the radius of the superhelix shows the same dependence on the initial angle, \( \theta_0 \), for both the Resistive-Force Theory prediction and the simulation result. However,
looking at the two insets in Figure 4.4, there seems to be an opposite dependence of radius with the length of the helix; $\rho_{th}$ increases as $L$ increases, while $\rho_{sim}$ decreases. This contrasting dependence could be due to the different behaviour of $\gamma_{fil}$ and $\gamma_{GMM}$ on the length $L$ seen in Figure 4.2.

4.2.2 Pitch of the Superhelix

To calculate the pitch of the superhelical trajectory, the $z$-coordinates corresponding to the same time step as two consecutive minimum $x$ values were subtracted from each other; this was then divided by $L$ to obtain the dimensionless quantity $\tilde{\Lambda}_{sim}$. Graphs showing the dependence of the pitch against the different initial values of $\theta_0$, for helices of varying lengths, for both the Resistive-Force Theory approximation and the Grand Mobility Matrix simulation results, are then plotted in Figure 4.5. Looking at the insets in Figure 4.5, it can be seen that, for both $\tilde{\Lambda}_{th}$ and $\tilde{\Lambda}_{sim}$, the pitch decreases as the length of the helix increases. This is in contrast to the results found for the radius of the superhelix, which showed opposite dependence on $L$ for $\bar{\rho}_{th}$ and $\bar{\rho}_{sim}$.

From the above, it is found that assigning an effective friction coefficient leads to conflicting results. Therefore, how to remedy this situation will be considered next.

![Figure 4.5](image-url) Plots of the initial condition the pitch for helices with $N = 4$, $\chi = 0.733$ and $\alpha_0 = 0$ with different lengths $L$ vs. $\theta_0$, with: (a) plot of $\Lambda_{th}$ calculated from Eq. (4.3) with $\gamma = \gamma_{fil}$, and (b) plot of $\Lambda_{sim}$. The insets show the dependence of $\Lambda$ on the length of the helix $L$.
4.3 Finding a Better $\gamma$

The following choice for improving the drag coefficient ratio for a sedimenting helix is made. The expression for $\gamma_{\text{hel}}$ (in Eq. (4.4)) is set equal to $\gamma_{\text{GMM}}$ and solved for $\gamma^*_{\text{fil}}$.

$$\frac{\mu_3^3}{\mu_1^3} = -\gamma^*_{\text{fil}} + \frac{\gamma^*_{\text{fil}} - 1}{2} \sin^2 \chi - \gamma^*_{\text{fil}} + (\gamma^*_{\text{fil}} - 1) \cos^2 \chi.$$  \hspace{1cm} (4.5)

Having solved for $\gamma^*_{\text{fil}}$, this new ratio is plugged into the equations for the dimensionless radius and pitch of the superhelix, in Eqs. (4.2) and (4.3), and plotted for different initial values $\theta_0$.

![Figure 4.6](image.png)

**Figure 4.6** Plots of (a) $\tilde{\rho}$ and (b) $\tilde{\Lambda}$ vs. $\theta_0$ for the simulation (blue), prediction using new $\gamma_{\text{fil}}$ from Eqs. (4.3) and (4.4) (orange), and $\gamma^*_{\text{fil}}$ (green). The inset in (b) shows the $\tilde{\Lambda}$s shifted such that the values at $\theta_0 = \pi/4$ match.

The plots in Figure 4.6 compare the radius and pitch, for a helix of length $L = 200$: calculated from the numerical data, $\tilde{\rho}_{\text{sim}}$ and $\tilde{\Lambda}_{\text{sim}}$ (blue dots); from Eqs. (4.2) and (4.3) using $\gamma_{\text{fil}}$ (orange +); and from using the newly calculated $\gamma^*_{\text{fil}}$ from Eq. (4.5) in Eqs. (4.2) and (4.3) (green ×). It can be seen that for the radius, the $\tilde{\rho}(\gamma^*_{\text{fil}})$ shows a closer match to $\tilde{\rho}_{\text{sim}}$ than $\tilde{\rho}(\gamma_{\text{fil}})$. For the pitch, instead, while the values of $\tilde{\Lambda}(\gamma^*_{\text{fil}})$ differ from $\tilde{\Lambda}_{\text{sim}}$ more than $\tilde{\Lambda}(\gamma_{\text{fil}})$ for a given $\theta_0$, it can be seen that the plots of $\tilde{\Lambda}(\gamma^*_{\text{fil}})$ and $\tilde{\Lambda}_{\text{sim}}$ show a more similar dependence on $\theta_0$ than for the plot of $\tilde{\Lambda}(\gamma_{\text{fil}})$. This is further shown in the inset of Figure 4.6(b) where the $\tilde{\Lambda}$s were shifted, such that the values at $\theta_0 = \pi/4$ match, in order to better visualise the dependence on $\theta_0$.

Whilst the RFT radius and pitch of the superhelix using the friction ratios so far
considered show good qualitative agreement with the results obtained using the GMM dynamics, further analysis is done to find a better quantitative agreement.

Another $\gamma, \gamma^*$, is now calculated in order to reach exact quantitative agreement between the two theories. The previous ratio, $\gamma_{fil}^*$, was found by looking at the drag coefficients obtained through the two theories, and equating the GMM coefficients’ ratio to Eq. (4.4). In alternative, $\gamma^*$ is calculated by directly focusing on the properties of the superhelix and equating the numerically obtained radius, $\rho_{\text{sim}}$, to the expression for the radius in Eq. (4.2). To find $\gamma^*$, $\tilde{\rho}_{\text{sim}}(\theta_0 = \pi/4)$ is set equal to the expression for $\tilde{\rho}$, from Eq. (4.2), and solved for $\gamma$. Figure 4.7 shows the plots of the values of $\tilde{\rho}_{\text{sim}}$ and $\tilde{\Lambda}_{\text{sim}}$ (blue dots), and of $\tilde{\rho}(\gamma^*)$ and $\tilde{\Lambda}(\gamma^*)$ (orange line) vs. $\theta_0$. It can be seen that, when using $\gamma^*$, the radius $\tilde{\rho}(\gamma^*)$ matches $\tilde{\rho}_{\text{sim}}$ accurately. In Figure 4.7(b), $\tilde{\Lambda}(\gamma^*)$ is also shifted up by a factor of 207 (green ×) in order to better show the dependence on $\theta_0$. It can be noted that, with the shift, $\tilde{\Lambda}_{\text{sim}}$ and $\tilde{\Lambda}(\gamma^*)$ show great agreement.

![Figure 4.7](image)

*Figure 4.7* Plots of (a) $\tilde{\rho}$ and (b) $\tilde{\Lambda}$ for the simulation (blue), prediction using $\gamma^*$ (orange) vs. $\theta_0$. In (b) $\tilde{\Lambda}^*(\gamma^*)$ shifted up by 207 (green) is plotted to better show the dependence on $\theta_0$.

In this Section, two different methods to evaluate a new $\gamma$ were introduced and examined. It is shown that, using $\gamma^*$, the results for the radius of the superhelical trajectory found through RFT and the ones numerically calculated using the GMM show exact agreement. Additionally, an equivalent dependence of the pitch on the initial orientation, $\theta_0$, is recovered. Though to match $\tilde{\Lambda}(\gamma^*)$ and $\tilde{\Lambda}_{\text{sim}}$ quantitatively, an apparently arbitrary shift is introduced. This shift is found to decrease as the length of the helix increases.
4.4 Euler Angles

Having looked at the trajectory of the sedimenting helix, the changes in its orientation are now studied. According to the results found in Chapter 3, the symmetry axis of the helix, $e_3 = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta)$ in the lab frame, is found to perform one full rotation (given by the Euler angle $\phi$) around $Z$ while travelling down a single pitch $\tilde{\Lambda}$ of the superhelix, and has a frequency of $2\pi/\tilde{T}$. Meanwhile, the helix is rotating (with Euler angle $\psi$) around its main axis of symmetry with a frequency much faster than $2\pi/\tilde{T}$, thus completing, in one period $\tilde{T}$, a number of turns of the order $\epsilon^{-2}$, where $\epsilon = \lambda/L$.

In Figure 4.8, the plots of $\phi$ vs. $t$, for helices of lengths $L = 200$ and $L = 400$ with different initial values of $\theta_0$, show that the behaviour of $\phi$ with respect to time does not depend on $\theta_0$. Here the initial cases of $\theta_0 = 0$ and $\theta_0 = \pi/2$ are omitted as these initial conditions do not lead to a superhelical trajectory.

As the helix is expected to perform one full rotation of $\phi$ while travelling down a single pitch of the superhelix, with a frequency of $2\pi/\tilde{T}$, in Figure 4.9, $\phi$ vs. $t$ is plotted on the same graph as $x$ vs. $t$ (with $x$ re-scaled to fit). It can be seen that at the time $t$ corresponding to each rotation of the angle $\phi$, given by a change of $2\pi$ (troughs of the blue line), $x$ is at the same value. This implies that after exactly one rotation of the helix along its symmetry axis, the helix is at the same $x - y$ position but one pitch $\tilde{\Lambda}$ lower, as is expected from the theory.

As already mentioned, it is predicted that the helix rotates around its axis of symmetry with a frequency such that the helix complete $O(\epsilon^{-2})$ turns in one period $\tilde{T}$. The period $T_{\text{sim}}$ of a full turn of the superhelix (time taken by the helix
Figure 4.9  The rotation of the helix about its symmetry axis ($\phi$; blue) and the rotation along the superhelical trajectory ($x$ position oscillations, yellow) are commensurate. The plot shows the two measures as a function of time for a helix with $N = 4$, $\chi = 0.733$, $\alpha_0 = 0$ with initial orientation $\theta_0 = \pi/4$, $\phi_0 = 0$ and $\psi_0 = 0$.

to travel down a single pitch $\Lambda_{\text{sim}}$ is, therefore, found by taking the time difference between two consecutive minima of the $x$ values. The number of rotations about the helix’s axis of symmetry within one period $T_{\text{sim}}$ is calculated and shown in Table 4.1.

<table>
<thead>
<tr>
<th>$L$</th>
<th>$\nu$</th>
<th>$\nu/\epsilon^{-2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>117</td>
<td>7.31</td>
</tr>
<tr>
<td>300</td>
<td>123</td>
<td>7.69</td>
</tr>
<tr>
<td>400</td>
<td>126</td>
<td>7.88</td>
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<tr>
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<td>128</td>
<td>8.00</td>
</tr>
<tr>
<td>600</td>
<td>129</td>
<td>8.06</td>
</tr>
<tr>
<td>700</td>
<td>130</td>
<td>8.13</td>
</tr>
<tr>
<td>800</td>
<td>131</td>
<td>8.19</td>
</tr>
</tbody>
</table>

Table 4.1  Table showing number of rotations of $\psi$ per period $T_{\text{sim}}$, $\nu$. Table also shows the number of rotations per period divided by $\epsilon^{-2}$.

where $\epsilon = 0.25$ for all values of $L$. This table shows that, in one full turn of the superhelix $T_{\text{sim}}$, the helix performs a number of rotations about its major axis that is of the order of $\mathcal{O}(\epsilon^{-2})$ as was predicted using Resistive-Force Theory.
4.4.1 Sedimentation in Almost Horizontal Orientations

From Figure 4.4, it can be seen that for a helix with the initial conditions \( \theta_0 = 0 \) and \( \theta_0 = \pi/2 \), the radius of the trajectory, \( \hat{\rho}_{\text{sim}} \) and \( \hat{\rho}_{\text{th}} \), is zero. This implies that for these initial conditions, a helix with an integer number of turns (\( \alpha_0 \neq 0 \)) does not follow a superhelical trajectory when sedimenting.

For \( \theta_0 = 0 \), the helix starts in a vertical configuration, and it maintains that orientation as it sediments vertically down. Instead, when helix starts in an almost horizontal orientation, \( \theta_0 \to \pi/2 \), in Resistive-Force Theory [3], the solutions to the equations of motion change. It is found that the transitional value of \( \theta_0 \) to enter this different regime is given by Eq. (4.6).

\[
\theta_0^{(\text{tr})} \approx \frac{\pi}{2} - \left| \frac{4 \epsilon \gamma}{\pi c_0 (\gamma - 1) \sin 2\chi} \sin \alpha_0 \right|.
\] (4.6)

For \( \theta_0 > \theta_0^{(\text{tr})} \), the dynamics of the Euler angles and spatial trajectories change significantly. The regime where \( \theta_0 > \theta_0^{(\text{tr})} \) is stable for helices with \( |\alpha_0| < \pi/4 \). It was found, instead, that when \( |\alpha| > \pi/4 \) and \( \theta_0 > \theta_0^{(\text{tr})} \), the trajectory is linearly unstable and is pushed away from the horizontal orientation in quasi-periodic oscillations of \( \theta(\hat{t}) \). These oscillations in \( \theta \) result in a superhelical-like spatial trajectory no longer characterised by the same equations for the radius and the pitch. The irregularity was classified by examining the power spectrum of \( \hat{X}(\hat{t}) \) for a helix with \( \alpha_0 = -1.2 \) and initial orientation \( \theta_0 = \pi/2 - 0.03 \) in Figure 4.10

Figure 4.10 shows the power spectrum of \( \hat{X}(\hat{t}) \) for a helix with \( |\alpha_0| > \pi/4 \) found by using RFT (red dashed line) and by evaluating the dynamics of the GMM (black line). In agreement with the results from RFT, the black line in the spectrum in Figure 4.10 has a main peak, which is associated to the superhelical component of the trajectory, as well as other frequencies which show that the trajectory is not purely helical.

4.5 Varying the Initial Conditions

Figure 4.11 shows a representative example of a helix with \( N = 4 \) and \( \chi = 0.733 \) to summarise these findings, as was done in Figure 3.9 in Section 3.5. The
Figure 4.10  Black line: power spectrum of $\tilde{X}(\tilde{t})$ for a helix with $N = 4$, $\chi = 0.733$, $\alpha_0 = -1.2$ with initial orientation $\theta_0 = \pi/2 - 0.03$, $\phi = 0$, and $\psi = 0$ evaluated by solving the dynamics of the GMM. Red dashed line: power spectrum of $\tilde{X}(\tilde{t})$ for a helix with $N = 4$, $\chi = 0.733$, $\alpha_0 = -1.3$ with initial orientation $\theta_0 = \pi/2 - 0.05$, $\phi = 0.2$, and $\psi = 0.2$ evaluated using RFT (see Figure 3.8(b)).

geometric parameter, $\alpha_0$, which controls how close to an integer number of turns the helix is, is varied within the range $[-\pi/2, \pi/2]$; and initial orientation, $\theta_0$, is varied within the range $[0, \pi/2]$ to delineate the parameter space. For each set of parameters, the amplitude of oscillations of $\theta(t)$ is plotted, in Figure 4.11, in order to infer the type of spatial trajectory performed by the helix. When the amplitude of oscillations of $\theta$ is small, for $\theta_0 \in [0, \pi/2]$, the helix is performing the superhelical trajectory, while for larger amplitudes of oscillation the helix enters a regime where its spatial trajectory is linearly unstable. The red dashed line, in Figure 4.11, shows the analytical prediction for the boundary between the superhelical and horizontal orientations $\theta_0^{(tr)}$, Eq. (4.6), where the new ratio of mobility coefficients, $\gamma^*$, found in Section 4.3 was used. The solid lines are the analytical predictions, $\alpha_0 = \pm \pi/4$, for the threshold between the linearly stable horizontal orientations and quasi-superhelical trajectories with large oscillations of $\theta(\tilde{t})$. 
Figure 4.11  State diagram for a helix with \( N = 4 \) and \( \chi = 0.733 \), for a given combination of \( \alpha_0 \) and \( \theta_0 \), with \( \phi_0 = \psi_0 = 0 \). The colour indicates the amplitude of oscillations of \( \theta(\tilde{t}) \) in a steady state or at long times, if the steady state is not reached, see the main text. a) The dashed line gives the analytical prediction for the boundary between the superhelical and horizontal orientations \( \theta_0^{(tr)} \), Eq. (4.6), using \( \gamma^* \) found in Section 4.3. The solid lines are the analytical predictions, \( \alpha_0 = \pm \pi/4 \), for the threshold between the linearly stable horizontal orientations and quasi-superhelical trajectories with large oscillations of \( \theta(\tilde{t}) \).

4.6  Concluding Remarks

In this Chapter, the sedimentation of a helical filament in a viscous fluid based on a Rotne-Prager-Yamakawa (RPY) level numerical approximation was computed. The helix was approximated as a collection of spheres and its GMM was found using the method introduced by Palanisammy and Den Otter \[^1\] and implemented by Joost de Graaf. The dynamics was then solved for the given GMM and initial conditions of the helix. These results are then compared to the RFT predictions found in Chapter 3. Here qualitative agreement is found as the same dependence of the radius and pitch on the initial orientation \( \theta_0 \) is recovered. Furthermore, it is found that, by tuning the friction ratio of translational mobilities (\( \gamma \)), good quantitative agreement for the RFT and numerical radius is reached. The pitch, using the unfitted ratio, \( \gamma_{fil} \), gives closer numerical agreement with RPY results but with a different dependence on \( \theta_0 \). On the other hand, using the ratio \( \gamma^* \) for the pitch shows the same dependence on \( \theta_0 \) but at the cost of the quantitative agreement.
It is found that for most initial orientations the helix performs a superhelical trajectory when sedimenting, with the superhelix having a pitch and radius in agreement with the RFT approximation. Additionally, also in agreement with the RFT predictions, the helix is found to complete a full rotation about its minor axis (by the angle $\phi$) in the same period it takes for it to travel down a single pitch, $\tilde{\Lambda}$ of the superhelix.

This shows that RFT, for a sedimenting helical filament, can produce good qualitative and semi-quantitative approximations for the trajectory when compared to the results obtained from a method that includes hydrodynamic interactions. So far, the GMM method [11], introduced in Chapter 2, was tested against the known results of spheres and rods, in Section 2.6.2 and against the RFT for a helix sedimenting in this Chapter. In the following chapters, further analysis of the behaviour of anisotropic particles sedimenting at low-Reynolds number using the GMM is done.
Chapter 5

L-Shape and C-Shape Sedimentation

Having, so far, studied the sedimentation of a rigid helix using two different methods (RFT and GMM), the focus of this chapter will be on the sedimentation of two non-chiral shapes; the L-shape and the C-shape. There are two reasons why the sedimentation of an L-shape and a C-shape are looked at here. First an L-shape, with an initial orientation that is parallel to the direction of gravity, is studied. This can be considered as an extension to the sedimenting rod but with a ‘kink’ added to one end. At first thought one would think that, as the short leg of the L-shape goes to zero, the results for a rod sedimenting are recovered. That is that the initial orientation, with respect to the vertical, remains constant as the object sediments ($\theta(t) = \theta_0$). However, it is found that that is not the case for an L-shape with a short leg, $l_1$, much shorter than the long leg, $l_2$, (i.e. $l_1 \ll l_2$). This behaviour will be examined and understood by considering the structure of the $11 \times 11$ grand mobility matrix.

Second, the sedimentation of the C-shape sedimenting at an angle to the plane of gravity is introduced. This is done based on the conclusions by Krapf and Witten [2, 10] that particles containing certain asymmetric properties will sediment performing a chiral trajectory. Therefore, for this part, a C-shape with an initial orientation that is at an angle to the plane of gravity is considered. Krapf et al. argue that the structure of the $3 \times 3$ sub-block of the mobility matrix, which contains the translational-rotational coupling terms, called the twist matrix, determines whether the sedimentation trajectory is chiral. Because
the twist matrix is a $3 \times 3$ square matrix, it can have either one or three real eigenvalues. In the case of a single real eigenvalue, the sign of the eigenvalue gives the chirality. With three real eigenvectors, the simple chirality of the object’s trajectory is no longer present, and the motion becomes more complicated and depends on initial conditions. Having calculated the GMM for a C-shape, it is found that its twist matrix has three real eigenvalues. Solving for the dynamics then shows that, when the C-shape is not parallel to the plane of gravity, it sediments performing a complex chiral trajectory with properties that depend on the initial orientation.

When looking at both the sedimentation parallel to the plane of gravity and sedimentation outside the plane of gravity, similar sedimentation behaviour and trajectories were found for the L- and C-shapes. Therefore, in this chapter, only the results for the L-shape will be outlined when studying the sedimentation in the plane of gravity; and, similarly, results for the sedimentation out of the plane of gravity will be shown solely for the C-shape. At the end of the chapter, however, a comprehensive state diagram will be shown for both shapes (Figures 5.6 and 5.7).

5.1 The Sedimentation of L-shaped Particles
Parallel to the Plane of Gravity

Figure 5.1 Sketch of a sedimenting L-shape, which indicates the quantities relevant to the analysis, with $l_1$ representing the short leg and $l_2$ the long leg. Examples of an L-shape with equal legs, one with $a \approx 3 : 1$ leg ratio and the rod with a small kink are shown on the right-hand side of the figure.
In this section, the sedimentation of L-shapes is studied where the analysis will be done both by using RFT and the RPY implementation.

Two L-shapes were created using the composite sphere approach. The first, considered in this section, is built up using a base of $3 \times 3$ spheres arranged in a square, with a distance between the spheres of 2.01. The squares are subsequently stacked to form both arms of the L-shape, see Figure 5.1. The second, is a straight line of single beads, spaced 2.01 apart, with a single bead at the end placed perpendicular to the line. This second L-shape is convenient to approach the limit of a straight rod, as will be examined in Section 5.1.4.

### 5.1.1 Resistive-Force Theory

In this Section the Resistive-Force Theory for the L-shape is introduced. The lab frame is $\{x, y\}$ and the body frame $\{1, 2\}$. The drag force acting on leg 1, $\mathbf{F}(1)$, and the one acting on leg 2, $\mathbf{F}(2)$, are given by:

\[
\mathbf{F}(1) = -K_{||}(1)(\mathbf{U} \cdot \mathbf{e}_1)\mathbf{e}_1 - K_{\perp}(1)(\mathbf{U} - (\mathbf{U} \cdot \mathbf{e}_1)\mathbf{e}_1),
\]

\[
\mathbf{F}(2) = -K_{||}(2)(\mathbf{U} \cdot \mathbf{e}_2)\mathbf{e}_2 - K_{\perp}(2)(\mathbf{U} - (\mathbf{U} \cdot \mathbf{e}_2)\mathbf{e}_2),
\]

where $\mathbf{e}_1$ and $\mathbf{e}_2$ point in the direction of leg 1 and 2, respectively, as shown in Figure 5.1. The force due to gravity, in the body frame, is given by:

\[
\mathbf{F}(g) = -F(\sin \theta \mathbf{e}_1 + \cos \theta \mathbf{e}_2).
\]

Representing the velocity $\mathbf{U}$ as $\mathbf{U} = U_1 \mathbf{e}_1 + U_2 \mathbf{e}_2$, the forces become:

\[
\mathbf{F}(1) = -K_{||}(1)U_1 \mathbf{e}_1 - K_{\perp}(1)U_2 \mathbf{e}_2,
\]

\[
\mathbf{F}(2) = -K_{||}(2)U_2 \mathbf{e}_2 - K_{\perp}(2)U_1 \mathbf{e}_1.
\]

The force balance condition $\mathbf{F}(1) + \mathbf{F}(2) + \mathbf{F}(g) = 0$ gives the following expressions for the velocity of the sedimenting L-shape:

\[
U_1 = -\frac{F \sin \theta}{K_{||}(1) + K_{\perp}(2)},
\]

\[
U_2 = -\frac{F \cos \theta}{K_{||}(2) + K_{\perp}(1)}.
\]
The centre of mass of each leg is given by $R_{CM}^{(i)} = \frac{l_i^2}{2} e_i$, where $l_i$ is the length of leg $i$, so that the centre of mass of the L-shape is:

$$R_{CM} = \frac{l_1^2}{2(l_1 + l_2)} e_1 + \frac{l_2^2}{2(l_1 + l_2)} e_2 \quad (5.8)$$

The torques with respect to the origin of the body frame are then expressed as,

$$T_{total} = (R_{CM}^{(1)} \times F^{(1)}) + (R_{CM}^{(2)} \times F^{(2)}) + (R_{CM} \times F^{(q)}) = 0 \quad (5.9)$$

Solving for $\theta$ this then gives:

$$\tan \theta = \frac{l_1 l_1 + 2l_2}{l_2 l_2 + 2l_1} \quad (5.10)$$

where the friction coefficients were approximated as: $K_{\perp(i)} = 4\pi \mu l_i$ and $K_{\parallel(i)} = 2\pi \mu l_i$.

The angle of sedimentation, $\alpha$, is then given by

$$\tan \alpha = \frac{U_x}{U_z} = \frac{|-\cos \theta U_1 e_1 + \sin \theta U_2 e_2|}{|\sin \theta U_1 e_1 + \cos \theta U_2 e_2|}, \quad (5.11)$$

where $U_1$ and $U_2$ are given by Eqs. (5.6) and (5.7) respectively and $\theta$ is given by Eq. (5.10). These equations, obtained through RFT, will be compared to results from the RPY-based algorithm in a later section.

### 5.1.2 Hydrodynamic Resistance Tensor of an L-Shape

Following the method introduced in Section 2.4.3, the resistance tensor for an L-shape, using RFT, is now evaluated. The integrals, in Eqs. (2.29)-(2.31), are carried out by integrating over the two legs of the L-Shape; keeping in mind that the end point of the first integral must match the starting point of the second one. Given an L-Shape, of the form in Figure 5.1, the two integrals to be computed are one along the $x$-axis from $-l_1$ to 0 and the other in the $z$ direction from 0 to $l_2$. Performing these integrals, the resulting resistance tensors are found to be:

$$\Gamma = \begin{pmatrix}
K_{\parallel} l_1 + K_{\perp} l_2 & 0 & 0 \\
0 & K_{\perp} l_1 + K_{\parallel} l_2 & 0 \\
0 & 0 & K_{\perp} l_1 + K_{\parallel} l_2
\end{pmatrix}, \quad (5.12)$$
The full resistance matrix, given by \( \text{C}^{\text{T}} \text{R} \text{C} \), is then inverted to find the mobility shape for and L-Shape slender object and it is found to have the form:

\[
\text{M} = \begin{pmatrix}
\mu_1^1 & 0 & \mu_3^3 & 0 & \mu_5^5 & 0 \\
0 & \mu_1^2 & 0 & \mu_3^4 & 0 & \mu_5^6 \\
\mu_3^1 & 0 & \mu_3^3 & 0 & \mu_5^5 & 0 \\
0 & \mu_4^2 & 0 & \mu_3^4 & 0 & \mu_4^6 \\
\mu_5^1 & 0 & \mu_3^3 & 0 & \mu_5^5 & 0 \\
0 & \mu_6^2 & 0 & \mu_6^4 & 0 & \mu_6^6 \\
\end{pmatrix},
\]

(5.15)

and this chequered pattern is consistent with the form of Grand Mobility Matrix obtained from the implemented code introduced in Section 2.6. Solving for the equations of motion using the mobility matrix of a general L-shape gives,

\[
\begin{pmatrix}
\dot{x}(t) \\
\dot{y}(t) \\
\dot{z}(t) \\
\dot{q}_0(t) \\
\dot{q}_1(t) \\
\dot{q}_2(t) \\
\dot{q}_3(t)
\end{pmatrix} = \begin{pmatrix}
\frac{1}{2}G \left( \mu_1^3 - \mu_3^1 + \cos 2\theta(t) \left( \mu_3^3 + \mu_1^1 \right) + \sin 2\theta(t) \left( \mu_3^3 + \mu_1^1 \right) \right) \\
0 \\
\frac{1}{2}G \left( \mu_1^1 + \mu_3^3 + \cos 2\theta(t) \left( \mu_3^3 - \mu_1^1 \right) - \sin 2\theta(t) \left( \mu_3^3 + \mu_1^1 \right) \right) \\
\frac{1}{2}G \sin \left( \frac{\theta(t)}{2} \right) (\sin \theta(t)\mu_3^3 - \cos \theta(t)\mu_5^3) \\
0 \\
\frac{1}{2}G \cos \left( \frac{\theta(t)}{2} \right) (\cos \theta(t)\mu_3^3 - \sin \theta(t)\mu_5^3) \\
0
\end{pmatrix},
\]

(5.16)

in velocity and quaternion notation. The quaternions are expressed in terms of Euler angles as: \( q_0 = \cos(\theta(t)/2) \), \( q_1 = 0 \), \( q_2 = \sin(\theta(t)/2) \) and \( q_3 = 0 \), where \( \phi(t) = \phi_0 = 0 \) and \( \psi(t) = \psi_0 = 0 \). Next, solving for,

\[
\frac{d}{dt} \cos \left( \frac{\theta(t)}{2} \right) = \frac{1}{2}G \sin \left( \frac{\theta(t)}{2} \right) (\sin \theta(t)\mu_5^1 - \cos \theta(t)\mu_5^3),
\]

(5.17)
and simplifying the resulting expression for $\theta(t)$ by considering the $t \to \infty$ limit, the final orientation for a sedimenting L-shape is found to be:

$$\theta_f = 2 \arctan \left( -\frac{\mu_1}{\mu_3} - \sqrt{(\mu_3^2 + \mu_1^2)} \right)$$  \hspace{1cm} (5.18)$$

Substituting $\theta_f$ for $\theta(t)$ in the expression for $\dot{x}(t)$ and $\dot{z}(t)$ in Eq. (5.16), the angle of sedimentation in the long-time limit is found to be:

$$\tan \alpha = \frac{\mu_1^3 - \mu_3^3 + \cos 2\theta_f (\mu_3^3 + \mu_1^3) + \sin 2\theta_f (\mu_3^3 - \mu_1^3)}{\mu_1^3 + \mu_3^3 + \cos 2\theta_f (\mu_3^3 - \mu_1^3) - \sin 2\theta_f (\mu_3^3 + \mu_1^3)}$$  \hspace{1cm} (5.19)$$

These new expressions, found for the final orientation and angle of sedimentation, are plotted in Figure 5.2 using both mobility matrix coefficients obtained using RFT and the ones obtained for the GMM.

5.1.3 Numerical Results using the RPY Approximation

Figure 5.2 The steady-state sedimentation orientation and trajectory for an L-shape. (a) The time $t \to \infty$ angle of the L-shape with respect to the vertical $\theta$ and (b) the angle that the trajectory makes with respect to the vertical, $\alpha$, as a function of the length of the long leg $l_2$ (in terms of the RPY bead radius $a$ for a fixed length of $l_1 = 24a$ of the short leg.

First, the steady-state sedimentation of an L-shape was examined and compared to the predictions from RFT. That is, for time $t \to \infty$, the orientation of the L-shape with respect to the vertical, $\theta$, and the angle that the trajectory makes with respect to the vertical, $\alpha$, were evaluated and plotted in Figure 5.2. The green line in (a) and (b) is the angle found using Eqs. (5.10) and (5.11), respectively. Eqs. (5.18) and (5.19), evaluated using the mobility matrix found using RFT in Section 5.1.2 (red line) and using the Grand Mobility Matrix coefficients (orange
Finally, the blue dots in the figure show the orientation and angle of sedimentation found using the dynamics code for the GMM of each L-shape. It was found that using RFT to reproduce the mobility matrix of an L-shape resulted in a matrix of the same form as the GMM. However, it can be seen, in Figure 5.2, that the RFT mobility coefficients reproduced lead to an orientation and trajectory that is not in agreement with the results reproduced with the RPY algorithm. Furthermore, the discrepancies obtained in the figure above could be attributed to the approximations involved in calculating the GMM. For future work, this could be checked by substituting the RPY functions with higher order approximations when computing the GMM \[11\].

Note that, for the RPY results, $\theta \neq \theta_0$ and $\alpha \neq \alpha_0$ as the L-shape reorients toward a stable and unique sedimentation configuration that is dependent only on $l_1$ and $l_2$. Figure 5.2 shows $\theta$ and $\alpha$ as a function of $l_1/l_2$ for a fixed value of $l_1 = 24$. Only the L-shape with equal arm lengths ($l_1 = l_2$) sediments vertically ($\alpha = 0$) after an initial transient, and it reorients itself with $\theta = \pi/4$. All other values of the ratio $l_1/l_2 \neq 1$ lead to a finite value of $\alpha$.

Figure 5.3 The (a) steady-state sedimentation orientation and (b) sedimentation trajectory for an L-shape for different initial orientations, $\theta_0$, and for different leg length ratios, $l_2 : l_1$.

It is found, see Figure 5.3, that the orientation angle $\theta$ (and therefore $\alpha$) is independent of the initial orientation $\theta_0$ and that it appears to converge toward $\theta_s = 0.31\pi$ in the limit $l_1/l_2 \to 0$. This is a contradictory result, as in the rod limit $l_1/l_2 \to 0$, the orientation is expected be $\theta = \theta_0$, see Section 2.6.2. The next section will explore the reason behind this apparent lack of convergence.
5.1.4 Convergence to the Rod-Like Limit

Here, the ‘line’ variant of the L-shape, see Figure 5.1, is considered in order to study how a small perturbation on a rod affects its sedimentation. The $6 \times 6$ sub-block of the GMM, which covers translation and rotation, has the following shape for an object with three symmetry planes (i.e. a rod):

$$
\mu_{tr} = \begin{pmatrix}
\mu_1^1 & 0 & 0 & 0 & 0 & 0 \\
0 & \mu_2^2 & 0 & 0 & 0 & 0 \\
0 & 0 & \mu_3^3 & 0 & 0 & 0 \\
0 & 0 & 0 & \mu_4^4 & 0 & 0 \\
0 & 0 & 0 & 0 & \mu_5^5 & 0 \\
0 & 0 & 0 & 0 & 0 & \mu_6^6
\end{pmatrix},
$$

(5.20)

where all listed elements $\mu_i^j$ are nonzero. When a small perturbation is made to this object, which eliminates one of the symmetry planes, the shape of the tensor is changed. Let the perturbation be as follows. The main body of the almost rod is along the $z$-axis and there is a small perturbation at in the $x-z$ plane. For example, a single bead at the end of the rod is shifted out of register along the positive $x$-axis. Then the shape of the tensor becomes with a chequered pattern, like in Eq. (5.15), where couplings in the translational and rotational $3 \times 3$ sub-blocks, as well as couplings between translation and rotation are introduced. When only a gravitational force is acting on the perturbed rod, the translational and orientational dynamics decouple. That is, the rod reorients as it sediments, but the value of $\alpha$ does not impact $\theta$. The dynamics of $\theta$ are governed by the equation

$$
\dot{\theta} = G \left( \mu_3^3 \cos \theta - \mu_5^5 \sin \theta \right),
$$

(5.21)

where the dot denotes the derivative with respect to time and $\theta(t = 0) = \theta_0$. The steady-state solution is obtained by setting $\dot{\theta} = 0$ and reads

$$
\tan \theta_s = \frac{\mu_3^3}{\mu_5^5}.
$$

(5.22)

This value of $\theta_s$ is independent of initial angle, and can be shown to be stable against perturbations. This goes against the result for a sedimenting rod which sediments with an orientation that is equal to its initial orientation, and therefore dependent on the initial angle. The reason why the rod limit is not recovered is because the decoupled orientational dynamics persist for all perturbations and
the two coupling terms scale equally with the limit of the short leg, $l_1$, going to zero.

## 5.2 C-Shape Outside of Plane of Gravity

Here, we define a C-shape, parametrised by,

$$\mathbf{r}_c = (\cos \alpha, 0, -\sin \alpha).$$  \hspace{1cm} (5.23)

The angle $\alpha$ takes its values from the interval $[0, \alpha_0]$, where $\alpha_0$ determines how much a full circle the shape spans. Examples of such C-shapes are shown in Figure 5.4.

![Diagram of a C-shape made up of spheres for a C-shape with: $\alpha_0 = \pi/2$ (left), $\alpha_0 = \pi/3$ (centre), and $\alpha_0 = \pi$ (right).](image)

**Figure 5.4** Diagram of a C-shape made up of spheres for a C-shape with: $\alpha_0 = \pi/2$ (left), $\alpha_0 = \pi/3$ (centre), and $\alpha_0 = \pi$ (right).

The focus now will be on the sedimentation of a C-shape, as shown in Figure 5.4, with initial orientation such that it is at an angle to the plane of gravity. Consider a C-shape with an initial orientation determined by a rotation about its $x$-axis and a rotation about its $y$-axis (as defined in Figure 5.4), $\beta_x$ and $\beta_y$ respectively; note that when $\beta_x = 0$ and $\beta_y = 0$, the C-shape is within the $x-z$ plane. A general C-shape is found to have a mobility matrix of chequered form such as the one introduced for the L-Shape in Eq. (5.15). The sub-block of the mobility matrix with the translational-rotational coupling terms, called the twist matrix, for the C-shape is found to have 3 real eigenvalues; according to Krapf et al., this implies that the chiral motion becomes complicated and depends on initial conditions.
The quaternions expressed in terms of the angles, in this case, are
\[ q_0 = \cos \beta_x/2 \cos \beta_y/2, \quad q_1 = \sin \beta_x/2 \cos \beta_y/2, \quad q_2 = \cos \beta_x/2 \sin \beta_y/2, \quad \text{and} \quad q_3 = \sin \beta_x/2 \sin \beta_y/2. \]
Using the mobility matrix, in Eq. (5.15), and considering the new expressions for the quaternions, the resulting equations of motion are less straightforward as those found in Eq. (5.16). Therefore, only trajectories using GMM for the C-shape and the dynamics code are studied here.

Figure 5.5  Sedimentation trajectory of a C-shape with \( \alpha_0 = \pi/2 \) with initial orientation \( \beta_x = \pi/5 \) and \( \beta_y = 2\pi/5 \). (a) show the 3-D view of the trajectory and (b) shows the view from above of the x-y plane and the inner.

Figure 5.5 shows the sedimentation trajectory for a C-shape with \( \alpha_0 = \pi/2 \) and initial orientation \( \beta_x = \pi/5 \) and \( \beta_y = 2\pi/5 \). It is found that the trajectory is chiral and that its handedness depends on the initial angle \( \beta_x \); for \( \beta_x \in (0, \pi) \) it is left-handed and for \( \beta_x \in (\pi, 2\pi) \) it is right-handed. The chiral trajectory, drawn by the C-shape as it sediments, looks like a Spirograph figure. This shape is defined by two main radii: an inner one (orange dashed circle) and an outer one (green dashed circle). To further analyse the chiral trajectories for the C-shape, and their dependence on the initial orientation of the object, the initial orientations \( \beta_x \) and \( \beta_y \) were varied in the range from 0 to 2\( \pi \) and the value of the inner radius of the trajectory for each set of parameters was plotted in the state diagram in Figure 5.6.

In the darker blue areas in Figure 5.6, there is no inner (or outer) radius for the trajectories as for these initial orientations the non-chiral trajectories, where the C-shape reaches a steady orientation and angle of sedimentation, are recovered. It can be seen that, whilst the inner radius of the trajectory increases towards the centre of the ‘islands’, the outer radius decreases. At the centre of the ‘islands’, it is found that the inner and outer radii of the trajectory coincide and a superhelical trajectory is recovered.
Figure 5.6  State diagram for a C-shape with $\alpha_0 = \pi/2$. For a given combination of $\beta_x$ and $\beta_y$. The colour indicates: (a) the value of the inner radius of the chiral trajectory in a steady state or at long times and (b) the value of the outer radius of the chiral trajectory in a steady state or at long times.

Figure 5.7  State diagram for an L-shape with $l_1 = 24$ and $l_2 = 62$. For a given combination of $\beta_x$ and $\beta_y$. The colour indicates the value of the inner radius of the chiral trajectory in a steady state or at long times.

Figure 5.7 instead, shows the state diagram for an L-shape with $l_1 = 24$ and $l_2 = 62$ where the value of the inner radius of the trajectory is plotted for each set of parameters $\beta_x$ and $\beta_y$ in the range from 0 to $2\pi$. It can be seen that the state diagrams for the L- and C-Shapes show strong similarities, and both are characterised by the presence of islands.
5.3 Concluding remarks

This Chapter looked at the sedimentation of two particles similar to each other, the L-Shape and the C-Shape. First an L-shape sedimenting parallel to the plane of gravity was studied using RFT and the GMM. Whilst it is found that RFT recovers a shape of the mobility matrix that is in agreement with the Grand Mobility Matrix, RFT fails to predict both the final orientation and angle of sedimentation of the L-shape. This can be seen in Figure 5.2. In conclusion, RFT fails to predict the dynamics for an L-shape and a method which includes hydrodynamic interactions is more useful to try and capture the reality of the dynamics for an L-shape.

Examining the issue further, it is found that an L-shape, when sedimenting, reorients itself to a preferred orientation that depends on the ratio of the two legs \((l_1 : l_2)\) and is independent of its initial orientation, \(\theta_0\), see Figure 5.3. Even in the rod-like limit, where the ratio of \(l_1/l_2 \to 0\), no dependence on the initial orientation is recovered, which is in contrast to the behaviour of a straight rod sedimenting. This apparent inconsistency can be explained by looking at the mobility matrix which shows that even the slightest perturbation on the rod leads to the decoupled orientational dynamics.

For this thesis, no in-depth analysis was done to study the behaviour of a C-shape approaching the rod-limit. However, when looking at the GMM of a C-shape with an almost rod-like shape, the matrix presents itself with off-diagonal coupling coefficients. Given the conclusions, reached in Section 5.1.4, the presence of these off-diagonal elements implies that the rod behaviour is not recovered for a C-shape in the rod-limit either. For future work, it would be of interest to further analyse the behaviour of the sedimentation of an L- and C-shape in the rod-like limit, using higher order approximations of the GMM.

Next, the sedimentation of a C-shape that is at an angle to the plane of gravity was examined. As the C-shape has a twist matrix that has three real eigenvalues, it is expected for it to sediment with a complicated chiral trajectory, which depends on the initial conditions [2]. It is found that the C-shape does indeed sediment with a chiral trajectory that is not as simple as a superhelical trajectory. The properties of this trajectory, including its chirality, depend on the initial conditions imposed on the system. This dependence can be summarised in Figure 5.6. It is then found, in Figure 5.7, that an L-Shape possesses a state diagram with strong
similarities to that of a C-Shape.

Having shown that non-chiral asymmetric particles can also sediment with a chiral trajectory given the right set of initial conditions, the next Chapter will look at the sedimentation of a Möbius strip, bringing the focus back onto chiral particles.
Chapter 6

Möbius Strip Sedimentation

In this Chapter, the focus will shift back to chiral particles, namely the Möbius strip. However, before moving on to the Möbius strip, the mobility matrix of a stadium-shaped particle, shown in Figure 6.1, is examined. The stadium can be considered a simpler, non-chiral version of the Möbius strip. Looping shapes made with a thin band, such as the stadium and Möbius strip, can be described by using the recently developed Slender Ribbon Theory [4, 62], introduced in Chapter 2, from which an approximation of the shape’s mobility matrix can be calculated. Koens and Lauga derived expressions for the mobility matrix coefficients for a stadium-shaped particle [4], as well as other shapes. Their results will be compared to the GMM coefficients, obtained using the RPY bead setup, for a stadium in the following section.

6.1 Stadium

A stadium is a particle of shape shown in Figure 6.1 where, in this parametrisation, the angle $\alpha$ determines how the ribbon sits relative to the base; when $\alpha = 0$ the ribbon lies completely flat in the plane like a disk, and when $\alpha = \pi/2$ the ribbon sits perpendicular to it like a cylinder. Using SRT, the expressions relating the forces and torques to the velocity and angular velocity found by Koens and
Lauga \cite{4} are:

\[
F_x = -\frac{8\pi (6L_3^2 - 2L_3(2L + 13) + 6L - (L_2 - 7) \cos 2\alpha + 25)}{\beta_2} U e_x + \frac{16(L_3 - 3) \sin 2\alpha}{\beta_2} \Omega e_y, \quad (6.1)
\]

\[
F_y = -\frac{8\pi (6L_3^2 - 2L_3(2L + 13) + 6L - (L_2 - 7) \cos 2\alpha + 25)}{\beta_2} U e_y + \frac{16(L_3 - 3) \sin 2\alpha}{\beta_2} \Omega e_x, \quad (6.2)
\]

\[
F_z = \frac{8\pi \left( \cos 2\alpha + 2L_3 - 5 \right)}{3 \cos 2\alpha - 2L_3(2 - L_3) - 3} U e_z, \quad (6.3)
\]

\[
T_x = -\frac{16(2L_3^2 - L_3(4L + 5) + 2(4L - 1) + (L_3 - 2) \cos 2\alpha)}{\pi \beta_2} \Omega e_x + \frac{16(L_3 - 3) \sin 2\alpha}{\beta_2} U e_y, \quad (6.4)
\]

\[
T_y = -\frac{16(2L_3^2 - L_3(4L + 5) + 2(4L - 1) + (L_3 - 2) \cos 2\alpha)}{\pi \beta_2} \Omega e_y + \frac{16(L_3 - 3) \sin 2\alpha}{\beta_2} U e_x, \quad (6.5)
\]

\[
T_z = \frac{4}{\pi(L_3 - 2)} \Omega e_z. \quad (6.6)
\]

Putting the coefficients of the above equations into a resistance matrix and
inverting it results in a mobility matrix of the form:

\[ M = \begin{pmatrix}
\mu_1^1 & 0 & 0 & 0 & \mu_5^1 & 0 \\
0 & \mu_2^2 & 0 & \mu_4^2 & 0 & 0 \\
0 & 0 & \mu_3^3 & 0 & 0 & 0 \\
0 & \mu_2^4 & 0 & \mu_4^4 & 0 & 0 \\
\mu_5^5 & 0 & 0 & 0 & \mu_5^5 & 0 \\
0 & 0 & 0 & 0 & 0 & \mu_6^6
\end{pmatrix} \tag{6.7} \]

where a diagonal matrix is recovered for the case \( \alpha = \pi/2 \). This in agreement with the shape of matrix for a slender cylinder evaluated by Johnson and Wu \[124\].

The GMM obtained for a stadium, however, is of chequered form like the one for the L-shape and C-shape, see Eq. (5.15). The equations derived by Koen and Lauga do not seem to account for the cross-coupling terms between \( x \) and \( z \), and \( y \) and \( z \). Another inconsistency found between the SRT mobility matrix and the GMM is in the order of magnitudes of the coefficients. For SRT, the torque coefficients in the diagonal of the \( 3 \times 3 \) bottom-right sub-block of the mobility matrix are found to be of one order of magnitude larger than the translational coefficients in the diagonal of the \( 3 \times 3 \) top-left sub-block of the mobility matrix, whilst for the GMM, the torque coefficients are of four orders of magnitude smaller than the translational ones. The cross-coupling terms, instead, are found to be, with respect to the corresponding translational coefficients, of one order of magnitude smaller for SRT and of six to eight orders of magnitude smaller in the GMM. Eqs. (6.8) and (6.9) show an example of \( 6 \times 6 \) mobility matrix obtained for a stadium with \( \alpha = \pi/4 \). Note that the coefficients for each matrix were scaled with respect to the given matrix’ \( \mu_1^1 \) term.

\[ M_{\text{SRT}} =
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0.25112176 & 0 \\
0 & 1 & 0 & 0.25112176 & 0 & 0 \\
0 & 0 & 0.80066284 & 0 & 0 & 0 \\
0 & 0.25112176 & 0 & 11.16045632 & 0 & 0 \\
0.25112176 & 0 & 0 & 0 & 11.16045632 & 0 \\
0 & 0 & 0 & 0 & 0 & 10.03601937
\end{pmatrix} \tag{6.8} \]
\[ \mathcal{M}_{\text{GMM}} = \left( \begin{array}{cccccc}
1 & 0 & 1.14 \times 10^{-6} & 0 & -3 \times 10^{-8} & 0 \\
0 & 1 & 0 & -3 \times 10^{-8} & 0 & 6 \times 10^{-8} \\
1.14 \times 10^{-6} & 0 & 0.77782040 & 0 & 6 \times 10^{-8} & 0 \\
0 & -3 \times 10^{-8} & 0 & 5.0597 \times 10^{-4} & 0 & -0.02 \times 10^{-8} \\
-3 \times 10^{-8} & 0 & 6 \times 10^{-8} & 0 & 5.0597 \times 10^{-4} & 0 \\
0 & 6 \times 10^{-8} & 0 & -0.02 \times 10^{-8} & 0 & 4.3507 \times 10^{-4} \\
\end{array} \right) \]

This disagreement between the two results could be attributed to the fact that, in SRT, an infinitesimally thin ribbon (its thickness is \( \ll \) than its width, which in turn is \( \ll \) than its length) is considered, while the spheres, in the RPY-bead model, give the stadium a non-zero thickness. To test this assumption, the mobility matrix of a stadium with a radius as big as computationally possible, whilst maintaining reasonable ratios between the three lengths of the shape, was evaluated. For this matrix, the chequered shape persists and the SRT result is not recovered. To further reach the thin ribbon limit, it is possible a larger bead-model stadium needs to be drawn, however, it is not currently possible due to the computational limitation that arises from a limit in the computer’s memory. The more likely cause of the discrepancy, however, is the RPY method’s inclusion of the hydrodynamic couplings between the parts of the stadium.

Nonetheless, the dependence of the mobility matrix coefficients on the geometric parameter, \( \alpha \), of the stadium are compared for the SRT and GMM results.

The plots in Figures 6.2 and 6.3 show the dependence on the parametric angle \( \alpha \) of the translational and rotational mobility coefficients of stadium calculated through SRT (blue dots) and from the GMM (orange +).

In this section, results for a stadium obtained from Slender Ribbon Theory and from the GMM evaluated using the RPY-bead method were compared. Here, no good quantitative or qualitative agreement was found. Further analysis should be done to better understand whether this disagreement stems from a differing definition of the stadium shaped particle. The following sections will shift the focus to the sedimentation of a Möbius strip.
Figure 6.2  Plot showing the dependence of the translational mobility coefficients of a stadium on the parametric angle $\alpha$. The comparison between the translational coefficients obtained using SRT (blue dots) and GMM (orange +) is shown for: (a) the $M[1,1]$ coefficient and (b) the $M[3,3]$ coefficient. Here all coefficients were normalised with respect to the $M[1,1]$ of a stadium with $\alpha = \pi/2$ obtained for the given theory.

Figure 6.3  Plot showing the dependence of the rotational mobility coefficients of a stadium on the parametric angle $\alpha$. The comparison between the rotational coefficients obtained using SRT (blue dots) and GMM (orange +) is shown for: (a) the $M[4,4]$ coefficient and (b) the $M[6,6]$ coefficient. Here all coefficients were normalised with respect to the $M[4,4]$ of a stadium with $\alpha = \pi/2$ obtained for the given theory.

6.2  The Möbius Strip

A Möbius strip parametrised by:

$$\mathbf{r}_m = \left( R + \frac{w}{2} \cos \frac{\chi}{2} \right) \cos \chi, \left( R + \frac{w}{2} \cos \frac{\chi}{2} \right) \sin \chi, \frac{w}{2} \sin \frac{\chi}{2} \right),$$  \hspace{1cm} (6.10)$$

where $R$ is the radius of the centre circle of the strip, $w$ is the width, and $\chi$ is a
parameter which runs from 0 to $2\pi$.

Figure 6.4  *Diagram of a Möbius strip, made up of spheres. Here the strip has $R = 30$ and $w = 14$. The Möbius lies in the $x$-$y$ plane, with its twisted part in the $x$-direction.*

The Möbius strip is made up of spheres and shown in Figure 6.4. A Möbius strip with a centre circle radius of 30 and band width of 14 (comprising of 7 beads) was constructed and its Grand Mobility Matrix was evaluated. The dynamics for the sedimentation of this given Möbius strip were then calculated. As expected, the resulting sedimentation trajectories are chiral, where the chirality depends on the Möbius strip’s chirality; a left-handed Möbius strip has a right-handed trajectory and a left-handed strip has a right-handed trajectory, see numbered peaks in Figure 6.5.

Figure 6.5  *Plot showing the view from above ($\tilde{X}$-$\tilde{Y}$ plane) of the sedimentation of: (a) a right-handed Möbius strip and (b) a left-handed Möbius strip. For (a) the sedimentation is left-handed, and in (b) the sedimentation is right-handed. The numbers indicate the order that the periodic trajectory follows.*
Much like for the helix, it is found that the motion of the sedimenting Möbius depends on the initial conditions of its orientation, namely of the Euler angles $\theta$ and $\psi$. The dynamics for various initial conditions of $\theta_0$ and $\psi_0$, in the range $\theta, \psi \in [0, 2\pi]$ were run and, by looking at the radius of the helical-like trajectory with respect to time, different types of trajectories were identified.

## 6.3 Types of Trajectory

### 6.3.1 Case 1: 2 Disks

In the first scenario, which gives a rosette-like shape when viewed from above (in the $x$-$y$ plane), there are four main radii that can be defined. These can be seen as a superposition of two concentric disks: $r_{\text{in}}^1$, $r_{\text{out}}^1$, $r_{\text{in}}^2$, and $r_{\text{out}}^2$. Within this scenario, there are then three distinct sub-cases which can be identified:

- $r_{\text{out}}^1 > r_{\text{out}}^2 > r_{\text{in}}^2 > r_{\text{in}}^1$: Here, the second disk is inside the first disk. The evolution of the radius with respect to time and the view from above of this trajectory are plotted in Figure 6.6(a) and (b) respectively.

![Figure 6.6](image)

**Figure 6.6** Plot showing an example of trajectory with 2 disks of a Möbius strip sedimenting, (a) is the evolution of the radius of the chiral trajectory with time, and (b) is the $x$-$y$ plane view of the trajectory. Four main radii, from two concentric disks are found. The outer, $r_{\text{out}}^1$ (orange), and inner, $r_{\text{in}}^1$ (green) radius of the first disk; and the outer, $r_{\text{out}}^2$ (red), and inner, $r_{\text{in}}^2$ (purple) radius of a second disk that is within the first disk.

- $r_{\text{out}}^1 > r_{\text{out}}^2 > r_{\text{in}}^1 > r_{\text{out}}^2$: Trajectories within this scenario have a radius with respect to time and a view from above ($x - y$) of the trajectory as shown in Figure 6.7(a) and (b) respectively.

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Figure 6.7  Plot showing a second type of trajectory with 
two disks of a Möbius strip sedimenting, (a) is the evolution of the radius of the chiral trajectory with time, and (b) is the x-y plane view of the trajectory. Four main radii, from two concentric disks are found. The outer, $r_{1\text{out}}$ (orange), and inner, $r_{1\text{in}}$ (green) radius of the first disk; and the outer, $r_{2\text{out}}$ (red), and inner, $r_{2\text{in}}$ (purple) radius of the second disk, where $r_{1\text{out}} > r_{2\text{out}} > r_{1\text{in}} > r_{2\text{in}}$.

• $r_{2\text{out}} > r_{1\text{out}} > r_{2\text{in}} > r_{1\text{in}}$: Finally, trajectories in this third sub-scenario have a radius and a view from above ($x - y$) as seen in Figure 6.8(a) and (b) respectively.

Figure 6.8  Plot showing a third type of trajectory with 2 disks of a Möbius strip sedimenting, (a) is the evolution of the radius of the chiral trajectory with time, and (b) is the x-y plane view of the trajectory. Four main radii, from two concentric disks are found. The outer, $r_{1\text{out}}$ (orange), and inner, $r_{1\text{in}}$ (green) radius of the first disk; and the outer, $r_{2\text{out}}$ (red), and inner, $r_{2\text{in}}$ (purple) radius of the second disk, where $r_{2\text{out}} > r_{1\text{out}} > r_{2\text{in}} > r_{1\text{in}}$. 

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6.3.2 Case 2: Oscillations

In this second case the radius’ evolution with time is a constant oscillation and, therefore, two main radii are identified: an outer one $r_{\text{out}}$ and an inner one $r_{\text{in}}$. Trajectories within this scenario have an evolution of radius with respect to time and a view from above ($x$-$y$) of the trajectory as shown in Figure 6.9.

Figure 6.9 Plot showing the oscillation type of trajectory, (a) is the evolution of the radius of the chiral trajectory with time, and (b) is the $x$-$y$ plane view of the trajectory. Two main radii are identified in this case: $r_{\text{out}}$ (orange) and $r_{\text{in}}$ (green).

6.3.3 Case 3: Tooth and Down Tooth

In this case three main radii are identified: an outer, $r_{\text{out}}$, and inner, $r_{\text{in}}$ one as well as a middle one, $r_{\text{mid}}$, which is closer to the value of $r_{\text{in}}$ for the ‘down tooth’ case and closer to $r_{\text{out}}$ for the ‘tooth’ case. The plots of the radius with respect to time and of the $x$-$y$ view of the trajectory are shown in Figures 6.10 and 6.11 for the ‘tooth’ and ‘down tooth’ case, respectively.

6.3.4 Case 4: Unstable

So far, the different types of trajectories introduced have a stable, repetitive behaviour for the radius of the trajectory. For this final case, however, the trajectories show an unstable and ‘chaotic’ trajectory, and no relevant constant radii are individuated. An example of such trajectory is shown in Figure 6.12. Note that not all ‘unstable’ scenarios have a behaviour as shown in the figure.

Additionally, to show the instability of the trajectory for this case, the power
Figure 6.10 Plots of (a) the radius vs. $t$ and (b) the $x$-$y$ plane view of the trajectory of Möbius strip sedimenting in the ‘tooth’ scenario. Three main radii are identified: an outer, $r_{\text{out}}$ (orange), and inner $r_{\text{in}}$ (green) one, and a middle one, $r_{\text{mid}}$ (red).

Figure 6.11 Plots of (a) the radius vs. $t$ and (b) the $x$-$y$ plane view of the trajectory of Möbius strip sedimenting in the ‘down tooth’ scenario. Three main radii are identified: an outer, $r_{\text{out}}$ (orange), and inner $r_{\text{in}}$ (green) one, and a middle one, $r_{\text{mid}}$ (red).

Figure 6.12 Plots of (a) the radius vs. $t$ and (b) the $x$-$y$ plane view of the trajectory of Möbius strip sedimenting in the ‘unstable’ scenario. Here no main radii are found due to the ‘chaotic’ trajectory.
spectrum of the radius of the trajectory, $r(t)$, is plotted in Figure 6.13. The many frequencies in the power spectrum further illustrates the presence of many modes in the trajectory.

![Figure 6.13](image.png)

**Figure 6.13**  *Power spectrum of the radius of the trajectory, $r(t)$ corresponding to the trajectory in Figure 6.12.*

### 6.3.5 Contour Plot

The motion of the sedimenting Möbius depends on the initial conditions of its orientation, $\theta_0$ and $\psi_0$, and in this Section, so far, multiple distinct types of sedimentation trajectory were described. Figure 6.14 shows a representative example of a Möbius with $R = 30$ and $w = 14$ to show the dependence of the type of spatial trajectory on $\theta_0$ and $\psi_0$.

Note, in the contour plot, the presence of ‘islands’, a feature that also appeared in the contour plot for a sedimenting C-shape, in Figure 5.6. Further analysis on the islands will be done in a later section.

Whilst the types of spatial trajectory so far identified have distinct behaviours, they all have an innermost and an outermost radius. The contour plots showing the values of these two radii for the different sets of initial conditions are shown in Figure 6.15 where, for both (a) and (b), the radius was divided by the length-scale 30 (the radius of the Möbius strip) and its log was taken to better show the dependence on the initial conditions. Here approximate values for the radii of the ‘Unstable’ trajectories were used.

Similar patterns appear on the contour plots for both the inner most radius
Figure 6.14  State diagram for a Möbius strip with \( R = 30 \) and \( w = 14 \) for a given combination of \( \theta_0 \) and \( \psi_0 \). The colour indicates the type of spatial trajectory.

Figure 6.15  State diagram for a Möbius strip with \( R = 30 \) and \( w = 14 \) for a given combination of \( \theta_0 \) and \( \psi_0 \). The colour indicates the value of: (a) the inner radius, and (b) the outer radius of the chiral trajectory in a steady state or at long times. Here, for both (a) and (b), the radius was divided by the length-scale 30 (the radius of the Möbius strip) and its log was taken to better show the dependence on the initial conditions.

and outermost radius, in Figure 6.15(a) and (b) respectively, and these are in agreement with the state diagram for the different types of trajectory. This shows that the type of spatial trajectory can be inferred by looking at the values of the radii of the chiral sedimentation. Having studied the spatial dynamics of a sedimenting Möbius strip, the orientational dynamics will now be examined.

Given the distinct nature of these contour plots, further analysis was done by
looking at the Euler angles and their Fourier Transforms.

6.4 Euler Angles

The orientational dynamics of a sedimenting Möbius strip are now studied. For most initial conditions, the three Euler angles \( \theta, \phi \) and \( \psi \) are found to have an oscillatory behaviour, so to better analyse and distinguish the different behaviours, their Fourier Transforms were calculated. The frequency of the main peak in the FFT log-log plot was taken and the contour plot for the different initial conditions, \( \theta_0 \) and \( \psi_0 \), was plotted and shown in Figure 6.16(a), (b) and (c) for the angles \( \theta, \phi \) and \( \psi \) respectively; where all the FFTs calculated are real.

![Contour plots](image)

**Figure 6.16** State diagram for a Möbius strip with \( R = 30 \) and \( w = 14 \) for a given combination of \( \theta_0 \) and \( \psi_0 \). The colour indicates the value of the main FFT peak of: (a) \( \theta(t) \), (b) \( \phi(t) \), and (c) \( \psi(t) \).

It can be seen that similar contour patterns, to the ones obtained when looking at the radii, are recovered when looking at the Euler angles’ behaviour. Additionally, the dependence on \( \theta_0 \) and \( \psi_0 \) of \( \theta(t) \) and \( \psi(t) \) appear to be the same.
6.5 The Islands

One of the main features of the contour plot is the presence of two types of islands. In particular, the islands dominated by the oscillatory behaviour of the radius, light blue islands in Figure 6.14, are found to be surrounded by a ‘wall’ of diverging radius (effectively a straight trajectory). A close-up of such an island is shown in Figure 6.17, where the colour indicates the value of $\log(r_{in}/30)$, and the values of the radius along the black lines are plotted in Figures 6.18 and 6.19.

![Figure 6.17](image)

**Figure 6.17** State diagram zooming in on an island for a Möbius strip with $R = 30$ and $w = 14$ for a given combination of $\theta_0 \in [0.4\pi, \pi]$ and $\psi_0 \in [0, 1.1\pi]$. The colour indicates the value of $\log r_{in}/30$. The values of the radius on the black lines, one at constant $\psi_0 = 0.9\pi$ and one at $\theta_0 = 0.7\pi$, are then plotted in Figures 6.18(a) and 6.19(a).

The plots of the value of the inner radius of the trajectory at constant $\psi_0 = 0.9\pi$ and $\theta_0 = 0.7\pi$ are shown in Figures 6.18(a) and 6.19(a). Here, it can be seen that there is a critical value $\theta_0^{(cr)}$ (in Figure 6.18(a)) and $\psi_0^{(cr)}$ (in Figure 6.19(a)) for which the radius diverges. In both of these plots, the behaviour of $r_{in}$, on the left of the critical value $\theta_0^{(cr)}$ (or $\psi_0^{(cr)}$), follows a clear diverging curve.

A power law of the form $\beta(\theta_0^{(cr)} - \theta_0)^\alpha$ ($\psi_0$ for constant $\theta_0 = 0.7\pi$) is assumed as the divergence law on the left side of Figure 6.18(a) (Figure 6.19(a)). To find the power law exponent ($\alpha$), the log-log plots of $r_{in}$ vs. $\theta_0^{(cr)} - \theta_0$ ($\psi_0^{(cr)} - \psi_0$) are shown in Figure 6.18(b) (Figure 6.19(b)). The slope of the lines in the log-log
Figure 6.18  Plots showing the divergence of the radius of the chiral trajectory at $\psi_0 = 0.9\pi$ for $\theta_0 \in [0.79\pi, 0.81\pi]$. (a) shows the plot of $r_{in}$ vs. $\theta_0$ and (b) is the log-log plot of $r_{in}$ vs. $\theta_0^{(cr)} - \theta_0$. The slope of (b) gives the exponent of the power law of the divergence on the left of the critical values in (a).

Figure 6.19  Plots showing the divergence of the radius of the chiral trajectory at $\theta_0 = 0.7\pi$ for $\psi_0 \in [0.93\pi, 0.97\pi]$. (a) shows the plot of $r_{in}$ vs. $\psi_0$ and (b) is the log-log plot of $r_{in}$ vs. $\psi_0^{(cr)} - \psi_0$. The slope of (b) gives the exponent of the power law of the divergence on the left of the critical values in (a).

gives $-\alpha$. From Figures 6.18(b) and 6.19(b), it is found that the power law which fits the diverging curves on inside of the wall is $x^{-1}$. The curves heading towards the critical value from outside the islands, instead, follow a less clear divergence law. It is likely that these divergences imply that the trajectory at the boundary of the islands is straight.
6.6 Concluding Remarks

In the first section of this chapter, the mobility coefficients of stadium shaped particle were calculated using the RPY-bead method and compared to results found using Slender Ribbon Theory [4]. Whilst some qualitative agreement is found in the dependence of mobility coefficients on the parametric angle $\alpha$, see Figures 6.2 and 6.3, the two methods appear to mostly disagree both qualitatively and quantitatively. The nature of the disagreement is unclear so far and further analysis is needed. Though a likely cause is the inclusion of the hydrodynamics couplings in the RPY method, which SRT does not consider.

The following sections, instead, focused on the sedimentation of another chiral particle, the Möbius strip. As expected, the Möbius strip, when sedimenting, performs a chiral trajectory with an opposite handedness to the handedness of the strip itself. Additionally, the properties of the chiral trajectory depend on the initial conditions imposed on the Euler angles $\theta$ and $\psi$. The state diagrams for a given combination of $\theta_0$ and $\psi_0$, in Figures 6.14-6.16, show a similar pattern, which includes the presence of so-called islands.

Further analysis showed that some of the islands are surrounded by a wall of diverging radius. A divergence that follows the $x^{-1}$ power law is found when approaching the wall from inside the island. No clear divergence law was found, however, when approaching the wall from outside the island.

For future work, it would be interesting to find expressions to describe the radius and pitch of the sedimentation trajectory of a Möbius strip, as was done for the sedimenting helix in Chapter 3.

So far, in this thesis, the dynamics of the sedimentation of various shapes of particles was examined using RFT and the RPY-bead method introduced in Chapter 2. The following chapter, however, will employ RFT to study the dynamics of a rigid helix in a simple shear flow.
Chapter 7

A Rigid Helix in a Shear Flow

The previous chapters focused on the dynamics of particles sedimenting due to gravity. Understanding the connection between the shape’s properties and the chiral trajectory could allow chiral sedimentation to be used as a tool to identify objects at the microscopic scale, such as colloidal particles and cells [2]. However, of great interest, is also the dynamics of particles in a shear flow. For example, the motion of a single particle in a simple shear flow would improve the understanding of suspension hydrodynamics [125], and it plays roles in other industrial processes, such as paper-making [126].

For rotationally symmetric ellipsoids at low Reynolds number and in the absence of Brownian motion, the trajectories make closed orbits, known as Jeffery Orbits [127], with analytic solutions that depend only on the particle’s aspect ratio and its orientation with respect to the gradient axis. Helical particles, in addition to performing Jeffery-like orbits, experience a net drift [12, 14, 21], in the direction perpendicular to the plane of shear, with a sign dependent on the chirality. The underlying physics of this drift, which is at the origin of swimming bacteria assuming a particular orientation with respect to an external flow (rheotaxis) [128], has been adopted to use shear flows in order to separate chiral objects [11, 13–15, 63, 129–131].

The behaviour of fibres and other particles in shear flows plays an important role in a wide range of commercially important processes. For example, Lundell _et al._ [126], have looked at the fluid dynamics involved in paper-making, where shear flow plays a role in the forming process. Wang _et al._ [16], instead, studied the self-diffusion, induced by shear, of curved fibres suspended in an incompressible
Newtonian fluid. Fibres with certain curvatures, including those with helical shapes, appear in multiple contexts, such as DNA, which is a double helix and always right-handed; the helically shaped bacteria (*Leptospira biflexa* [28]); and rigid helical screws [13]. And, more specifically, there have been multiple studies on the dynamics of a helix in a shear flow. For example, Kim and Rae [11] investigated the motion of screw-sensed particles in a shear flow, where they calculated the forces and torque using SBT. Here they found that the fundamental component of the motion is a rotation of the particle along the shear flow. Later, Makino and Doi [12], computationally simulated the motion of helices in a shear flow. They found that these drift in a direction perpendicular to the plane of shear, with the sign determined by the particle’s chirality as expected. The drift experienced by helices in a shear flow has been examined in considerable detail theoretically [11, 15, 63, 132] and experimentally [13, 14, 129]. In experiment, Marcos et al. [14], have shown that a micro-scale shear can quickly separates chiral objects with high efficiency at low Reynolds number, since the helix experiences a drift in two opposite directions depending on its chirality. Furthermore, recent theoretical work [132] sees the derivation a generalised version of the Jeffery equations for the angular dynamics of a helicoidal object in a shear flow, where a new constant from the chirality of the object is included.

In this chapter, the focus will be on a rigid helix in a simple shear flow, where the forces and torques are approximated using RFT. Here the drag forces and torques, acting on a helix, calculated in Chapter 3, expressed in Eqs. (3.8)-(3.13), are used. Expressions for the forces and torques due to the shear are calculated in the following section.

### 7.1 Forces and Torques due to Shear

In this section, the forces and torques acting on a helix in a shear flow are calculated. Consider a shear flow, restricted to the $\{X, Y\}$ plane as in Figure 7.1 moving in the $X$ direction with a shear rate $\dot{\gamma}$ so that the shear velocity in the lab frame is given by

$$V_s^{lab} = \dot{\gamma} y_0 \hat{X}.$$  \hspace{1cm} (7.1)

The force and torque due to the shear flow are then calculated, following a method similar to the one used in finding the components of the drag force and torque.
Figure 7.1  Diagram of a helix with orientation $\theta_0 = \pi/2$ and $\phi_0 = 0$ in a shear flow restricted to the $\{X,Y\}$ plane.

acting on a body (Chapter 2.4). First, the shear velocity is transformed from the lab frame to the body frame, using the rotation matrix $D$ in Eq. (2.9), and is found to be

$$V^{bf}_s = (A_1 Y \dot{\gamma}, A_2 Y \dot{\gamma}, A_3 Y \dot{\gamma}),$$

(7.2)

where

$$Y = y_0 + C_1 R \cos \alpha + C_2 R \sin \alpha + C_3 R \frac{\lambda}{2\pi} \alpha,$$

(7.3)

represents a point on the helix in the lab frame in the Y-direction and,

$$A_1 = \cos \theta \cos \phi \cos \psi - \sin \phi \sin \psi,$$

(7.4)

$$A_2 = -(\cos \theta \cos \phi \sin \psi + \sin \phi \cos \psi),$$

(7.5)

$$A_3 = \sin \theta \cos \phi,$$

(7.6)

$$C_1 = \cos \theta \sin \phi \cos \psi + \cos \phi \sin \psi,$$

(7.7)

$$C_2 = -\cos \theta \sin \phi \sin \psi + \cos \phi \cos \psi,$$

(7.8)

$$C_3 = \sin \theta \sin \phi.$$

(7.9)

The shear force and torque are then calculated by performing the following integrations,
\[
\mathbf{F}_s = \int \mathbf{dF}_s ds = \int \left[ K \parallel (\mathbf{V}_s \cdot \mathbf{t}) \mathbf{t} + K \perp (\mathbf{V}_s - (\mathbf{V}_s \cdot \mathbf{t}) \mathbf{t}) \right] ds, \quad (7.10)
\]
\[
\mathbf{T}_s = \int \mathbf{r}_h \times \mathbf{dF} ds, \quad (7.11)
\]

where \( ds = \lambda / 2\pi \sec \chi d\alpha \) and \( \mathbf{t} = (\sin \chi \sin \alpha, \sin \chi \cos \alpha, \cos \chi) \) as defined in Eq. (3.5); and the integrals are performed over the range \( \alpha \in [-\pi N + \alpha_0, \pi N - \alpha_0] \). The integrals are performed with the aid of Mathematica \cite{133} and the final expressions for the three components of the force and torque due to the shear are then given by,

\[
F_{s1}^1 = \frac{1}{24\pi} \left[ 12A_1 \gamma \left( 2\pi x_2 - C_1 \Delta_2 \tan \chi \right) \right. \\
\left. - (\gamma - 1) \sin \chi \cos \chi \left( 3 \tan \chi \left( (1 + \Delta_1)(4\pi A_1 x_2 - 2A_3 C_2) \\
+ A_2 C_3 \right) - 2 A_2 C_3 \sin^2 \alpha_0 + 12 A_3 C_3 (\Delta_2 + (-1)^N \cos \alpha_0) \right. \\
\left. - 4 \Delta_2 (A_1 C_1 - A_2 C_2) \sin \alpha_0 \tan^2 \chi \right) \right], \quad (7.12)
\]
\[
F_{s2}^2 = \frac{1}{24\pi} \left[ 12A_2 \gamma \left( 2\pi x_2 - C_1 \Delta_2 \tan \chi \right) \right. \\
\left. + (\gamma - 1) \sin \chi \left( 6 A_3 C_1 \sin \chi (\Delta_1 - 1) + 4\pi \Delta_2 A_3 x_2 \right. \\
\left. - \sin \chi \left( 3 A_1 C_3 (\Delta_1 + \cos \alpha_0) - 12\pi A_2 x_2 (\Delta_1 - 1) \right. \\
\left. - 4\Delta_2 \tan \chi (A_2 C_1 (2 + \cos^2 \alpha_0) - A_1 C_2 \sin^2 \alpha_0) \right) \right) \right], \quad (7.13)
\]
\[
F_{s3}^3 = \frac{1}{4\pi} \left[ 2A_3 \gamma \left( 2\pi x_2 - C_1 \Delta_2 \tan \chi \right) \right. \\
\left. - (\gamma - 1) \cos^2 \chi \left( 4\pi A_3 x_2 + 2(-1)^N A_1 C_3 \cos \alpha_0 \tan \chi \right. \\
\left. - 2\Delta_2 \tan \chi (2\pi A_2 x_2 + A_3 C_1 - A_1 C_3) \right. \\
\left. + \tan^2 \chi (A_1 C_2 - A_2 C_1) - \Delta_1 \tan^2 \chi (A_1 C_2 + A_2 C_1) \right) \right], \quad (7.14)
\]
\[T^1_s = -\frac{1}{144\pi^2} \left[ 6\gamma \left( 2(\pi L)^2 A_2 C_3 - 3 A_3 C_2 \tan^2 \chi (1 + \Delta_1) \right) \\
- 6 \tan \chi (A_2 C_2 - A_3 C_3)((-1)^N \cos \alpha_0 + \Delta_2) \right) \\
- (\gamma - 1) \sin^2 \chi \left( 36 A_3 C_3 \cot \chi \left( \Delta_2 (3 - (\pi L)^2) + 3(-1)^N \cos \alpha_0 \right) \right) \\
+ 2 \tan (A_1 C_1 - A_2 C_2) \left( (-1)^N \cos \alpha_0 (6 \cos^2 \alpha_0 + \Delta_1) \right) \\
- \Delta_2 (1 - 6 \cos^2 \alpha_0) + 9 (2\pi A_1 x_2 - A_3 C_2) (\cos 2 \alpha_0 + 3 \Delta_1 + 2) \\
+ 6 A_2 C_3 (3 (\cos 2 \alpha_0 + \Delta_1) + (\pi L)^2 (2 \cos 2 \alpha_0 - 3 \Delta_1)) \right] \right], \quad (7.15)\]

\[T^2_s = \frac{1}{72\pi^2} \left[ 3\gamma \left( 18\pi \Delta_2 A_3 x_2 + 2 (\pi L)^2 A_1 C_3 - 3 A_3 C_1 \tan^2 \chi (1 + \Delta_1) \right) \\
- 6 A_1 C_2 \tan \chi ((-1)^N \cos \alpha_0 - 1) \right) \\
- (\gamma - 1) \sin^2 \chi \left( 72\pi A_3 x_2 \cot \chi ((-1)^N \cos \alpha_0 + \Delta_2) \right) \\
+ \tan (9 (\pi A_2 x_2 + \frac{1}{2} A_3 C_1) (3 \Delta_1 - 2 + \cos 2 \alpha_0) + A_1 C_3 (11 (\pi L)^2 \\
- 9 (\cos 2 \alpha_0 + \Delta_1)) + \tan \chi (A_1 C_2 + A_2 C_1) (6 (-1)^N \cos^3 \alpha_0 \right) \\
+ 8 \Delta_2 (\cos^2 \alpha_0 + 2)) - 4 A_1 C_2 \tan \chi (2 (-1)^N \cos \alpha_0 + 9 \Delta_2) \right) \]. \quad (7.16)\]

\[T^3_s = -\frac{1}{8\pi^2} \tan \chi \left[ \gamma \left( 2\Delta_2 (2\pi A_2 x_2 - A_1 C_3) - 2(-1)^N A_1 C_3 \cos \alpha_0 \right) \\
+ A_1 C_2 \tan \chi (1 + \Delta_1) - A_2 C_1 \tan \chi (1 - \Delta_1) \right) \\
+ (\gamma - 1) \sin^2 \chi \left( 4\pi A_3 x_2 \cot \chi - 2 \Delta_2 (2\pi A_2 x_2 + A_3 C_1 - A_1 C_3) \right) \\
+ (-1)^N A_1 C_3 \cos \alpha_0 - A_1 C_2 \tan \chi (1 + \Delta_1) \\
+ A_2 C_1 \tan \chi (1 - \Delta_1) \right) \]. \quad (7.17)\]

where \( \Delta_1 = \frac{\sin 2\alpha_0}{2\pi L} \), \( \Delta_2 = \frac{(-1)^N \sin \alpha_0}{\pi L} \), and in order to work with dimensionless quantities, the forces and torques were divided by:

\[F \rightarrow \frac{K_0 \lambda L \dot{\gamma}}{\cos \chi}, \quad (7.18)\]

\[T \rightarrow \frac{K_0 \lambda^2 L \dot{\gamma}}{\cos \chi}, \quad (7.19)\]
and \( L \) and the components of the velocities \( U \) and angular velocities \( \Omega \) were replaced with their dimensionless counterparts:

\[
U \rightarrow \frac{U}{\lambda \dot{\gamma}}, \quad \Omega \rightarrow \frac{\Omega}{\dot{\gamma}}, \quad L \rightarrow \frac{L}{\lambda}. \tag{7.20}
\]

### 7.2 Numerical Setup

Unlike the case of the helix sedimenting due to gravity, the equations of motion here do not have a straightforward dependence on the velocity and angular velocity components, and directly solving the differential equations for the Euler angles becomes computationally expensive. Therefore, in this section an alternative algorithm is introduced.

With the requirement that net forces and torques vanish, the equations of motion for this setup are

\[
F + F_s = 0, \tag{7.21}
\]
\[
T + T_s = 0. \tag{7.22}
\]

These equations are then set up in the form,

\[
M \begin{pmatrix} U \\ \Omega \end{pmatrix} + b = 0
\]

where \( M \) is a (6 × 6) matrix containing the coefficients of the velocity and angular velocity, \( U \) and \( \Omega \) respectively, and \( b \) is a 6-vector containing all the terms that are dependent on the Euler angles. Once the matrix \( M \) and vector \( b \) are determined, the inverse of \( M \) is found in order to obtain

\[
w = \begin{pmatrix} U \\ \Omega \end{pmatrix} = -M^{-1} \cdot b \tag{7.23}
\]

Given the expression for \( w \) found in Eq. (7.23), the following step is to transform the velocities from the body frame to the lab frame by applying the transpose of
the rotation matrix $D$ expressed in Eq. (2.9). Similarly,

$$
M_A = \begin{pmatrix}
\sin \psi & -\cos \psi \sin \theta & 0 \\
\cos \psi & \sin \psi \sin \theta & 0 \\
0 & \cos \theta & 1
\end{pmatrix},
$$

(7.24)
is used in order to relate the angular velocities to the Euler angles. Combining these elements, the following set of differential equations for the positions in the lab frame and the Euler angles of the body is obtained:

$$
\frac{\partial}{\partial t} \begin{pmatrix}
X \\
Y \\
Z \\
\theta \\
\phi \\
\psi
\end{pmatrix} = \left( D^T \cdot U \right) 
\begin{pmatrix}
M_A^{-1} \\
\Omega
\end{pmatrix}.
$$

(7.25)
The resulting equations of motion are then solved using Scientific Python [120] by employing the fourth-order Runge-Kutta time-stepping method [121].

Given this numerical setup, in what follows a helix with $N = 4$ number of turns and an angle $\chi = 0.733 \approx 42^\circ$ is considered for different initial conditions of the variables $\alpha_0$, $\theta_0$ and $\psi_0$; where $\alpha_0$ represents how much the helix deviates from having an integer number of turns $N$, and $\theta_0$ and $\psi_0$ are the initial conditions of two of the Euler angles. No dependence on the initial value of $\phi$ is found, therefore $\phi_0 = 0$ is used for this Chapter.

### 7.3 Helix in the Shear Plane

#### 7.3.1 Dependence on End-Points Orientation

Here the dependence on the initial condition $\psi_0$ is studied and in order to determine the effect that its value has on the behaviour of the helix in the shear flow, the trajectories for a relatively long helix with $N = 4$, $\alpha_0 = 0$ and $\chi = 42^\circ$ were evaluated for the initial orientations $\theta_0 = \pi/2$, $\phi_0 = 0$; where for $\theta_0 = \pi/2$ the helix lies in the shear plane. The numerical calculations were performed for
varying initial values of the angle $\psi_0$; where the angle $\psi$ represents the rotation of the helix about its 3-axis as shown previously in Figure 3.6. For $\psi = 0$ the end points of the helix point downwards while for $\psi = \pm \psi$ they point upwards.

The plots for the trajectories in the $x$, $y$ and $z$ directions are shown in Figure 7.2 for the initial conditions $\psi_0 = 0, \pi/2, \pi, 3\pi/2$.

![Figure 7.2](image.png)

**Figure 7.2** Plots of a) $\tilde{x}$, b) $\tilde{y}$, and c) $\tilde{z}$ vs. $\tilde{t}$ for a helix with $N = 4$, $\chi = 0.733$, $\alpha_0 = 0$ and initial orientation $\theta_0 = \pi/2$, $\phi_0 = 0$ for different values of $\psi_0$ (0 blue line, $\pi/2$ orange line, $\pi$ green line and $3\pi/2$ red line).

Depending on the initial value of $\psi$, the helix is seen traveling in the positive (when $\psi_0 \in (0, \pi]$) or negative (when $\psi_0 \in (\pi, 2\pi]$) $x$ direction, see Figure 7.2(a). It can also be noticed, that when the helix starts with an initial configuration where its ends point upwards (green lines in Figure 7.2), there is almost no displacement in the $x$ and $y$ directions, in Figure 7.2(a) and (b). In Figure 7.2(b), for the initial condition $\psi_0 = 0$, a sudden oscillation in the trajectory in the $y$-direction can be seen. This is because, the helix is found to be stable in the configuration with its ends pointing downwards ($\psi_0 = 0$) only for a limited period, after which it re-orientates itself into the more stable configuration with its ends pointing upwards ($\psi_0 = \pi$). This will be explored further when looking at the behaviour of the Euler angles in the next section.

Finally, in agreement with the predictions and results for a helix in a shear flow outlined at the start of this chapter, Figure 7.2(c) shows that for all values of $\psi_0$,
the helix experiences a lateral drift in the negative $z$ direction (i.e. the direction perpendicular to the shear plane). The velocity in the $z$ direction is found to be independent of the initial conditions imposed on $\psi$. Further analysis shows that the values of the velocity in the $x$ direction, found by taking the gradient of the $x - t$ plots, show a sinusoidal dependence on $\psi_0$. These results can be seen in Figure 7.3.

![Figure 7.3](image)

**Figure 7.3** Plots showing the dependence on the value of $\psi_0$ for a) the velocity in the $x$-direction, $\tilde{U}_x$, and b) the velocity in the $z$-direction, $\tilde{U}_z$. The values of the velocities plotted are obtained from the numerical calculations introduced in the previous section.

### 7.3.2 Euler Angles

The changes in the helix’s orientation are now studied. It is found that plots of the Euler angles $\theta$, $\phi$, and $\psi$ show the same behaviour for all the different values of $\psi_0$ after long times where a steady state has been reached. The plots are shown in Figure 7.4.

Figure 7.4(a) shows that, at long times, the value of $\theta$ settles at the value of its initial orientation $\theta_0 = \pi/2$, meaning that a helix in the plane of the shear will stay within that plane as it moves. The value of $\psi$, in Figure 7.4(c), after some time, settles at $\pi$ regardless of its starting value; this implies that independently of its initial orientation, the helix will end up in the configuration with its free ends pointing upwards, as shown in Figure 3.6. In Figure 7.4(c), the initial orientation, $\psi_0$, seems to be initially stable but after a long time it destabilises and the helix re-orientates itself to the preferred orientation $\psi_0 = \pi$. This delayed re-orientation causes some oscillations in $\theta_0$, seen in Figure 7.4(a), after which the helix settles back to an orientation with its major axis in the plane of shear ($\theta = \pi/2$). Finally, in Figure 7.4(b), the angle $\phi$ is seen to be linearly decreasing in time, meaning
that the helix is completing a full rotation about its minor axis with every $2\pi$ increment of its $\phi$ angle. The period of this rotation and its dependence on the number of turns, $N$, of the helix are then computed in a later Section.

### 7.3.3 Jeffery Orbits

Putting together everything that was found for a helix with its major axis within the plane of the shear, it can be concluded that the helix does indeed perform Jeffery-like orbits while also experiencing a lateral drift. Where the drift arises from the coupling of translation and rotation during the Jeffery-like orbit flipping motion in the shear flow. To better observe this, the orientation trajectory of the helix’s major axis is shown in Figure 7.5 for different initial values of $\theta_0$.

To further study the effects of chirality on the trajectory, the forces and torques for a left-handed helix (opposite chirality to the helix so far considered) were calculated. It was then found that the direction of lateral drift perpendicular to the shear plane depends on the chirality of the helix; with a drift in the negative...
Figure 7.5 Projection of the trajectories of the orientation of the helix’s major
axis for different initial values of $\theta_0$: $\theta_0 = 0$ (blue), $\theta_0 = \pi/10$ (orange), $\theta_0 = \pi/5$ (green), $\theta_0 = 3\pi/10$ (red), $\theta_0 = 2\pi/5$ (purple), $\theta_0 = 9\pi/20$ (magenta), and $\theta_0 = \pi/2$ (olive).

$z$-direction for a right-handed helix, and in the $+z$-direction for a left-handed
one. This is in agreement with conclusions drawn by Marcos et al. [14], who
argue that the origin of chirality-dependent drift at low Reynolds number can be
qualitatively understood for the case of a helix.

Their argument is as follows: consider a right-handed helix aligned with a simple
shear flow, and decompose the velocity at a small filament of the helix into
components perpendicular and parallel to it. Drag on a thin rod in low Reynolds
number flow has a greater resistance when oriented perpendicular rather than
parallel to the flow [30]. Since the flows at the top and bottom halves of the helix
are in opposite directions, both halves have a drag component along $-z$. Thus, a
right-handed helix aligned with the shear flow drifts in the $-z$ direction. Reversing
the chirality of the helix or the sign of the shear produces a drift along $+z$.

Additionally, it is found that the left-handed helix travels in the opposite $x$-
direction to the right-handed helix but with the same dependence on $\psi_0$, and
regardless of the value set for $\psi_0$, it settles to an orientation of $\psi = 0$ with its
ends pointing downwards (see Figure [3.6]).

7.3.4 Changing Number of Turns

As seen in Figure 7.4 the angle $\phi$ is linearly decreasing in time, meaning that the
helix is constantly completing full rotations about its minor axis. It is found that
this period of rotation of $\phi$ does not depend on the initial orientation $\psi_0$ of the
helix, but it does, however, depend on the number of turns, \( N \), of the helix.

Figure 7.6  
Plots showing the dependence on the number of turns of the helix, \( N \) for a) the period of rotation of \( \phi \), b) the velocity in the \( x \)-direction, \( \tilde{U}_x \), and c) the velocity in the \( z \)-direction, \( \tilde{U}_z \). Where in b) the blue dots are the values of \( \tilde{U}_x \) and the orange crosses are the absolute values of the velocity, \( |\tilde{U}_x| \). The helix considered has \( \chi = 0.733 \) and \( \alpha_0 = 0 \).

Figure 7.6 shows the dependence of the period of rotation of \( \phi \), \( |\tilde{U}_x| \) and \( \tilde{U}_z \) with respect to the number of turns, \( N \), of the helix. It can be seen that the direction of \( \tilde{U}_x \) changes depending on whether \( N \) is even or odd; to better show the dependence of the magnitude on \( N \), the absolute values of velocity in the \( x \)-direction are also plotted (orange markers in Figure 7.6(b)). When plotted against \( N \), the period of oscillation of \( \phi \), in Figure 7.6, appears to increase linearly with \( N \).

### 7.4 Helix Outside the Shear Plane

#### Behaviour of \( \theta \)

For values of \( \theta_0 \neq \frac{\pi}{2} \) the helix is found to perform a kayaking motion with varying amplitude, which depends on the initial orientation \( \theta_0 \), as can be seen in Figure 7.7. The further away from a starting orientation where the helix’s
major axis is perpendicular to the shear plane, the wider the amplitude of the kayaking motion becomes. Here the observed kayaking motion is found to be stable and consistent at long times. For \( \theta_0 \) approaching \( \frac{\pi}{2} \), however, it is observed, in Figure 7.7(b), that the orientation is initially unstable and visibly oscillates. These oscillations appear to dissipate as a period of time passes, after which the angle \( \theta \) will settle into the \( \frac{\pi}{2} \) orientation, as seen in Figure 7.7(b). This means that there is a critical angle \( \theta_{0c} \approx \frac{\pi}{2} \), where the helix is almost completely within the plane of shear, such that, when \( \theta_0 \geq \theta_{0c} \), the helix is drawn into the plane of shear. Here the Jeffery-like orbit behaviour, observed in the previous Section, is recovered.

![Figure 7.7](image-url)

**Figure 7.7** Plot of \( \theta \) vs. \( \tilde{t} \) for initial conditions of a) \( \theta_0 \in [0, \pi/2] \), and b) for values of \( \theta_0 \rightarrow \pi/2 \). This is done for helix with \( N = 4 \), \( \chi = 0.733 \), \( \alpha_0 = 0 \) and initial orientation \( \phi_0 = 0 \) and \( \psi_0 = \pi/2 \).
**Behaviour of ψ**

For initial conditions where the helix does not start in the shear plane, the angle \( \psi \) linearly decreases with time, meaning that the helix is constantly spinning about its major axis. For initial configurations where the helix is almost parallel to the shear plane (\( \theta_0 \to \frac{\pi}{2} \)), instead, the helix will settle in the configuration with its free ends pointing up (\( \psi = 0 \)), as is the case for the helix in the shear plane.

### 7.5 Non-integer Number of Turns

Having so far considered a helix with an integer number of turns, \( \alpha_0 = 0 \), now a helix with \( \alpha_0 \neq 0 \) is considered. The code was run for values of \( \alpha_0 \) ranging between \( -\frac{\pi}{2} \) to \( \frac{\pi}{2} \), and \( \theta_0 \) ranging between 0 and \( \frac{\pi}{2} \). For each set of these initial conditions, the amplitude of the oscillations of \( \theta \), when the dynamics have reached a steady state, is measured and the results are plotted in Figure 7.8 as a function of \( \alpha_0 \) and the initial value \( \theta_0 \).

![State diagram for a helix with \( N = 4 \), \( \chi = 0.733 \) and initial orientation \( \phi_0 = 0 \) and \( \psi_0 = \pi/2 \), for a given combination of \( \alpha_0 \) and \( \theta_0 \). The colour indicates the amplitude of oscillations of \( \theta(t) \) in a steady state or at long times, if a steady state is not reached.](image)

**Figure 7.8** State diagram for a helix with \( N = 4 \), \( \chi = 0.733 \) and initial orientation \( \phi_0 = 0 \) and \( \psi_0 = \pi/2 \), for a given combination of \( \alpha_0 \) and \( \theta_0 \). The colour indicates the amplitude of oscillations of \( \theta(t) \) in a steady state or at long times, if a steady state is not reached.

In the previous section, it was found that a helix with its major axis at an angle to the plane of shear (\( \theta_0 \neq \pi/2 \)) performs a kayaking motion as it drifts in the \( -z \)-direction. This kayaking motion, given by periodic oscillations of \( \theta(t) \) becomes more amplified as \( \theta_0 \) increases from 0, see Figure 7.7(a). This behaviour can also be observed in the state diagram in Figure 7.8. In this plot, an increase in the
size of oscillations of $\theta(t)$ (where the colour in the diagram becomes redder) is seen as the value of $\theta_0$ ($y$-axis) increases. As the value of $\theta_0$ further increase and approaches $\pi/2$, however, the oscillation amplitude decreases. This is consistent with the observation, in Figure [7.7(b)], that $\theta$ tends to the constant value of $\pi/2$ for initial configurations where the helix lies almost completely in the shear plane ($\theta_0 \approx \pi/2$).

It was previously seen that as $\theta_0$ increases in value, the oscillations of $\theta$ increase in amplitude leading to a bigger kayaking motion in Figure [7.7]. This behaviour can now also be seen in the state diagram in Figure 7.8 where the colour indicates an increase in the size of oscillations for bigger $\theta_0$ values. It can also be noticed that as the values of $\theta_0$ approach $\pi/2$, the oscillations decrease. This is consistent with the observation that $\theta$ tends to the constant value of $\pi/2$ for initial configurations where the helix lies almost completely in the shear plane.

7.6 Concluding Remarks

In this Chapter, it was found that a helix placed in a shear flow, with its major axis of symmetry in the shear plane, performs Jeffery-like orbits and experiences a lateral drift in the positive (or negative) $z$-direction. The sign of the drift depends on the chirality of the helix, as well as on the parity of its number of turns ($N$ even or odd). It is also found that, regardless of the initial value of $\psi_0$, a right-handed helix will settle into an orientation with its free ends pointing upwards ($\psi = \pi$) and a left-handed helix will settle with it free ends pointing downwards ($\psi = 0$). Additionally, the period of rotation of the helix about its minor axis is independent of the initial condition of $\psi_0$ imposed, but shows a linear dependence on the number of turns of the helix, $N$.

Leaving the shear plane ($\theta_0 = \pi/2$) and examining a helix where its major axis is at an angle with the plane of shear, a kayaking motion appears. The amplitude of this kayaking motion depends on the initial angle that the helix’ major axis makes with the shear plane; as $\theta_0$ increases from 0 the kayaking motion becomes wider. There is, however, a critical value of $\theta_0$, $\theta^*_{0} \lesssim \pi/2$, such that, instead of having a kayaking motion, the helix is drawn into the orientation with its major axis in the plane of shear and the Jeffery-like orbits are recovered. This behaviour can then clearly be observed in the state diagram in Figure 7.8 where, in the blue region at the top of the graph, the helix is performing the Jeffery-like orbits,
and it can be seen that this region is delimited by both $\theta_0^c \approx \pi/2$ and a condition on $\alpha_0$, such that $\alpha_0 < |\alpha_0^c|$. For further work, it could be of interest to find an analytical approximation for these critical values of $\theta_0$ and $\alpha_0$. 
Chapter 8

Conclusions

In summary, in this thesis, the dynamics of chiral and anisotropic particles that perform chiral trajectories when sedimenting were studied. Additionally, the dynamics of a rigid helix in a shear flow were calculated by employing RFT. Here, the major findings, and how they connect to the literature, are summarised. The possibility for experimental implementation, where applicable, is briefly discussed.

Krapf and Witten [2, 10] found that, while all chiral particles sediment with a chiral trajectory, chiral trajectories can also be performed by non-chiral particles. Krapf and Witten discussed that this behaviour is obtained from particles with an asymmetry which is reflected in the particle’s mobility matrix. Consequently, the Chapters 3-6 looked at the sedimentation of helices, L- and C-shapes, and Möbius, where the dynamics were evaluated by employing Resistive Force Theory and an RPY-level approximation method. Where the accuracy of the RPY-based calculation of the Grand Mobility Matrix was confirmed in Chapter 2 by benchmarking the simulation against the literature results for a sphere and a straight rod.

Chapters 3 and 4 studied the sedimentation dynamics of a rigid helix. In Chapter 3 the dynamics were evaluated by employing RFT. It is found that for most initial orientations the helix performs a superhelical trajectory when sedimenting, where the handedness of the trajectory is opposite to the handedness of the sedimenting helix itself. Here, approximate expressions for the radius and pitch of the superhelical trajectory are found in Eqs. (3.48) and (3.49). From these, it was concluded that the experimental observation of these superhelical trajectories is unlikely for macroscopic helices in confined geometries. According
to Eq. \((3.48)\), the radius of the superhelical trajectory in physical units, \(L\tilde{\Lambda}\), scales as \(L^2/\lambda\), which implies a very wide trajectory. In turn, the size of the tank used in such an experiment should be significantly larger than \(L\tilde{\Lambda}\), implying rather wide geometries. Worse still, the pitch of the superhelical trajectory is significantly larger than its radius, implying not only wide, but also very tall fluid tanks. For instance, consider a helix with \(L = 10\ \text{cm}\), \(\chi = 0.733\) and four full turns, \(N = 4\) and \(\alpha_0 = 0\). If the radius of the helical filament is \(r = 0.5\ \text{mm}\), the ratio of the friction coefficients becomes \(\gamma \approx 1.26\) (using Eqs. \((3.3)\) and \((3.4)\) for \(K_{\parallel}\) and \(K_{\perp}\)). With these parameters, and selecting \(\theta_0 = \pi/4\), \(\rho \approx 2L = 20\ \text{cm}\) and \(\Lambda \approx 285L = 28.5\ \text{m}\) is obtained. As RFT can, at best, produce semi-quantitative approximations of actual drag forces on extended objects, the applicability of these results was verified in the following chapter.

Consequently, chapter 4 looked at the sedimentation of a helix using the RPY numerical computation introduced in Chapter 2.6. The helix was approximated as a collection of spheres and its GMM was calculated using the method introduced by Palanisamy and Den Otter \([1]\) and implemented by Joost de Graaf. It was found that for most initial orientations the helix performs a superhelical trajectory when sedimenting, with the superhelix having a pitch and radius in agreement with the RFT approximation. Additionally, also in agreement with the RFT predictions, the helix completes a full rotation about its minor axis (by the angle \(\phi\)) in the same period it takes for it to travel down a single pitch, \(\tilde{\Lambda}\) of the superhelix. This chapter showed that RFT, for a sedimenting helical filament, can produce good qualitative and semi-quantitative approximations for the trajectory when compared to the results obtained from a method that includes hydrodynamic interactions. Considering the results found for other shapes, this appears to be a fortuitous agreement.

Chapter 5 then looked at the sedimentation of the L-Shape and the C-Shape. First an L-shape sedimenting parallel to the plane of gravity was studied using RFT and the GMM. RFT recovered a shape of the mobility matrix in agreement with the GMM, however, it failed to find both a final orientation and angle of sedimentation of the L-shape in agreement with the RPY results. Examining the issue further, it was found that an L-shape, when sedimenting, re-orients itself to a preferred orientation that depends on the ratio of the two legs and is independent of its initial orientation. Even in the rod-like limit, where the ratio of \(l_1/l_2 \to 0\), no dependence on the initial orientation is recovered, which is in contrast to the behaviour of a straight rod sedimenting. This apparent inconsistency can be
explained by looking at the mobility matrix which shows that even the slightest perturbation on the rod leads to the decoupled orientational dynamics. The second part of Chapter 5 then evaluated the sedimentation dynamics of a C-shape at an angle to the plane of gravity. It was found that the C-shape sediments with a chiral trajectory that is not as simple as a superhelical trajectory. The properties of this trajectory, including its chirality, depend on the initial conditions imposed on the system.

The following particle shape studied was the Möbius strip and its achiral version, the stadium. In the first section of Chapter 6, the mobility coefficients of stadium shaped particle were calculated using the RPY-bead method and compared to results found using Slender Ribbon Theory [4]. Whilst some qualitative agreement was found in the dependence of mobility coefficients on the parametric angle $\alpha$, the two methods disagreed both qualitatively and quantitatively. The nature of the disagreement remains unclear and further analysis is needed. The following sections, instead, focused on the sedimentation of the Möbius strip. As expected, the Möbius strip, when sedimenting, performs a chiral trajectory with an opposite handedness to the handedness of the strip itself. Additionally, the properties of the chiral trajectory depend on the initial conditions imposed on the strip’s initial orientation. Furthermore, a rich state diagram, highlighting a wide range of behaviours exhibited by the Möbius strip, was found.

In the final chapter, Chapter 7, RFT was employed to study the dynamics of a rigid helix in a simple shear flow. It was found that a helix placed in a shear flow, with its major axis of symmetry in the shear plane, performs Jeffery-like orbits and experiences a lateral drift in the positive (or negative) $z$-direction. The sign of the drift depends on the chirality of the helix, as well as on the parity of its number of turns ($N$ even or odd). Additionally, it was found that, regardless of the initial value of $\psi_0$, a right-handed helix will settle into an orientation with its free ends pointing upwards ($\psi = \pi$) and a left-handed helix will settle with it free ends pointing downwards ($\psi = 0$). This behaviour is analogous to that of a helix sedimenting in a horizontal orientation ($\theta_0 = \pi/2$). The dynamics of a helix where its major axis is at an angle with respect to the shear plane, which delimits the two regions of behaviour, kayaking and Jeffery orbits, was found.

Overall, it was shown that the sedimentation of anisotropic or chiral particles is chiral and with a handedness dependent on the handedness of the particle
(if the particle is chiral) or the initial orientation (if the particle is achiral). For a sedimenting helix, a superhelical trajectory is recovered and expressions for the superhelix’s radius and pitch are calculated. The C-shape and Möbius strip sediment with a more complex chiral trajectory. Therefore, for future work, it would be interesting to find analytic expressions to describe these trajectories as well as correct the discrepancies between SRT and the RPY method. Furthermore, in agreement with multiple observations [11–18], it was found that a helix in a shear flow experiences a lateral drift with a direction that depends on the handedness of the helix. Better understanding the dependence of this lateral drift on the properties of the helix can help progress in fields such as enantiomer separation [63].

Given the work presented in this thesis, possible areas of future research are now outlined, some of which arise from the current limitations of the methods implemented. This thesis largely focused on the implementation of RPY-level approximations of the mobility matrix, for a rigid body made up of a collection of spherical beads, based on the assumption that the fluid is a Newtonian fluid.

This thesis has highlighted the utility of using the GMM to analyse the sedimentation behaviour of complex-shaped particles. The results have shown that the use of RPY-level approximations in the GMM can effectively capture the dynamics of these particles. Therefore, for future work, one could substitute the RPY-level approximations in the GMM with higher-order approximations. Doing so could confirm the current results of the thesis as well as give further insight into the results of an L-shape approaching the rod limit, which is a counter-intuitive result. Furthermore, to gain a better understanding of the sedimentation behaviours found for the L- and C-Shapes, it could be of interest to study other similar shapes, such as T-Shape, Z-Shape, or H-Shape, and eventually adding chirality by twisting the H-Shape. Given their higher degree of symmetry compared to the L-Shape, the T-Shape, and Z-Shape could exhibit less rich state diagrams when looking at the sedimentation behaviour. Similarly, the H-Shape, which is even more symmetric than the others, may have an even simpler state diagram. Moreover, studying the behaviour of a twisted H-Shape could give a better understanding of how chirality affects the sedimentation of asymmetric shapes.

The sedimentation of the Möbius strip produced a complex state diagram with several distinct regions of behaviour that were highly dependent on the initial orientation of the strip. Further research into this topic could include examining
the effects of additional twists and exploring the role of twist parity in the sedimentation behaviour. This research also opens up interesting questions for micro- and nano-scale robotics — for example if the coupling is reversible (which is expected in the low-Reynolds regime) then the rotation of a Möbius strip would cause perpendicular motion, allowing the Möbius strip to be used as a propeller with a simpler geometry than a helix.

The GMMs calculated throughout the thesis are only 6x6 sub-blocks, and cannot be used to look at an object in a shear flow. In the future, building on the code in order to correctly obtain the full $11 \times 11$ Grand Mobility Matrix, which considers the strain and stress, would enable the comparison of the current RFT results for a helix in a shear flow with the results using the RPY method.

An ambitious, longer-term project could explore the possibility of modifying the RPY approximations in order to account for properties of non-Newtonian fluids, and therefore enable the investigation of the behaviour of rigid particles in non-Newtonian fluids. Understanding the flow properties of these fluids and how they interact with other particles can provide valuable insights into many natural and industrial processes, from the flow of blood in the human body to the behaviour of industrial slurries.
Appendix A

Pair Mobilities

The approximate analytical expressions for the mobility matrix of two interacting spherical particles, outlined in [1] are summarised here. Using auxiliary functions $x$, $y$, and $z$ in the dimensionless distance $\tilde{r}_{ij} = \frac{r_{ij}}{a}$, the elements of the mobility matrix read as [1, 11]:

\begin{align}
\mu_{V,i,\alpha}^{F,j,\beta} &= x_{F,j}^{i} \hat{r}_{ij}^{\alpha} + y_{F,j}^{i} P_{\alpha\beta}, \\
\mu_{\Omega,i,\alpha}^{F,j,\beta} &= y_{F,j}^{i} \epsilon_{\beta\gamma} \hat{r}_{ij}^{\gamma}, \\
\mu_{\Omega,i,\alpha}^{T,j,\beta} &= x_{T,j}^{i} \hat{r}_{ij}^{\alpha} + y_{T,j}^{i} P_{\alpha\beta}, \\
\mu_{E,i,\alpha\beta}^{F,j,\gamma} &= x_{E,j}^{i} \hat{r}_{ij}^{\alpha} \hat{r}_{ij}^{\beta} + y_{E,j}^{i} \left( \hat{r}_{ij}^{\alpha} P_{\beta\gamma} \hat{r}_{ij}^{\gamma} + \hat{r}_{ij}^{\beta} P_{\alpha\gamma} \hat{r}_{ij}^{\gamma} + \hat{r}_{ij}^{\beta} P_{\alpha\delta} \hat{r}_{ij}^{\delta} \right), \\
\mu_{E,i,\alpha\beta}^{S,j,\gamma\delta} &= x_{E,j}^{i} d_{\alpha\beta} d_{\gamma\delta} + y_{E,j}^{i} \left( \hat{r}_{ij}^{\alpha} P_{\beta\gamma} \hat{r}_{ij}^{\gamma} + \hat{r}_{ij}^{\beta} P_{\alpha\gamma} \hat{r}_{ij}^{\gamma} + \hat{r}_{ij}^{\beta} P_{\alpha\delta} \hat{r}_{ij}^{\delta} \right) + z_{E,j}^{i} \left( P_{\alpha\gamma}^{i} P_{\beta\delta}^{i} + P_{\beta\gamma}^{i} P_{\alpha\delta}^{i} - P_{\alpha\beta}^{i} P_{\gamma\delta}^{i} \right),
\end{align}

where $r_{ij} = x_{j} - x_{i}$ is the difference vector between particles $i$ and $j$, $\hat{r}_{ij} = \frac{r_{ij}}{|r_{ij}|}$ is the parallel unit vector, $d_{ij} = \hat{r}_{ij} \otimes \hat{r}_{ij} - \frac{1}{3} I$ is the traceless dyadic, and $P_{\alpha\beta} = I - \hat{r}_{ij} \otimes \hat{r}_{ij}$ is the perpendicular projection. The remaining elements then follow.
from the symmetry relations

\[ \begin{align*}
V_{j,\beta} &= \Omega_{i,\alpha}^\delta, \\
T_{i,\alpha} &= \mu_{F,j,\beta}, \\
S_{i,\alpha} &= \mu_{E,j,\gamma}^\delta, \\
S_{i,\alpha} &= \mu_{E,j,\gamma}^\delta.
\end{align*} \tag{A.7} \]

In the Rotne-Prager-Yamakawa approximation, used in this thesis, the auxiliary functions are given by \[1\]

\[ \begin{align*}
X^{V,i}_{F,j} &= \delta_{ij} + (1 - \delta_{ij}) \left( \frac{3}{2} \tilde{r}_{ij}^{-1} - \tilde{r}_{ij}^{-3} \right), \\
Y^{V,i}_{F,j} &= \delta_{ij} + (1 - \delta_{ij}) \left( \frac{3}{4} \tilde{r}_{ij}^{-1} + \frac{1}{2} \tilde{r}_{ij}^{-3} \right), \\
Y^{\Omega,i}_{F,j} &= - (1 - \delta_{ij}) \frac{3}{4} \tilde{r}_{ij}^{-2}, \\
X^{\Omega,i}_{T,j} &= \frac{3}{4} \delta_{ij} + (1 - \delta_{ij}) \frac{3}{4} \tilde{r}_{ij}^{-3}, \\
Y^{\Omega,i}_{T,j} &= \frac{3}{4} \delta_{ij} - (1 - \delta_{ij}) \frac{3}{8} \tilde{r}_{ij}^{-3}, \\
X^{E,i}_{F,j} &= (1 - \delta_{ij}) \left( \frac{9}{4} \tilde{r}_{ij}^{-2} - \frac{18}{5} \tilde{r}_{ij}^{-4} \right), \\
Y^{E,i}_{F,j} &= (1 - \delta_{ij}) \frac{6}{5} \tilde{r}_{ij}^{-4}, \\
Y^{E,i}_{T,j} &= - (1 - \delta_{ij}) \frac{9}{8} \tilde{r}_{ij}^{-3}, \\
X^{E,i}_{S,j} &= \frac{27}{20} \delta_{ij} - (1 - \delta_{ij}) \left( \frac{27}{4} \tilde{r}_{ij}^{-3} - \frac{81}{5} \tilde{r}_{ij}^{-5} \right), \\
Y^{E,i}_{S,j} &= \frac{9}{20} \delta_{ij} + (1 - \delta_{ij}) \left( \frac{9}{8} \tilde{r}_{ij}^{-3} - \frac{18}{5} \tilde{r}_{ij}^{-5} \right), \\
Z^{E,i}_{S,j} &= \frac{9}{20} \delta_{ij} + (1 - \delta_{ij}) \frac{9}{10} \tilde{r}_{ij}^{-5}.
\end{align*} \tag{A.10-20} \]

For future work, these functions could then be substituted with higher-order approximations \[11\].
Appendix B

Basis Matrices

Due to the combination of multiple ranks in the grand mobility tensor, standard numerical methods for square matrices cannot be employed. As a result, the strain rate and stress are rewritten as a linear combination of ‘basis matrices’, $e_\kappa^E$ and $e_\kappa^S$, and their corresponding ‘dual basis matrices’, $e_\kappa^E$ and $e_\kappa^S$.

The strain rate of the flow field is rewritten as,

$$E^\infty = \sum_\kappa e_\kappa^E \mathcal{E}_\kappa^\infty,$$

$$\mathcal{E}_\kappa^\infty = e_\kappa^E : E^\infty,$$  \hspace{1cm} (B.1)

where the set of coefficients $\mathcal{E}_\kappa^\infty$ make up a column vector $\mathcal{E}^\infty$ and the colon denotes a double contraction. The strain rate is then converted between matrix and vector representation by

$$S = \sum_\kappa e_\kappa^S S_\kappa,$$

$$S_\kappa = e_\kappa^S : S,$$  \hspace{1cm} (B.3)

where the Greek index $\kappa$ runs from 1 to 5. The corresponding five basis matrices
to convert the stress from the vector $\mathbf{S}$ to the matrix $\mathbf{S}$ are

$$
\mathbf{e}_1^S = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{e}_2^S = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \mathbf{e}_3^S = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},
$$

(B.5)

$$
\mathbf{e}_4^S = \frac{1}{3} \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \mathbf{e}_5^S = \frac{1}{3} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.
$$

The reciprocal basis are then given by,

$$
\mathbf{e}_1^* = \frac{1}{2} \mathbf{e}_1^S, \quad \mathbf{e}_2^* = \frac{1}{2} \mathbf{e}_2^S, \quad \mathbf{e}_3^* = \frac{1}{2} \mathbf{e}_3^S, \quad \mathbf{e}_4^* = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{e}_5^* = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.
$$

(B.6)

Several symmetry rules, derivable from the Lorentz reciprocal theorem, are satisfied by the particle-particle grand mobility matrices in Eq. (2.36). Consequently, by choosing

$$
\mathbf{e}_E^\kappa = \mathbf{e}_S^\kappa, \quad \mathbf{e}_S^\kappa = \mathbf{e}_S^\kappa,
$$

(B.7)

$$
\mathbf{e}_E^S = \mathbf{e}_S^S,
$$

(B.8)

as the basis matrices for the strain rate, the particle-particle grand mobility matrices in Eq. (2.37) will also satisfy these symmetries, resulting in a symmetric grand mobility matrix for the cluster, in Eq. (2.42). Although convenient, the imposition of symmetry is not compulsory to the approach taken by Palanisamy and Den Otter [1].

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Appendix C

Sub-Matrices of Grand Resistance Matrix

The force and torque related sub-matrices of the grand resistance matrix, in Eq. (2.41) are given by,

\[
\xi_F^V = \sum_{i,j=1}^{N} \xi_{V,j}^{F,i}, \quad (C.1)
\]

\[
\xi_F^\Omega = \sum_{i,j=1}^{N} \left[ \xi_{\Omega,j}^{F,i} - \xi_{V,j}^{F,i} \epsilon_j \right], \quad (C.2)
\]

\[
\xi_F^\varepsilon = \sum_{i,j=1}^{N} \left[ \xi_{\varepsilon,j}^{F,i} + \xi_{V,j}^{F,i} \varphi_j \right], \quad (C.3)
\]

\[
\xi_T^V = \sum_{i,j=1}^{N} \left[ \xi_{V,j}^{T,i} + \epsilon_i \xi_{V,j}^{F,i} \right], \quad (C.4)
\]

\[
\xi_T^\Omega = \sum_{i,j=1}^{N} \left[ \xi_{\Omega,j}^{T,i} - \xi_{V,j}^{T,i} \epsilon_j - \epsilon_i \xi_{V,j}^{F,i} \epsilon_j + \epsilon_i \xi_{V,j}^{F,i} \right], \quad (C.5)
\]

\[
\xi_T^\varepsilon = \sum_{i,j=1}^{N} \left[ \xi_{\varepsilon,j}^{T,i} + \xi_{V,j}^{T,i} \varphi_j + \epsilon_i \xi_{V,j}^{F,i} \varphi_j + \epsilon_i \xi_{\varepsilon,j}^{F,i} \right], \quad (C.6)
\]

where \( \epsilon_j \) are the 3 \( \times \) 3 matrices

\[
\epsilon_{j,\alpha\beta} = \epsilon_{\alpha\beta}(r_j) = \epsilon_{\alpha\beta\gamma}r_{j,\gamma}, \quad (C.7)
\]
\[ \varphi_{j,\alpha\kappa} = \varphi_{\alpha\kappa}(r_j) = \sum_{\beta} (e^E_{\kappa})_{\alpha\beta} \epsilon_{j,\beta}, \quad (C.8) \]

with \( \epsilon \) being the Levi-Civita tensor and \( e^E_{\kappa} \) being the basis matrices defined in Appendix [B]

Finally, the stress-related sub-matrices of the grand resistance matrix are

\[ \xi^S_V = \sum_{i,j=1}^N \left[ \xi^S_{V,j} + \psi_i \xi^F_{V,j} \right], \quad (C.9) \]

\[ \xi^S_\Omega = \sum_{i,j=1}^N \left[ \xi^S_{\Omega,j} - \xi^S_{V,j} \varphi_j - \psi_i \xi^F_{V,j} + \psi_i \xi^F_{\Omega,j} \right], \quad (C.10) \]

\[ \xi^S_\varepsilon = \sum_{i,j=1}^N \left[ \xi^S_{\varepsilon,j} + \xi^S_{V,j} \varphi_j + \psi_i \xi^F_{V,j} \varphi_j + \psi_i \xi^F_{\varepsilon,j} \right], \quad (C.11) \]

with the \( 5 \times 3 \) matrices

\[ \psi_{i,\kappa\alpha} = \psi_{\kappa\alpha}(r_i) = \sum_{\beta} r_{i,\beta} (e^S_{\kappa})_{\beta\alpha}, \quad (C.12) \]

where the basis matrices \( e^S_{\kappa} \) were defined in Appendix [B]
Bibliography


