DYNAMICS OF SINGLE SEMIFLEXIBLE FILAMENTS IN A VISCOUS FLUID

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THESIS

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Abstract

Numerous cellular functions rely on semiflexible filaments as structural elements (F-actin, microtubules), locomotive organs (flagella, cilia) or carriers of information (DNA). Flexible and semiflexible polymers are also commonly encountered in technological applications, specifically in chemical engineering and materials sciences. A thorough description of the physics involved can be achieved only through a detailed modeling and understanding of their mechanical properties and dynamics. With recent advances in nanofabrication techniques and experimental capabilities using microfluidic devices, there has been a renewed interest in the dynamics of semiflexible polymers. In this work, we present a detailed and efficient simulation method for solutions of short single semiflexible polymers using slender body theory in Stokes flow. An algorithm is developed that takes into account the inextensibility and elasticity of the filament, and accounts for hydrodynamic as well as Brownian forces. This is tested against theoretically known and experimentally verified equilibrium properties and scaling laws. We then focus on flow fields commonly observed in microfluidic devices, particularly the dynamics of bio-polymers in linear shear flows and near hyperbolic stagnation points. In linear shear flow, Brownian fluctuations dislodge the filament from an otherwise stable axis resulting in a characteristic tumbling motion. A sub-linear growth of tumbling frequency with shear rate is obtained that matches with experimental observations. Also, interesting non-linear behavior of the filament shape is observed in the case of hyperbolic flow geometries that are prevalent in microfluidic devices used to separate, observe and manipulate single macromolecules. Thermal fluctuations are suppressed by the flow when the filament is aligned with the extensional axis, and this suppression is shown to
depend on the rate of extension of the external flow. Similarly, in the compressional regime, filaments undergo a buckling instability similar to Euler buckling of beams, taking on higher mode shapes with increasing flow strengths. Both suppression and buckling are attributed to a competition between tension and elasticity. Our study confirms the existence of this stretch-coil transition, which could also explain certain biophysical aspects of filament rearrangement in streaming and bio-locomotion. A detailed characterization of such behavior pertaining specifically to flow fields commonly seen in microfluidic devices will aid in the design of such devices constructed particularly for trapping, separating and precise control of single polymer molecules. Furthermore, the model developed here can be potentially extended to include interactions and electrokinetic phenomena that may then lead to solving problems in applications like DNA electrophoresis and polymer translocation through pores.
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Chapter 1

Introduction

Nature abounds with ingenious examples of rendering dynamical capabilities at the cellular level. These abilities require structural or functional elements with properties that enable them to perform, in the most efficient fashion, the basic tasks of locomotion, reproduction and growth. And a number of these cellular functions rely on semiflexible filaments\textsuperscript{1}. These are biological polymers that are highly inextensible and with a rigidity that energetically suppresses bending \cite{1}. Microfilaments (or actin filaments) are thin filaments found in the cytoplasm of most eukaryotic cells that are flexible and relatively strong. With their resistance to tensile and compressive forces at the subcellular scale, they play highly versatile roles in motility, cellular shape changes and mechanical support. Microtubules (rope-like polymers of tubulin proteins) are highly dynamic members that play critical roles in maintaining cell structure, intracellular transport and cell reproduction. Flagella are tail-like protrusions from a cell body that lash back and forth like a whip, and are responsible for locomotion of many micro-organisms and cells like spermatozoa. Cilia are similar slender protuberances that play roles in mobility and sensing. And of course, one of the most critical and well known macromolecules in all known life forms in Deoxyribonucleic acid (DNA). These single or double stranded polymers of simple units called nucleotides are contained in the nucleus or the cytoplasm and carry genetic instructions that are passed on across generations of cells. DNA has, over the years, gained the attention of scientists outside of biology too - their applications in forensics, bioinformatics, nanotechnology and anthropology are widespread.

Dynamics of semiflexible fibers in a viscous fluid are also key to understanding many

\textsuperscript{1}The terms filament, fiber and polymer will be used interchangeably in this work
interesting problems in engineering. Non-Newtonian bulk behavior of suspensions can, in many cases, be attributed to such fibers that make up their micro-structure [2, 3]. They are also relevant in understanding the rich and interesting area of soft materials. Semiflexible synthetic polymers are often encountered in technological applications, specifically in chemical engineering and materials sciences. With recent advances in nanofabrication techniques and experimental capabilities using microfluidic devices [4, 5, 6, 7], there has been a renewed interest in the dynamics of semiflexible polymers.

A thorough description of the biophysical processes involving these polymeric molecules can only be achieved through a detailed understanding and modeling of their mechanical properties and dynamics. Of particular interest is the behavior of semiflexible filaments in external flows that commonly occur in microchannels that may be used for separation, trapping and observation of single polymer molecules [4, 8]. For instance, G. I. Taylor’s classic four-roll mill [9] has been used widely to create hyperbolic stagnation points to trap drops and particles. Recently, this idea has been scaled down to successfully trap and manipulate micro- and nanoscale particles [6, 7]. In the vicinity of such a hyperbolic flow geometry, semiflexible polymers are known to display interesting non-linear dynamics as a result of the competition between elastic energy and tension - a situation well-known for inducing a buckling instability in filaments and pearling instability in membranes [10]. Another interesting application is the electrokinetic transport and separation of charged macromolecules [11, 5]. This problem, which requires the coupling of the hydrodynamic problem with the solution for the electric force acting on the polymer, holds the scope for theoretically explaining many observed phenomena in applications like DNA electrophoresis.

One common feature of the examples listed above is the large aspect ratio of length to characteristic thickness, ranging from order ten to many thousands in some biological settings. This fact has been historically exploited in many ways to develop models describing such polymers. One such model is the bead-spring model [12, 13]. Here, a polymer is modeled as a sequence of beads, each offering hydrodynamic resistance to flow of the surrounding
medium, and connected to each other with springs that provide for elastic and deformational properties of the chain as a whole. These are appropriate for very long chains, and detailed internal dynamics are not captured. A related class is the bead-rod model [14, 15] that uses rigid links with bending moments to connect beads. This latter model is prevalent in the study of short semiflexible biological polymers. However, hydrodynamic interactions are not naturally included in bead-rod models, in which drag only occurs at the beads, and the drag anisotropy of slender polymer segments is not captured by these models, with a few exceptions [15].

A very different approach is based on slender-body theory [16, 17, 18] for hydrodynamics, which exploits the aforementioned large aspect ratio of the fibers. This model does capture drag anisotropy due to the slenderness, and can be easily extended to include hydrodynamic interactions within and between filaments. This model, along with Euler-Bernoulli elasticity, has been used recently [3, 19, 20] to model non-Brownian flexible filaments in flow. Versions of this model have been used to study forced dynamics of stiff polymers [21, 22]. The primary appeal of using this model lies in the reduction of a filament-fluid interaction problem to a relatively simple equation describing the filament centerline, along with constraints imposed by the physics of the problem under consideration. Numerical methods based on this approximation have been designed [3] that reduce computational cost as compared to grid based methods that may be required if the problem was not simplified to a set of coupled equations describing the filament centerline.

1.1 The Low-Reynolds-Number Limit

The motion of a Newtonian fluid is governed by the Navier-Stokes equations, which are obtained by applying Newton’s second law to a material particle inside the fluid. In situations in which inertia can be neglected with respect to viscous forces, these equations simplify to
[23] the Stokes equations\(^*\):

\[-\nabla p + \mu \nabla^2 \mathbf{u} = 0, \quad \nabla \cdot \mathbf{u},\]

which describes the conservation of momentum and mass associated with a fluid of velocity \(\mathbf{u}(\mathbf{x})\), pressure \(p(\mathbf{x})\) and dynamic viscosity \(\mu\). The Stokes equations provide a good approximation to the flow field when the Reynolds number

\[Re = \frac{\rho U a}{\mu}\]

is very small. Here, \(U\) and \(a\) are representative values of velocity and length. A quick calculation using the length scales associated with micro-organisms or single cells (0.1 to 100 micrometers), the properties of water (density of 1 kilogram per cubic metre and viscosity of about 1 centipoise at room temperature) and motion of such particles in the range of a few micrometers to millimetres per second shows us that the Reynolds number ranges from \(10^{-6}\) to \(10^{-4}\). This substantiates the use of Stokes equations for these so-called creeping flows [25].

Now, if we assume we have a filament in the flow, and let \(\partial S\) denote its surface and \(\mathbf{u}_{\partial S}\) its surface velocity. Imposing the no-slip condition on \(\partial S\) and the requirement that far away, the velocity equals a background velocity \(\mathbf{u}^\infty(\mathbf{x})\) which is also a solution to the Stokes equations gives:

\[\mathbf{u} = \mathbf{u}_{\partial S} \text{ on } \partial S, \quad \mathbf{u} \to \mathbf{u}^\infty \text{ for } ||\mathbf{x}|| \to \infty.\]

A full formulation of this problem would yield integral equations that are very expensive to solve numerically. Instead, the slenderness of the filament is exploited to reduce it to an equation of the filament centerline, using the fundamental solutions of the Stokes equations.

The Stokeslet is one such fundamental solution - it is the Green’s function of the Stokes equations.

\(^*\)The implicit assumption is that the unsteady term is as insignificant as the non-linear convective term, sometimes justified as the Stokes number limiting to zero. See Guazzelli & Morris [24].
equations for a point force. The Stokeslet tensor is given by

$$G(x, x_0) = \frac{1}{8\pi \mu} \frac{I + \hat{r}\hat{r}}{|r|},$$

where $I$ is the identity tensor, $r = x - x_0$, $\hat{r}$ is the unit vector $\hat{r} = r/|r|$ and $\hat{r}\hat{r}$ is a dyadic product. The Stokeslet is sometimes represented [26, 25] without the factor $1/8\pi \mu$ and is called the Oseen tensor. Clearly, by its very definition:

$$u(x) = G(x, x_0) \cdot f(x_0).$$

In addition to the Stokeslet, higher order fundamental solutions (doublet and so on) can be constructed by differentiation of the Oseen tensor.

The premise of the slender body theory is that an approximation to the presence of a filament can be derived by placing a line distribution of such fundamental solutions on the filament centerline, and then employing the technique of matched asymptotics.

### 1.2 A Few Preliminaries

#### 1.2.1 The Slender Body Theory

The notion behind the development of slender body theory for hydrodynamics is that the disturbance felt due to the presence of a body whose length is much larger than its characteristic thickness is the same as that due to a particular line distribution of Stokeslets. This formulation exploits the strong shape anisotropy of the elongated filament. The idea of exploiting the slenderness of a body in viscous flow has been around since Cox [27, 28] and was developed in great detail by Batchelor [16], Keller & Rubinow [18] and Johnson [17]. Simply put, the flow very close to the body is similar to that near a cylinder with the no-slip condition imposed (the ‘inner flow’) which is then asymptotically matched to the flow far
away as felt due to the aforementioned line distribution (the ‘outer flow’).

Figure 1.1: The geometry of the slender body as considered in Section 1.2.1

We consider a filament of length $L$ parametrised by arclength $s \in [0, L]$ and $\mathbf{x}(s, t) = (x(s, t), y(s, t), z(s, t))$ represents the filament centerline (Figure 1.1). It is important to note that $s$ is assumed to be a material parameter, and is thus independent of time. If the filament were circular in cross-section with radius $r(s)$ such that $r(s) = 2\epsilon \sqrt{s(L - s)}$, we can define a slenderness parameter $\epsilon$ where $r(L/2) = \epsilon L$. A non-local slender body approximation [29, 3] of the centerline velocity is given by

$$8\pi \mu \left( \frac{\partial \mathbf{x}(s, t)}{\partial t} - \mathbf{u}_0(\mathbf{x}(s, t), t) \right) = -\Lambda[f](s) - K[f](s), \quad (1.6)$$

where $f$ is the force per unit length on the filament and $\mu$ is the fluid viscosity. Here, $\Lambda[f](s)$ is the local operator defined as

$$\Lambda[f](s) = [-c(I + \hat{\mathbf{p}}(s)) + 2(I - \hat{\mathbf{p}}(s))] \cdot f(s). \quad (1.7)$$
Here, \( c = \log(\epsilon^2 e) \) and \( \hat{p} = x_s \) is the unit tangential vector along the axis of the filament, where the subscript refers to differentiation with respect to arclength. The integral operator \( K[f](s) \) is given by

\[
K[f](s) = \int_0^L \left( \frac{I + \dot{r}(s, s') \dot{r}(s, s')}{|r(s, s')|} \cdot f(s') - \frac{I + \hat{p}(s) \hat{p}(s)}{|s - s'|} \cdot f(s) \right) \, ds',
\]

(1.8)

where \( r(s, s') = x(s) - x(s') \), caps denote unit vectors and \( \dot{r} \) and \( \hat{p} \hat{p} \) are dyadic products. This approximation for the velocity of the centerline is accurate to the order \( O(\epsilon^2 \log\epsilon) \) and is uniformly valid for the specific choice of filament radius as described above [17].

Clearly, the operators \( \Lambda \) and \( K \) depend on the shape of the filament at any given time. The local operator, as we shall henceforth call \( \Lambda \), accounts for drag anisotropy due to the slenderness of the filament. This can be easily seen if we consider the part \(-c(I + \hat{p} \hat{p})\); for a needle-like rigid body, inverting this operator suggests that drag on the body for translations perpendicular to the axis are twice that for translations parallel to the axis - a well-known hydrodynamic result [25]. The remainder terms are non-local corrections that capture the global effect on the fluid velocity from the presence of the filament.

The fluid velocity \( u(x) \) at any point \( x \) in the flow and not on the filament is approximated by

\[
8\pi\mu (u(x) - u_0(x)) = -\int_0^L \left( \frac{I + \dot{r}(s') \dot{r}(s')}{|r(s')|} + \frac{\epsilon^2 I - 3\dot{r}(s') \dot{r}(s')}{2 |r(s')|^3} \right) \cdot f(s') \, ds',
\]

(1.9)

where now \( r(s') = x - x(s') \). Note that (1.9) follows directly from (1.5), with the additional second term representing a doublet.

To study the dynamic of several filaments in say a suspension of fibers, one can simply add up the contribution to the total velocity field from each individual filament. This works due to the superposition principle for linear Stokes flow. Particularly, the centerline equation

\[
\]
gets modified as

\[ 8\pi\mu \left( \frac{\partial \mathbf{x}_\beta(s, t)}{\partial t} - \mathbf{u}_0(\mathbf{x}_\beta(s, t), t) \right) = -\Lambda_\beta[\mathbf{f}_\beta](s) - K_\beta[\mathbf{f}_\beta](s) - \sum_{\alpha=1, \alpha \neq \beta}^N \Upsilon_\alpha(\mathbf{x}_\beta(s)), \tag{1.10} \]

where the summation is over \( 1 \leq \alpha \leq N \) filaments, with the contribution of the filament \( \beta \) omitted, as it is accounted by the other terms as in (1.6). Here \( \Upsilon_\alpha \) denote the terms on the right hand side of (1.9) evaluated to obtain the disturbance velocity due to filament \( \alpha \) on the centerline of filament \( \beta \).

1.2.2 Euler-Bernoulli Elasticity

The dynamic equation for forces on a single filament can be obtained by minimising the functional \( \mathcal{E} \) that represents the energy associated with the mechanical forces acting on it:

\[ \mathcal{E} = \frac{1}{2} \int_0^L \left[ A \mathbf{x}_{ss}^2 + T(\mathbf{x}_s^2 - 1) \right] ds. \tag{1.11} \]

Here, the first term represents elastic energy with \( A = EI \) being the flexural rigidity (product of Elastic modulus and the second moment of area) and \( T(s, t) \) is a Lagrangian multiplier that acts to keep the the filament locally inextensible \( (\mathbf{x}_s \cdot \mathbf{x}_s = \mathbf{p}^2 = 1) \) at all times. Physically, \( T(s, t) \) corresponds to a line tension along the filament centerline that acts to keep it at a constant length.

The total energy associated with one filament can be minimized by writing an Euler-Lagrange equation of \( \mathcal{E} \):

\[ \frac{\partial \mathcal{E}}{\partial \mathbf{x}} - \frac{\partial}{\partial s} \left( \frac{\partial \mathcal{E}}{\partial \mathbf{x}_s} \right) + \frac{\partial^2}{\partial s^2} \left( \frac{\partial \mathcal{E}}{\partial \mathbf{x}_{ss}} \right) = 0. \tag{1.12} \]

If \( \mathbf{f}(s) \) is the external force per unit length acting on the filament, this gives us:

\[ \mathbf{f}(s) = -(T(s)\mathbf{x}_s)_s + A\mathbf{x}_{ssss}. \tag{1.13} \]
Note that the second derivative of $x$ with respect to arclength is not zero in general as the filament is flexible.

### 1.2.3 Brownian Motion

At the length scales associated with bio-polymers, Brownian fluctuations become relevant and an additional term is required in Equation (1.13) to model thermal fluctuations in the solvent. This additional term is a stochastic force distribution $f^{br}$ that must satisfy the fluctuation-dissipation theorem of statistical mechanics. This relates the expectation values of the Brownian forces to the friction coefficient of the filament. More precisely, the Brownian force must satisfy:

\[ \langle f^{br}(s, t) \rangle = 0, \]
\[ \langle f^{br}(s, t)f^{br}(s', t') \rangle = 2k_B T M^{-1}\delta(t - t')\delta(s - s'), \]

where $\langle \cdot \rangle$ represents an ensemble average, $\delta$ is the Dirac delta function and $k_B T$ is the thermal energy. $M$ is the mobility tensor associated with the filament at that instant. A Brownian force that satisfies these statistics gets added to (1.13) and this captures the effect of stochastic thermal fluctuations.

### 1.3 How Flexible is Semiflexible?

Having briefly reviewed elasticity and Brownian fluctuations in the preceding sections, we are now in a position to ask the question that defines the very scope of this work - exactly how flexible is semiflexible? We have so far been rather informal about the definition of semiflexibility, and shall now define precisely what the term means.

For this, we first introduce the concept of persistence length ($\ell_p$). It can be thought of as a length scale at which thermal fluctuations and elastic forces in the filament strike
a balance. More rigorously, $\ell_p$ is the characteristic length associated with the exponential decay of tangent vector autocorrelation [1, 30]. In other words, tangent vectors lose memory of the direction of each other over this length:

$$\langle \hat{\mathbf{p}}(s) \cdot \hat{\mathbf{p}}(s') \rangle = \exp \left[ -\frac{|s - s'|}{\ell_p} \right].$$

(1.16)

A more handy relation that directly associates with the idea of a balance between elasticity and thermal fluctuations is [31, 32]

$$\ell_p = \frac{A}{k_B T}.$$  

(1.17)

If the tangential correlations decay rapidly, as in the case of many synthetic polymers, the persistence length is very small. Such polymers, for which $\ell_p \ll L$, are called flexible and presumably, they energetically favor coiled states. On the other end of the spectrum are extremely rigid (with respect to Brownian fluctuations) fibers with $\ell_p \gg L$ which almost do not give in to shape fluctuations due to Brownian forces. The semiflexible regime that we shall focus on in this work is where $\ell_p \approx L$. Within this regime, DNA and actin tend to be on the flexible end, whereas microtubules are on the stiffer side. As an example, in the classic experiments of Gittes et al. [1], microtubules were found to have a rigidity of $A \approx 10^{-23} Nm^2$ corresponding to a persistence length of $\ell_p \sim 5mm$ whereas the corresponding values for actin were $A \sim 10^{-26} Nm^2$ and $\ell_p \sim 18\mu m$.

1.4 Overview of current work

The focus of the current work is to describe the dynamics of single semiflexible biopolymers in Stokesian fluids. We start with implementing the model based on the slender body theory described in Section 1.2.1. Chapter 2 primarily deals with this implementation where we derive an equation governing the centerline of the filament along with a coupled tension equation that arises from the inextensibility condition. The associated computational
methods are described, along with justifications of the conditions and methods used.

Chapter 3 presents results and discussion regarding the dynamics of single fibers in purely Brownian solvents - those that do not have an imposed background flow field. We compare results from our algorithm to analytical and experimental results that describe the statistical properties of polymers, and draw physical conclusions from it. This also serves as a test case for the model.

In Chapter 4, we move ahead in applying the model to understand the dynamics of a single filament in an imposed flow field. The case of a linear shear flow is first considered, where we begin with non-Brownian fibers, and compare our results to previous works and established theory regarding the rotation of rigid filaments. A dynamical description of this system follows, and that leads to the full model where Brownian forces are considered as well. The interesting phenomenon of periodic tumbling is introduced and scaling laws associated with it are described herein.

The latter part of Chapter 4 deals with the fluctuations and dynamics of filaments near a hyperbolic stagnation point. The suppression of thermal fluctuations in the extensional regime and the buckling instability in the compressional regime are discussed in detail here. An analytical approximation for the suppression is derived based on a variational approach, that is reflected in our simulations. We also discuss numerical results from the ‘stretch-coil’ transition and buckling instability that have been observed in recent experiments.

We end by summarizing the findings and proposing ways to improve the model, to include physics that make it more directly applicable to corresponding experiments and a perspective on the myriad of interesting problems that such a description would allow us to solve.
Chapter 2

Single Filament Model

2.1 The Centerline Equation

As described in Chapter 1, the presence of the filament or fiber is felt only by the disturbance velocity of the line distribution of Stokeslets. In other words, the filament is assumed to have zero thickness. As such, the equation of motion of the centerline of the filament as given by the slender body theory in Section 1.2.1 is assumed to represent the dynamics of the entire filament. This approximation is valid in the very high-aspect-ratio limit which applies in the case of bio-polymers that we consider, with the characteristic thickness being a few orders of magnitude less that the characteristic length.

For our model, we consider a single filament far away from other filaments or walls. This can be thought to physically represent the setting in a microchannel experiment (a single DNA separation device, for instance) with the channel width being significantly larger than the filament size. This free-draining approximation allows us the use of slender body theory as described in Section 1.2.1 without significant modifications. Introducing the effect of confinement in this model is a topic of future interest, and a brief perspective will be provided in Chapter 5. For now, we neglect wall interactions without having to resort to modified Green’s functions of the Stokes equations [33, 15] or using auxiliary solutions to correct for the presence of boundaries [34].

Regarding hydrodynamic interactions, since we consider only single filaments in this study, the extra terms accounting for multiple filaments do not picture at all. Furthermore, the integral operator in Equation (1.6) which accounts for intra-chain interaction is also not
considered here. The assumption here is that the effect of filament motion on the background flow is small enough not to introduce significantly different dynamics as compared to that due to the shape anisotropy. Furthermore, the integral operator in Equation (1.8) is singular at \( s = s' \) and requires careful handling to make it suitable for numerical computations [3]. On the same lines, the filament is assumed not to cross over itself.

With these assumptions, we now write the centerline equation from Equations (1.6) and (1.7) that accounts for the motion of a filament of position \( \mathbf{x}(s, t) \) in a fluid with imposed velocity \( \mathbf{u}_0(\mathbf{x}(s, t), t) \) as:

\[
8\pi\mu \left( \frac{\partial \mathbf{x}(s, t)}{\partial t} - \mathbf{u}_0(\mathbf{x}(s, t), t) \right) = \left[ c(I + \mathbf{\hat{p}}(s)) - 2(I - \mathbf{\hat{p}}(s)) \right] \cdot \mathbf{f}(s). \tag{2.1}
\]

Here \( \mathbf{f}(s) \) is the force per unit length on the filament body, which we know from the discussion is Sections 1.2.2 and 1.2.3 to be

\[
\mathbf{f}(s) = -(T(s)\mathbf{x})_s + A\mathbf{x}_{ssss} + \mathbf{f}^{br}(s), \tag{2.2}
\]

where \( T(s) \) is the varying line tension, \( A \) is the rigidity of the filament which is assumed to be a homogeneous material property, and \( \mathbf{f}^{br}(s) \) is the stochastic Brownian force acting on the filament as described by the conditions in Equations (1.14) and (1.15). It is important to note here that twist elasticity is neglected [35]. Also, as mentioned earlier, we do not explicitly add any forces to maintain physical uniqueness of different filament point locations - excluded volume is assumed.

Regarding boundary conditions, the filament ends are ‘free’, i.e., there are no forces or moments acting at the ends of the filament. This is true for an untethered filament suspended freely in a fluid [32, 3, 22]. This gives

\[
\mathbf{x}_{ss}|_{s=0,L} = \mathbf{x}_{ssss}|_{s=0,L} = T|_{s=0,L} = 0. \tag{2.3}
\]
2.1.1 Non-dimensionalization

In the problems that we consider here, the imposed flow is assumed to be of a constant flow strength $\dot{\gamma}$. This immediately gives us a time scale $\dot{\gamma}^{-1}$. However, it is important to note that this might not be a suitable time scale to non-dimensionalize the velocity of the filament, which is affected by Brownian fluctuations. Clearly, another time scale comes into play here (and as we shall discover in Chapter 4, the ratio of these two scales has interesting physical implications) and this is $8\pi \mu L^4/A$. All lengths are made dimensionless using the contour length $L$ and forces with $A/L^2$.

For Brownian forces, following [32], we use a different scaling:

$$f^{br} = \left[ \sqrt{\frac{L}{\ell_p}} \frac{A}{L^2} \right] \xi, \quad (2.4)$$

where $\xi$ is the dimensionless Brownian force, and the ratio $\sqrt{L/\ell_p}$ is introduced so that the dimensionless noise has the second moment of the form:

$$\langle \xi(s, t) \xi(s', t') \rangle = 2 \Lambda^{-1} \delta(t - t') \delta(s - s'). \quad (2.5)$$

Here, $\Lambda$ is the local mobility tensor as described in Equation (1.7). Note that we have made use of Equation (1.17) to arrive at the above form. This, in addition to the condition of zero mean ($\langle \xi(s, t) \rangle = 0$) defines the Brownian force.

The non-dimensional centerline equation thus becomes

$$\frac{\partial x(s, t)}{\partial t} = \bar{\mu} u_0(x(s, t), t) - \Lambda \cdot \left[ -(T(s)x_s) + x_{ssss} + \sqrt{\frac{L}{\ell_p}} \xi(s) \right], \quad (2.6)$$

where all variables are now dimensionless. The parameter $\bar{\mu}$ is a ratio of the characteristic
fluid drag to the filament elastic force:

\[ \bar{\mu} = \frac{8\pi \mu \gamma L^2}{A/L^2}. \]  

(2.7)

This ratio, sometimes called an effective viscosity [3, 20], along with the ratio \( L/\ell_p \) control the relative importance of viscous, elastic and Brownian forces in this formulation. The only other parameter now is \( c = \log(\epsilon^2 \epsilon) \) which appears in the mobility operator \( \Lambda \) and this is taken to be a constant value for our purposes.

### 2.2 The Tension Equation

We recollect from our discussion in Section 1.2.2 that the line tension in Equation (2.2) acts in a way so as to keep it inextensible. This tension is configuration dependent and has to be evaluated at every instant based on the shape and viscous forces at that instant. What this means is that we need to construct, in addition to Equation (2.6), a coupled equation for that will evaluate the tension. This tension can be then fed into the force distribution to evaluate the position of the filament centerline.

For this, we consider the condition of inextensibility \( x_s \cdot x_s = 1 \) where \( x_s = \hat{p} \) is the unit tangent vector at \( s \). We can thus write:

\[ \frac{\partial}{\partial t} (x_s \cdot x_s) = 0 \Rightarrow x_s \cdot x_{ts} = 0, \]  

(2.8)

where we have used the fact that \( s \) is a material parameter to interchange the \( s \) and \( t \) derivatives. This condition can be combined with Equation (2.6) to get

\[ x_s \cdot \frac{\partial}{\partial s} \left( \bar{\mu} u_0(x(s, t), t) - \Lambda \cdot \left[ -(T(s)x_s)_s + x_{ssss} + \sqrt{\frac{L}{\ell_p}} \xi(s) \right] \right) = 0, \]  

(2.9)

where \( \Lambda = -c(I + x_s x_s) + 2(I - x_s x_s) \). Further simplification requires a ladder of differential
identities, derived from the filament inextensibility condition:

\[
x_s \cdot x_s = 1,
\]
\[
x_s \cdot x_{ss} = 0,
\]
\[
x_s \cdot x_{sss} = -x_{ss} \cdot x_{ss},
\]
\[
x_s \cdot x_{ssss} = -3x_{ss} \cdot x_{ssss},
\]
\[
x_s \cdot x_{sssss} = -3x_{ss} \cdot x_{ss} - 4x_{ss} \cdot x_{ssss}.
\]

The resulting form of the dimensionless line tension equation reads:

\[
2cT_{ss} + (2 - c)(x_{ss} \cdot x_{ss})T = \bar{\mu}x_s \cdot \frac{\partial u_0}{\partial s} + (2 - 7c)(x_{ss} \cdot x_{ssss}) - 6c(x_{ss} \cdot x_{ssss})
\]
\[
+ 2c \sqrt{\frac{L}{l_p}} (\xi_s \cdot x_s) + (2 + c) \sqrt{\frac{L}{l_p}} (\xi \cdot x_{ss}).
\]  

(2.10)

This is a second order inhomogeneous differential equation in \(T(s)\) and can be solved if the position and Brownian forces are known. This tension acts as a Lagrangian multiplier, constraining the motion of the filament in a way as to ensure inextensibility. This is ensured from the fact that this equation was derived beginning from \(x_s \cdot x_s = 1\) for all \(s\) at all time. In practice however, numerical errors will be introduced into our computations from the finite difference approximations that will be made to the derivatives, and additional correction might be required to ensure this constraint. This is accounted \[3\] by replacing the inextensibility condition in Equation (2.8) by

\[
\frac{\partial}{\partial t} (x_s \cdot x_s) = x_s \cdot \frac{1}{2}x_{ts} = \beta (1 - x_s \cdot x_s).
\]  

(2.11)

Clearly, this is equivalent to the original condition when \(x_s \cdot x_s = 1\) and acts to counter the error if there is one. The penalization parameter \(\beta\) is chosen based on the computational parameters. This modified constraint only changes the tension equation (2.10) with an
additional $-\beta(1 - x_s \cdot x_s)$ term on the right hand side.

2.3 Computational Methods

In this section, we discuss the numerical methods applied to the single filament model as described in the preceding sections. We shall also describe in detail how the stochastic terms are computed and conditioned for numerical stability.

2.3.1 Semi-Implicit Time Marching

The spatial derivatives in Equations (2.6) and (2.10) are discretized using second-order divided differences, and the time marching is performed using a second-order time-stepping scheme. The fourth derivatives of $x$ with respect to arclength in Equation (2.6) will yield a strict fourth-order stability limit on the time-step size. The obvious way to get past this constraint is to use an implicit scheme. Instead of making the entire equation implicit thus increasing computing cost, we use a semi-implicit scheme \[3\] wherein all occurrences of $x_{ssss}$ are treated implicitly. Specifically, we separate the terms in Equation (2.6) as

$$ \frac{\partial x}{\partial t} = M(x, x_{ssss}) + N(x). \tag{2.12} $$

Here, the terms in $M$ are to be treated implicitly, whereas $N$ is completely explicit.

Time-marching is second order accurate using a backward differentiation formula. For time-step $\Delta t$ and subscripts denoting time at which the term is being evaluated, we have:

$$ \frac{1}{2\Delta t}(3x^{n+1} - 4x^n + x^{n-1}) = M(2x^n - x^{n-1}, x_{ssss}^{n+1}) + 2N(x^n) - N(x^{n-1}). \tag{2.13} $$

To illustrate this, applying the above scheme to the centerline equation in (2.6) requires us
to first separate the terms that will be treated implicitly and explicitly:

\[
\frac{\partial}{\partial t} \mathbf{x} + \Lambda [x_{ssss}] = \bar{\mu} \mathbf{u}_0 - \Lambda \left( -T \mathbf{x}_s \right)_s + \sqrt{\frac{L}{\ell_p}} \xi = N(\mathbf{x}).
\] (2.14)

Here, the mobility operator $\Lambda$ acting on the fourth derivative (moved to the left hand side) is evaluated implicitly and the terms grouped into the right hand side are treated explicitly. This then becomes, following Equation (2.13) and using the definition of $\Lambda$:

\[
\frac{1}{2\Delta t} (3x^{n+1} - 4x^n + x^{n-1}) + (2 - c)x_{ssss}^{n+1} - (2 + c) [ (2x^n_s - x_{ss}^{n-1}) \cdot x_{ssss}^{n+1} ] (2x^n_s - x_{ss}^{n-1}) \\
= 2N(x^n) - N(x^{n-1}),
\] (2.15)

where the dyadic product has been simplified to show the numerical scheme. The only difference is the very first time step, where we do not have a previous time level available, and there we use a simple forward Euler step. And finally, the tension equation (2.10) introduces no constraint on the time-step and so is evaluated explicitly at the current time level.

As to spatial discretization, we consider $N$ equally spaced points on the filament with spacing $h$ such that $h = \Delta s = 1/(N - 1)$. Hence, the discrete points become $s_j = jh$ where $j = 1, 2, \ldots, N$. All spatial derivative are approximated by second-order divided differences, so the approximation is valid to an $O(h^2)$ error. Standard centered stencils are used wherever applicable, except at the boundaries where skewed operators are applied. The boundary conditions of forcelessness and momentlessness at the ends, from Equation (2.3), enter the system enforcing conditions on the finite difference stencils applied at or near the end points. For all the results presented in this work, we use 64 spatial points to discretize one filament, and the dimensionless time step is $\Delta t = 10^{-10}$. The aspect ratio $\epsilon$ is taken to be 0.01.
2.3.2 Evaluating Brownian Terms

Recollect from Section 1.2.3 that the Brownian forces are specified only by their mean and second moment - properties that make them satisfy the fluctuation-dissipation theorem. Numerically, this force distribution $\xi$ is approximated as:

$$\xi(s,t) = \sqrt{\frac{2}{\Delta s \Delta t}} \mathbf{B} \cdot \mathbf{w}, \quad (2.16)$$

where $\mathbf{w}$ is a random vector from a Gaussian distribution of zero mean and unit variance. $\Delta s$ is the spatial grid spacing and $\Delta t$ is the time step. $\mathbf{B}$ is the tensor square root of the resistance tensor $\Lambda^{-1}$. This approximation can be seen to satisfy Equation (2.5) directly.

The random vector $\mathbf{w}$ is generated from a uniform distribution at each evaluation. Calculating the square root of the inverse of the mobility tensor can be costly, especially since the tensor depends on the current position and this is updated at every time-step. For the operator $\Lambda$, we evaluate the form of $\mathbf{B}$ analytically using the following manipulation: we can represent the mobility operator $\Lambda$ in the form $(2 - c)(\mathbf{I} - \alpha \hat{p}\hat{p})$, where $\alpha = (2 + c)/(2 - c)$. Then assuming $\Lambda^{-1}$ to be of the form $(\mathbf{I} + \beta \hat{p}\hat{p})/(2 - c)$, one can write:

$$\Lambda \Lambda^{-1} = (\mathbf{I} - \alpha \hat{p}\hat{p})(\mathbf{I} + \beta \hat{p}\hat{p}) = \mathbf{I}. \quad (2.17)$$

This allows us to solve for $\beta$ and we get $\beta = \alpha/(1 - \alpha) = -(2 + c)/2c$ which then yields the form of $\Lambda^{-1}$:

$$\Lambda^{-1} = \frac{1}{2 - c} \left[ \mathbf{I} - \left( \frac{2 + c}{2c} \right) \hat{p}\hat{p} \right]. \quad (2.18)$$

Finding the tensor square root of $\Lambda^{-1}$ is now a similar exercise: we assume that $\sqrt{\Lambda^{-1}}$ is of the form $(\mathbf{I} + \gamma \hat{p}\hat{p})/\sqrt{(2 - c)}$ and then

$$(\mathbf{I} + \gamma \hat{p}\hat{p})(\mathbf{I} + \gamma \hat{p}\hat{p}) = \mathbf{I} + \beta \hat{p}\hat{p}.$$
One can solve for \( \gamma = -1 \pm \sqrt{1 + \beta} = -1 \pm \sqrt{(c - 2)/2c} \) where either of the roots may be used. This then gives the form of the inverse of the square root of the mobility tensor

\[
B = \sqrt{\Lambda^{-1}} = \sqrt{\frac{1}{2 - c}} \left[ I + \left( -1 \pm \sqrt{\frac{c - 2}{2c}} \right) \hat{p} \hat{p} \right], \tag{2.19}
\]

which goes into Equation (2.16). Of course, this method is possible only due to the form of \( \Lambda \); if hydrodynamic interactions were to be included, the mobility operator would include the integral in Equation (1.8) and a full square root algorithm or asymptotics must be applied.

There are two important points to notice at this point. The first is that the tension equation (2.10) has the spatial derivatives of the Brownian force \( \xi(s) \) appearing in it. Brownian forces at adjacent grid points can be completely uncorrelated and using Equation (2.16) directly in Equation (2.10) can lead to numerical instabilities resulting from the very large terms obtained by directly differentiating \( \xi(s) \). Noting that high wavenumber force fluctuations do not result in high wavenumber shape fluctuation owing to the strongly smoothing nature of the fourth derivative in Equation (2.6), one strategy to solve this problem will consist of applying a ‘low-pass-filter’ to the stochastic force distribution. This is achieved by taking a Fourier transform of \( \xi(s) \) which allows us to sort the distribution by wavenumber. The highest few wavenumbers (representing the sharpest gradients) are cut out and the distribution is transformed back. The magnitude of \( \xi(s) \) is then rescaled to conserve the total energy by matching the variance to that of Equation (2.5). It is important here to not cut out so many wavenumbers so as to lose the dynamics due to thermal fluctuations; we have filtered out not more than the top 40% of wavenumbers and this is seen not to affect the equilibrium properties (as will be described in detail in Chapter 3).

The other caveat is that the Brownian force in Equation (2.16) is proportional to the square root of the time-step. This means that during integration, the effective order of the time marching scheme is reduced from second to first order. This has been noted previously [12] and will result in a stricter time constraint to ensure stability and accuracy. The way to
get past this would be to implement specialized stochastic integration algorithms [36, 37, 38] like a mid-point scheme that are tailored to bring up the order of accuracy. This gain in order of accuracy is at the price of more evaluations at every time-step. Implementing a more accurate while at the same time economic scheme is a challenging open problem.

### 2.4 Summary

The centerline of the filament is modelled as a line distribution of singularities, following slender body theory. We neglect hydrodynamic interactions and account for only drag anisotropy, which gives the governing equation for the centerline as in Equation (2.6). Forces come into the equation based on Euler-Bernoulli elasticity, and Brownian forces are also accounted for. The inextensibility condition is enforced through a line tension equation. The coupled system of centerline and tension equations is solved with the boundary conditions of force and moment free ends.

The system is time-marched using a semi-implicit scheme, where all terms but the fourth order derivatives are treated explicitly using a second-order backward scheme. Terms involving the fourth derivative are treated implicitly to avoid strict time step constraints. All spatial derivatives are approximated by second order finite differences. The Brownian force is approximated as in Equation (2.16), where the square root of the inverse of mobility can be found analytically.
Chapter 3

Dynamics in the Absence of Background Flow

In this chapter, we apply our model to study the dynamics of semiflexible polymers in a Brownian solvent. There is no imposed flow field, and the only force driving the polymer is the Brownian force acting along its length. In such a case, the polymer is known to exhibit characteristic equilibrium properties. We begin by discussing the equilibrium properties of end-to-end distance and radius of gyration; this leads us to the sub-diffusive growth of the mean-square displacement of the end-to-end distance with time and the saturation values of the same. We end the chapter with a detailed description of the diffusive properties of the filament, over both short and long times. These properties, when compared against expected analytical measures, serve as a verification for our model before we apply it to cases with imposed background flows.

3.1 Equilibrium Length Properties

3.1.1 End-to-end Distance

When a polymer undulates due to thermal fluctuations, the arc-length is conserved due to inextensibility. This lets us define the end-to-end distance (sometime called ‘projection distance’ [31]) of the polymer - the straight line displacement \( R \) between its ends. Since the fluctuations are stochastic, we are interested in the mean value about which the end-to-end distance fluctuates. In other words,

\[
\langle R^2 \rangle = \langle |r_{ee}|^2 \rangle, \quad r_{ee} = x(L) - x(0), \tag{3.1}
\]
where we have defined the mean-square end-to-end distance $\langle R^2 \rangle$ as the ensemble average of the magnitude of the end-to-end vector $r_{ee}$ in equilibrium.

\[ r_{ee} = \int_0^L x_s ds. \]  

(3.2)

We now use the definition of the persistence length $\ell_p$ from Equation (1.16) as the length scale over which the autocorrelation of the tangent vector $x_s$ decays exponentially:

\[ \langle x_2(s_1) \cdot x_s(s_2) \rangle = exp \left( -\frac{|s_1 - s_2|}{\ell_p} \right), \]  

(3.3)

which allows us to rewrite Equation (3.1) using Equation (3.2) as

\[ \langle R^2 \rangle = \int_0^L \int_0^L \langle x_s(s_1) \cdot x_s(s_2) \rangle ds_1 ds_2 = 2 \int_0^L \int_0^{s_1} \langle x_s(s_1) \cdot x_s(s_2) \rangle ds_1 ds_2. \]  

(3.4)
Now, substituting for the integrand from Equation (3.3) above and performing the integration, we can arrive at the expression for the mean-square end-to-end distance in equilibrium:

\[
\langle R^2 \rangle = 2\ell_p L - 2\ell_p^2 (1 - e^{-L/\ell_p}).
\] (3.5)

Equation (3.5) allows us to find approximate values of the end-to-end distance when the filament approaches rigid or very flexible extremes. In the limit of very rigid fibers \((\ell_p/L \gg 1)\), Equation (3.5) can be expanded in an exponential series and to \(O((\ell_p/L)^{-2})\), we have:

\[
\langle R^2 \rangle = L^2 \left(1 - \frac{1}{3} \frac{L}{\ell_p} \right).
\] (3.6)

This physically makes sense, as one would expect minimal undulations as the filament becomes rigid with respect to Brownian fluctuations, and the end-to-end distance would be very close to the contour length. In the other end of the regime, where we have extremely flexible filaments \((\ell_p/L \ll 1)\), it is seen that to \(O((\ell_p/L)^2)\),

\[
\langle R^2 \rangle = 2\ell_p L = L^2 \left(\frac{2\ell_p}{L} \right).
\] (3.7)

Clearly, a very flexible filament is seen to have a small end-to-end distance as a result of coiling due to fluctuations.

The entire spectrum from very flexible to rigid is shown in Figure 3.2. Values from our simulations for \(\ell_p/L = 4, 9, 16\) and 25 are also shown. It must be noted here that our interest is in this range of persistence lengths, and most results are presented for these cases. Keeping in mind that the end-to-end distance is a stochastic variable defined only by an ensemble average, the data shown here is averaged from 50 different runs with different random sequences.

Wilhelm & Frey [39] have derived a probability distribution function for semiflexible filaments in Brownian solvents, and they observed a characteristic shift of the peak towards
Figure 3.2: Variation of mean-square end-to-end distance $\langle R^2 \rangle$ and mean square radius of gyration $\langle S^2 \rangle$ as a function of flexibility $R \sim L$ as the filament got stiffer, a result consistent with Equation (3.6) and one that has been experimentally verified [40]. The probability distribution as obtained from our simulations are shown in Figure 3.3, and this shift in peak is clearly seen.

The above discussion pertained to the equilibrium value of the end-to-end distance. Of course, a filament introduced to a Brownian solvent will take some time to reach this equilibrium value, and Figure 3.4(a) shows the the time evolution of a filament before it reaches the above value. The time scale associated with this will be elaborated on in Section 3.1.3 where we consider the mean-square displacement of the end-to-end distance.
3.1.2 Radius of Gyration

The radius of gyration is a widely used measure of the size of the polymer, and is significant in characterizing, for instance, the width of a micro-channel or pore that the polymer can pass through. It is the root-mean-square distance of the parts of the polymer from its center of mass:

\[
S^2 = \frac{1}{L^2} \int_0^L \int_0^L \langle (\mathbf{x}(s_1) - \mathbf{x}^0) \cdot (\mathbf{x}(s_2) - \mathbf{x}^0) \rangle \, ds_1 \, ds_2 \\
= \frac{1}{L^2} \int_0^L \int_0^{s_1} \langle (\mathbf{x}(s_1) - \mathbf{x}(s_2))^2 \rangle \, ds_2 \, ds_1,
\]

(3.8)
Figure 3.4: Time evolution of (a) mean-square end-to-end distance and (b) mean-square radius of gyration
where \( x^0 \) refers to the center of mass of the filament. This can be simplified [30] to get the expression for the equilibrium mean squared radius of gyration:

\[
\langle S^2 \rangle = \frac{\ell_p L}{3} - 2\ell_p^2 + \frac{2\ell_p^3}{L} - \frac{2\ell_p^4}{L^2}(1 - e^{-L/\ell_p}).
\] (3.9)

As with the end-to-end distance, we can use Equation (3.9) to approximate the mean square radius of gyration for the extreme cases. For very rigid rod-like polymers (\( \ell_p/L \gg 1 \)), one finds to \( O((\ell_p/L)^{-2}) \),

\[
\langle S^2 \rangle = \frac{L^2}{12} \left( 1 - \frac{1}{5} \frac{L}{\ell_p} \right).
\] (3.10)

The pre-factor of 1/12 corresponds to the radius of gyration of a perfectly rigid rod of unit length. Similarly, in the very flexible limit of \( \ell_p/L \ll 1 \), it can be shown that to \( O((\ell_p/L)^2) \),

\[
\langle S^2 \rangle = \frac{\ell_p L}{3} = L^2 \left( \frac{1}{3} \frac{\ell_p}{L} \right).
\] (3.11)

which, again, represents a small radius of gyration corresponding to a possibly highly coiled state.

Figure 3.2 shows the entire spectrum of \( S^2 \) as obtained from Equation (3.9). Shown along with it are values obtained by numerical simulation of the polymer model, for \( \ell_p/L = 4, 9, 16 \) and 25. The transient variation of \( S^2 \) to this equilibrium value over a characteristic time scale (which is the same as that we see with the end-to-end distance) is shown in Figure 3.4(b).

### 3.1.3 Mean-Square Displacement of End-to-end Distance

Validation with equilibrium values of end-to-end distance and radius of gyration does not tell us anything about the performance of the model before it reaches this equilibrium. As was mentioned before, there is a characteristic time scale (usually referred to as the longest relaxation time of the single filament) at which these equilibrium values are realized. To
account for the transient dynamics before this relaxation is achieved, we need a property that is time dependent and preferably one that shows a clear transition to equilibrium. For this, we use the mean-square displacement (MSD) of the end-to-end distance. The MSD is defined as

$$\Delta R(t) = \langle (R(t) - R(0))^2 \rangle.$$  \hspace{1cm} (3.12)

MSD of polymers with free boundary conditions has been previously studied analytically [31] and verified experimentally [40]. It is known to grow sub-diffusively like $t^{3/4}$, and for long times approach an equilibrium value of

$$\Delta R(t \gtrsim \tau) = \frac{2}{45} \left( \frac{L}{\ell_p} \right)^2,$$  \hspace{1cm} (3.13)

where $\tau$ is the longest relaxation time of the polymer. This is also the time scale at which both the end-to-end distance and the radius of gyration saturate to their aforementioned equilibrium values. Results from our simulations reproduce this behavior excellently. The sub-diffusive growth as $t^{3/4}$ is clearly seen, till it reaches the correct equilibrium asymptote. It must also be noted that the characteristic relaxation time is very close to that reported in the experiments of LeGoff et al. [40]. The ensemble averages from 50 runs for each value of flexibility ($\ell_p/L = 4, 9, 16$ and $25$) are shown in Figure 3.5.

It is interesting to note here that for very short times, $t/\tau < 10^{-3}$, both experiments [40] and theory [32] report a downturn in the slope to approximately $t^{7/8}$. Our numerical results seem to indicate a downturn too that qualitatively matches with previous findings.

### 3.2 Diffusivity of Centre of Mass

Diffusivity of a polymer in the absence of flow characterises transport due to Brownian fluctuations. Translational and rotational diffusivity of rigid rods are well studied problems [41]. The effect of flexibility on diffusivity, however, is relatively less studied especially in the
context of continuous space curve models like the slender-body theory. In our simulations, we track the position of the center of mass $x^0$ and this gives us the diffusivity, which is defined as the average square displacement per unit time. The definition, however, can yield different values based on the time scale - in the limit of $\delta t \to 0$ one gets what we shall call the short-time diffusivity; and when time is large enough that it is of the order of relaxation time scale $t \sim \tau$, the long-time diffusivity is obtained.
3.2.1 Short-time Diffusivity

As mentioned above, the short-time diffusivity of center of mass of the polymer is defined as (along each degree of freedom)

\[
D = \lim_{\delta t \to 0} \frac{\langle |\delta x^0|^2 \rangle}{2\delta t}.
\] (3.14)

For numerical simulations, the limit of \(\delta t \to 0\) is essentially a single time step \(\Delta t\) (which in our case is \(\sim 10^{-5}\) times the relaxation time scale). Then at each time, the displacement \(\Delta x^0\) is resolved into the components parallel to and perpendicular to the mean orientation of the filament, \(\Delta x^0_\parallel\) and \(\Delta x^0_\perp\) respectively. Short-time diffusivity of the center of mass in the parallel and perpendicular directions then become:

\[
D_\parallel = \frac{1}{2\Delta t} \langle |\Delta x^0_\parallel|^2 \rangle,
\] (3.15)

\[
D_\perp = \frac{1}{4\Delta t} \langle |\Delta x^0_\perp|^2 \rangle,
\] (3.16)

where the factor of 4 in the perpendicular direction is merely due to the fact that our simulations are in three dimensions and there are two degrees of freedom in the direction perpendicular to the mean orientation of the filament.

Figure 3.6(a) shows \(D_\parallel\) and \(D_\perp\) variation with flexibility. Doi & Edwards [41] predict a relation for the rigid limit that when manipulated shows an inverse dependence on \(\ell_p/L\). Our numerical results show that this dependence for short-time diffusivity extends well into the \(\ell_p = 4L\) case which is the most flexible case that was tested. Physically, this could be interpreted as parts of a more flexible chain (one with a smaller value of \(\ell_p/L\)) being less correlated with parts far away from it and thus allowing itself to be moved around more easily by thermal fluctuations. This random motion of the entire filament body transcends into higher diffusivity than a more rigid fiber.

Another point of interest is the ratio \(D_\parallel/D_\perp\). This indicates the relative ease of diffusing
Figure 3.6: (a) Short-time diffusivity and (b) long-time diffusivity of the filament center of mass for a range of semiflexible filaments. Subsets show same points on a log-log scale.
in a direction parallel to the filament axis as compared to one perpendicular to it. This ratio is known to be $\sim 2$ from comparing resistive forces along the two directions (Chapter 1). A crude approximation for the rigid limit is to apply the mobility tensor $\Lambda$ on a unit force parallel and perpendicular to the filament axis to obtain this ratio. This ratio can be easily seen to be $2c/(c - 2)$, where $c = \log(\epsilon^2 e)$. For $\epsilon = 0.01$, we get $D_{\parallel}/D_{\perp} \approx 1.61$. Of course, this is valid only for straight filaments. But it is interesting to note that from our simulations, this ratio is evaluated to be $\approx 1.57$.

### 3.2.2 Long-time Diffusivity

The long-time diffusivity of the center of mass is defined over a larger time scale, particularly of the order of the relaxation time $\tau$. Since now the polymer has all three degrees of freedom, the long-time diffusivity is defined as:

$$D = \lim_{t \to \infty} \frac{1}{6t} \left\langle |x^0(\tau + t) - x^0(\tau)|^2 \right\rangle,$$

(3.17)

where $\tau$ is the relaxation time and so this is evaluated after the polymer has undergone its time dependent transition to equilibrium. Figure 3.7 shows this diffusion over time and it is clearly Fickian. The diffusion constant can be evaluated for each value of flexibility and the dependence is shown in Figure 3.6(b). Here, as against what was seen in the case of short-time diffusivity, the dependence for the more flexible end of the spectrum is no longer $(\ell_p/L)^{-1}$, but towards the rigid rod limit the inverse dependence seems to show up, consistent with the Doi & Edwards definition.

### 3.3 Concluding Remarks

In this chapter, we applied our single filament model derived in Chapter 2 to the case where there is no background flow and the only forces causing the polymer to move around are
Brownian fluctuations. This enabled us to compare and validate the model against scaling laws and observed experimental characteristics of polymers in Brownian solvents.

The end-to-end distance (Section 3.1.1) and radius of gyration (Section 3.1.2) are both commonly used length scales. We have seen that when a polymer is placed in a solution at an arbitrary position, both end-to-end distance and radius of gyration saturate to an equilibrium value over a characteristic relaxation time. The equilibrium values are found to be consistent with analytically evaluated values. We also evaluated the mean-square displacement of the end-to-end distance which grows sub-diffusively with time till it reaches an equilibrium plateau. Both the growth rate with time and the equilibrium value were found

Figure 3.7: Diffusion of centre of mass for filaments of different flexibility
to be consistent with scaling available in the literature and recent experimental reports.

We then moved on to describe the short and long-time diffusivity of the filament center of mass. A Fickian diffusivity is observed, and the magnitude of the diffusivity approached the rigid rod scaling for almost straight filaments.
Chapter 4

Dynamics in Linear Shear and Hyperbolic Flows

Having verified our algorithm against analytical results, we now move on to the main application of the slender body model - that of deciphering the dynamics of polymers in an imposed flow. We focus particularly on the kind of flows seen commonly in micro-channel devices used to trap, separate and manipulate single filaments. Such applications arise in single polymer studies, genetic engineering and related experiments and the development of hydrodynamic ‘trap’ devices [6, 7] that make all the above possible. We begin by applying the slender body model to free filaments in a simple shear flow. Analytical results can be obtained for simplified cases (if one were to neglect Brownian forces), and numerical solutions enable us to explore more complicated cases. We then move on to studying the suppression of fluctuations and buckling instability that are displayed in the neighbourhood of hyperbolic stagnation points.

4.1 Linear Shear Flow

In this section, we are concerned about the dynamics of a filament placed in a laminar shear flow as depicted in Figure 4.1. In terms of the position vector $\mathbf{x} = (x, y, z)$ of the filament, the velocity felt by the body is of the form $\mathbf{u}_0 = (\dot{\gamma}y, 0, 0)$. Before we go on the general case of a filament in shear with Brownian forces, it is insightful to learn the dynamics in the absence of thermal fluctuations.
4.1.1 The Non-Brownian Case

The model as we derived it in Chapter 2 accounts for hydrodynamic as well as Brownian forces. In particular in Equation (2.6) for the filament centerline and Equation (2.10) for the line tension induced in the filament, not accounting for the noise term $\xi$ gives us the deterministic set of equations:

$$\bar{\mu} \frac{\partial \mathbf{x}(s,t)}{\partial t} = \bar{\mu} \mathbf{u}_0(\mathbf{x}(s,t),t) - \boldsymbol{\Lambda} \cdot \left[-(T(s)\mathbf{x}_s) + \mathbf{x}_{ssss}\right],$$  \hspace{1cm} (4.1)

$$2cT_{ss} + (2-c)(\mathbf{x}_{ss} \cdot \mathbf{x}_{ss}) T = \bar{\mu} \mathbf{x}_s \cdot \frac{\partial \mathbf{u}_0}{\partial s} + (2-7c)(\mathbf{x}_{ss} \cdot \mathbf{x}_{ssss}) - 6c(\mathbf{x}_{sss} \cdot \mathbf{x}_{sss}).$$  \hspace{1cm} (4.2)

Note that in this case, the time scale is the one associated with the shear rate, i.e. $\dot{\gamma}^{-1}$, and the centreline equations get modified to accommodate this change of non-dimensionalization. All other characteristic scales remain the same as before. $\bar{\mu} = 8\pi \mu \dot{\gamma} L^4 / A$ is the ratio between viscous and elastic forces, and $\boldsymbol{\Lambda} = -c(I + \mathbf{\hat{p}}\mathbf{\hat{p}}) + 2(I - \mathbf{\hat{p}}\mathbf{\hat{p}})$ is the mobility operator as we have defined before.

If the filament is flexible with respect to viscous forces, it can become unstable to buckling. A particularly simple case, however, is when the filament is rigid - such a rod would simply rotate about its center (which we assume is in the shear plane, Figure 4.2(a)) and possibly translate with the fluid. It turns out that the Equation (4.1) can be solved analytically and
Figure 4.2: (a) Straight filament in planar shear flow and (b) The dynamical analogue of a flow on a circle

this might give us some insight into the dynamics of such rotational motion.

For the analytical solution, we consider a perfectly straight filament with position vector \( \mathbf{x} = (x, y, z) \) in the dimensionless planar shear flow \( \mathbf{u}_0 = (y, 0, 0) \). Since the filament is now a rigid rod, we can solve for \( \theta \) which is the angle the filament makes with the \( x \)-axis. The slender body equations then have the exact solution:

\[
\mathbf{x}(s, t) = \left( \frac{1}{2} - s \right) \hat{\mathbf{e}}_\theta, \quad T = \frac{\bar{\mu} \sin 2\theta}{8c} s(s - 1),
\]

(4.3)

where \( s \in [0, 1] \) is the arclength and \( \hat{\mathbf{e}}_\theta = (\cos \theta, \sin \theta, 0) \). \( \theta \) then solves the non-linear ODE:

\[
\frac{\partial \theta}{\partial t} = -\sin^2 \theta.
\]

(4.4)

Assuming an initial angle of \( \theta(t = 0) = \theta_0 \), we then have the exact solution:

\[
\theta(t) = \cot^{-1}(t + \cot \theta_0).
\]

(4.5)

This solution is shown in [3] to be identical to \( O(\epsilon^2) \) the Jeffery orbit solution for a long
slender ellipsoid in a shear flow (as the filament is approximated by an ellipsoid for the slender body approximation [17]).

We can see from the solution in Equation (4.5) and the simulation results in Figure 4.3 that the filament rotates about its center to align with the shear plane. Figure 4.4 shows the case of a filament starting from $\theta_0 = 17\pi/18$. It is vital to note that the filament is assumed to have zero thickness the way the slender body theory is formulated, and once aligned with the plane of zero shear, it stays aligned till it is externally perturbed. The rotation is initially slow due to the low shear rate at small distances from the $x$-axis, and as $\theta$ approaches $\pi/2$, the angular speed is maximum. It slows down again as the shear rate lessens and then aligns with the flow ever so slowly. In fact, Tornberg & Shelley [3] note that for $\epsilon = 0.01$ (the value we use in our simulations), the filament takes only about 4% of the time period to cover 90% of the orbit, and most of the time is spent aligning with the $x$-axis. It can also be seen by dimensionalizing Equation (4.5) that the orbit is faster for a higher shear rate, which one would expect by intuition.

Another point of view of looking at Equation (4.5) is to think of it as a flow on a circle [42]. As shown in Figure 4.2(b), the system has fixed points at $\theta = n\pi$, all of which are half stable. These equilibria can be attained approaching only from one direction, and once there a filament will stay in equilibrium till externally perturbed. And if perturbed, it is
Figure 4.4: Angle of a straight filament $\theta$ with respect to the $x$-axis in a planar shear flow either pushed back to equilibrium or it takes a full turn to the next fixed point, based on the direction of perturbation. This approach is particularly insightful when we include Brownian forces, and we shall return to this soon.

When the filament in flexible (note that ‘flexible’ in this context refers to flexibility with respect to viscous forces), the equations are not so amenable to analytical treatment and we solve them numerically. The feature most predominant in flexible fibers is the buckling instability, caused by non-uniform tension developed in the filament due to hydrodynamic forces. A perfectly straight remains straight for the entire orbit, but the tiniest of perturbations (which is externally imposed in our simulations) leads to interesting buckling
patterns. Figure 4.5 shows slight buckling for (a) $\bar{\mu} = 2 \times 10^5$ and pronounced buckling for (b) $\bar{\mu} = 4 \times 10^5$. These results are in good agreement with those presented in [3]. The filament here is initially placed at $\theta_0 = 17\pi/18$. 

Figure 4.5: Buckling of a flexible filament for (a) $\bar{\mu} = 2 \times 10^5$ and (b) $\bar{\mu} = 4 \times 10^5$
As was mentioned before, this buckling is a result of the non-uniform tension induced in the filament due to the hydrodynamic forces that cause shape fluctuations. In the case of rigid rods, the tension is known to have a parabolic profile as in Equation (4.3). This tension is negative till the time where the filament is vertical, to resist compression; beyond that, the tension becomes positive, actively resisting elongation as the flow tends to straighten the filament out. But when the filament buckles, tension starts out negative and takes on more complicated patterns (Figure 4.6) to enforce inextensibility through the complex shapes that the filament takes.

![Graph showing tension induced in the filament as a result of buckling (solid blue line) for $\bar{\mu} = 4 \times 10^5$ and the corresponding values for a rigid rod (dashed red line) shown against arclength $s$.](image)

**Figure 4.6:** Tension induced in the filament as a result of buckling (solid blue line) for $\bar{\mu} = 4 \times 10^5$ and the corresponding values for a rigid rod (dashed red line) shown against arclength $s$.

### 4.1.2 Linear Shear with Brownian Fluctuations

A good place to start the discussion on linear shear flows with Brownian motion is to go back to Figure 4.2. As was mentioned earlier, a non-Brownian filament aligns itself with the shear plane and stays aligned. There are no perturbations that may cause it to move
out of plane once $\theta = n\pi$. Now if we consider Brownian forces acting along the filament, there is a possibility that the filament (or a part of it) may be pushed out of the stable axis once it aligns with the flow. One can visualize the effect, and intuitively predict that if the fluctuation causes the filament to rotate counter-clockwise (with reference to Figure 4.2), the shear tends to push it back to a position where the forces might be balanced. If however the fluctuation is such that the filament rotates clockwise, it now faces the shearing action of the background flow that drives it away from the shear plane and the filament takes a tumble. Figure 4.7 shows this possible tumbling mechanism.

![Figure 4.7: Descriptive cycle of one tumble of a filament](image)

Following the analysis of non-Brownian rods, we first attempt to understand the dynamics by considering a simpler case - that of perfectly straight filaments. It can be shown [32, 43] that the equation governing $\theta$ in this case, similar to Equation (4.4) for non-Brownian rods, is:

$$\frac{\partial \theta}{\partial t} = -\sin^2 \theta + \Xi,$$

(4.6)

where $\Xi$ is a stochastic term that is related to the rotational diffusivity of a rod [32]. This term becomes a control parameter in a saddle node bifurcation at $\Xi = 0$ [42]. The unstable branch in this bifurcation corresponds to the Brownian forces driving the filament out of the
stall line, where shear effects kick in and a new rotation cycle begins.

This predicted tumbling has been found to be consistent with experimental observations. Single DNA molecules observed using fluorescence microscopy \[44, 45\] do not show a steady extended state in shear flow, but instead undergo characteristic end-over-end tumbling motion.

![Figure 4.8: Typical filament angle evolution with time. Time is made dimensionless with the relaxation time \(\tau\), and angle is measured in radians](image)

Figure 4.8 shows the typical time trajectory of polymer orientation angle \(\theta\) with respect to the stall line. To find this angle, we introduce the radius of gyration tensor:

\[
G = \frac{1}{L^2} \int_0^L \int_0^{s_1} (x(s_1) - x(s_2))(x(s_1) - x(s_2)) ds_2 ds_1,
\]  

\((4.7)\)
where the product is now a dyadic. For the results presented here, the eigenvector corresponding to the largest eigenvalue of this tensor, evaluated at each time step, is defined as the mean orientation of the filament [44]. Figure 4.8 indicates the possibility of periodic tumbling, and this makes one wonder if there is indeed a characteristic frequency associated with this.

![Figure 4.9: Scaling of Tumbling frequency $\nu^*$ with Weissenberg number $Wi$ for a filament of $\ell_p/L = 4$](image)

It turns out that there is indeed a scaling that governs the tumbling frequency. Schroeder et al. [44] determined this scaling experimentally, and ascribed it to the net result of the stretch, align, flip and collapse phases in shear. A power law increase of tumbling frequency
as $\nu \propto \text{Wi}^{2/3}$ was reported, one that was consistent with analytical results for Brownian rods in strong shear flow. Here, $\text{Wi} = \dot{\gamma}\tau$ is the Weissenberg number defined as the ratio of the longest polymer relaxation $\tau$ to the time scale of the background flow $\dot{\gamma}^{-1}$.

Our numerical simulations reproduce this scaling in excellent quality as shown in Figure 4.9. Characteristic frequency of tumbling (made dimensionless with the polymer relaxation time, $\nu^* = \nu\tau$) is seen to scale as $\text{Wi}^{2/3}$, consistent with experimental observations.

### 4.2 Hyperbolic flows

We now focus on a family of flows commonly observed in microfluidic devices, particularly in four-roll mills and hydrodynamic trap devices. These flow fields are hyperbolic and a filament placed at the stagnation point displays interesting non-linear behavior. Tension induced in the filament can suppress fluctuations when aligned with the extensional axis, or can cause a buckling instability analogous to Euler buckling of beams [46] when aligned with the axis of compression. Recently, there have been attempts to study this ‘stretch-coil’ transition in macroscopic flows by electrodynamic forcing [47]. Young & Shelley [20] used slender body theory to describe the dynamics in the case of non-Brownian elastic filaments, extending the theory to predict transport of fibers in cellular flows like in the experiments of Wandersman et al. [47]. At the microscopic scale, this phenomenon can be particularly useful in designing devices meant to separate and trap single particle for long time scales like in the microfluidic device developed by Tanyeri et al. [6, 7]. A notable attempt at investigating this effect with the inclusion of thermal fluctuations is a recent work by Kantsler & Goldstein [4] where a variational method is used to justify experimentally observed trends.

Free polymers in Brownian solvents have been well studied [1, 31], but the effect of non-uniform tension has only begun to receive attention. Here, we consider both aforementioned phenomena that this non-uniform tension can induce: that of suppression of thermal fluctuations in extension, and the buckling instability in compression.
4.2.1 Suppression of Thermal Fluctuations

The filament is placed in an extensional flow \( \mathbf{u}_0 = (u, v, w) = (\dot{\gamma} x, -\dot{\gamma} y, 0) \) in such a way that the center of mass of the filament remains exactly at the hyperbolic stagnation point. This would correspond to a controlled microfluidic device [6, 4] that, by carefully controlled pressures at the entrances and exits, traps the filament at the center. Figure 4.10 (a) illustrates this set-up.

![Figure 4.10](image_url)

Figure 4.10: (a) Cross flow geometry with filament placed at the hyperbolic stagnation point. (b) Filament geometry as used in the analysis of suppression of fluctuations in extension

For the purpose of this section, we consider a filament aligned with the extensional axis (the horizontal axis in Figure 4.10 (b)). For simplicity of analysis, assume a two-dimensional system with the small amplitude fluctuations from a mean position represented by \( h(x) \) (Figure 4.10 (b)). Filament rotations away from the axis are assumed small [4] which allows us to approximate the mean position to be along the axis, and the end-to-end distance \( R \) of the filament is approximately the same as its contour length \( L \). Then, the energy of the filament (assumed to be placed with its center at the origin) is:

\[
E = \frac{1}{2} \int_{-L/2}^{L/2} \left[ A h_{xx}^2 + T(x) h_x^2 \right] \, dx. \tag{4.8}
\]
This follows from Equation (1.11).

The tension \( T(s) \) can be approximated if we assume a 2-D background flow \( u_0 = (x, -y) \) (made dimensionless by standard scales that we have been using). Note that thermal fluctuations will be introduced in Equation (4.8) as an external forcing and so we consider the governing equation for the non-Brownian rod as in Equation (4.1). For an almost straight filament, noting that \( x_{ss} = 0 \), the steady centerline equation reduces to:

\[
\bar{\mu}u_0 = -(2 - c)\mathbf{I} - (2 + c)x_s x_s \cdot (-T_s x_s) = 2cT_s x_s. \tag{4.9}
\]

The filament is assumed to lie along the \( x \)-axis between \( x = -L/2 \) and \( L/2 \). In dimensionless terms, this corresponds to a position vector \( \mathbf{x} = (-1/2 + s, 0) \), the unit tangent vector \( x_s = (1, 0) \) and a corresponding background velocity \( u_0 = (-1/2 + s, 0) \) for \( s \in [0, 1] \). Using this in Equation (4.9) along with the boundary conditions on tension, \( T(s = 0) = T(s = 1) = 0 \), the tension can be found to be

\[
T(s) = \frac{\bar{\mu}}{4c}(s^2 - s), \tag{4.10}
\]

which in dimensional terms gives the familiar form of non-uniform tension in an almost straight thread aligned with the extensional axis [16, 4]:

\[
T(x) = \frac{2\pi \mu \dot{\gamma}}{\ln(1/e^2\epsilon)} \left[ \frac{L^2}{4} - x^2 \right], \tag{4.11}
\]

where we have used \( \bar{\mu} = 8\pi \mu \dot{\gamma}L^4/A \) and \( c = \log(e^2\epsilon) \).

Using this expression for tension in Equation (4.8) and the Euler-Lagrange equation, we can derive a set of eigenfunctions \( W^{(n)}(x) \) and corresponding eigenvalues \( \lambda_n \) (see Appendix A for derivation and details) that satisfy the boundary conditions \( W^{(n)}_{xx}(x = \pm L/2) = W^{(n)}_{xxx}(x = \pm L/2) = 0 \), which represent respectively, force-free and moment-free ends. These eigenfunctions (shown here under the convenient rescaling \( \xi = \pi x/L \) and \( \Lambda_n = \lambda_n L^4/\pi^4 A \))
are governed by
\[ W^{(n)}_{\xi\xi\xi\xi} - \bar{\Sigma} \left[ \left( \frac{\pi^2}{4} - \xi^2 \right) W^{(n)}_\xi \right]_\xi = \Lambda_n W^{(n)}. \] (4.12)

Here, \( \bar{\Sigma} = \bar{\mu} / 4 \pi^4 \ln(1/\epsilon^2 e) \) is a dimensionless group that is a ratio of tensile force to elastic force, defined as:
\[ \bar{\Sigma} = \frac{2\mu\dot{\gamma}}{\pi^3 A \ln(1/\epsilon^2 e)}. \] (4.13)

Now, projecting the amplitude of fluctuations onto the basis \( \{ W^{(n)}(x) \} \) such that \( h(x) = \sum_n a_n W^{(n)}(x) \), it can be shown by integration of parts and the boundary conditions described above (Appendix A) that the energy decomposes exactly into contributions from each mode independently: \( E = L/2 \sum_n \lambda_n a_n^2 \). The principle of equipartition then allows us to derive the variance of the amplitudes \( a_n \) to be
\[ \langle a_m a_n \rangle = \frac{\delta_{mn} L^3}{\pi^4 \ell_p \Lambda_n}. \] (4.14)

Then, if the mean amplitude is assumed to be \( \langle a_n \rangle = 0 \), the mean filament fluctuation amplitude is \( \bar{h} = 0 \). Which tells us that the local variance \( V(x) = \langle [h(x) - \bar{h}]^2 \rangle \) is
\[ V(x; \bar{\Sigma}) = \frac{L^3}{\ell_p \pi^4} \sum_{n=1}^{\infty} \frac{W^{(n)}(x; \bar{\Sigma})^2}{\Lambda_n(\bar{\Sigma})}. \] (4.15)

For the case of \( \bar{\Sigma} = 0 \), Equation (4.12) is a one-dimensional biharmonic equation which can be solved analytically (Appendix A), and \( \Lambda_n \) grows like \((n + 1/2)^4\). For \( \bar{\Sigma} \neq 0 \), a numerical solution is straightforward and Figure 4.11 shows \( V(x, \bar{\Sigma}) \) from Equation (4.15) evaluated to the first 1000 terms for four different values of \( \bar{\Sigma} \); the suppression of amplitude fluctuations with increasing strain rate is evident. Here, \( \bar{V}_e \) is the mean end point fluctuation, \( \bar{V}_e = [V(-L/2) + V(L/2)]/2 \).

Following Kantsler & Goldstein [4], we note that the eigenfunctions for \( \bar{\Sigma} \neq 0 \) are strikingly similar to those for \( \bar{\Sigma} = 0 \) (Appendix A), with the peaks flattened out mirroring the
Figure 4.11: Normalized local variance as predicted by Equation (4.15) for $\bar{\Sigma} = 0$ (blue), 1 (red), 10 (green) and 100 (magenta).

suppression of amplitude fluctuations by the extensional flow. Furthermore, the form of $V(x, \bar{\Sigma})$ in Equation (4.15) is such that the first few terms dominate, a fact reflected in the ‘W’ shape corresponding to the fundamental mode in Figures 4.11 and 4.12. Simulations show that the variance closely follows the predicted pattern with fluctuations being suppressed as $\bar{\Sigma}$ increases (Figure 4.12).

A clearer picture of the suppression of amplitude fluctuations is the magnitude of variance of the filament end fluctuations, $\bar{V}_e$. Figure 4.13(a) shows that for small $\bar{\Sigma}$, this value is almost the same as that for $\bar{\Sigma} = 0$. However, for $\bar{\Sigma} > 1$ the variance is heavily suppressed.
The scaling $\ell_p/L^3$ follows from Equation (4.15) and removes the dependence on flexibility. Figure 4.13(b) indicates that the mean angle of the filament with respect to the $x$-axis is also suppressed for $\tilde{\Sigma} \gtrsim 1$, a useful result that validates our assumption in developing the equation for tension in the filament as in Equation (4.11).

4.2.2 The Buckling Instability

Buckling of elastic rods is a well studied problem in elasticity [46] with many applications in mechanical engineering. In classical solid mechanics, an elastic rod undergoes buckling if
Figure 4.13: (a) Variance of filament-end fluctuations in case of three dimensional amplitude fluctuations and the corresponding values for the projection on the $x$-$y$ plane, as obtained from simulations. The theoretical prediction from Equation (4.15) is shown by the solid line. (b) Variance of mean filament orientation with respect to the axis.
for a given length the compressional force exceeds a critical value, or the length exceeds a
threshold value for a given force. An analogous buckling has been reported, for instance in
the buckling of microtubules by molecular motors [48] and the buckling of microtubules due
to compressive forces inside a lipid bilayer held in tension [49, 50]. More recently, Becker
& Shelley [2] predicted bifurcations to shape instabilities in the hydrodynamic analog of
this phenomenon. Their model was applied to studying the dynamics of macroscopic non-
Brownian elastic filaments in cellular flow [20], and verified by corresponding experiments
where arrays of hyperbolic flows were generated by electrodynamic forcing [47].

However, at the microscopic level, Brownian forces come into play and this so called
‘stretch-coil’ transition is rounded by thermal fluctuations. An theoretical explanation of
buckling near hyperbolic points is yet incomplete, and we present here results from applying
our slender body model to this very problem. Such numerical results, along with experimental
studies like the recent work of Kantsler & Goldstein [4] using microfluidics, aim towards
achieving a comprehensive understanding of the full problem.

The compressional case is set up quite similar to the extensional case from the previous
section, but with $\dot{\gamma}$ being negative this time. For convenience, we shall only talk about
the magnitude of $\dot{\gamma}$ and hence of $\tilde{\Sigma}$, with the negative sign in this case being implied. The
geometry and terminology is as depicted in Figure 4.14 (a).

A simplified dynamical analysis of a straight non-Brownian rod on the lines of what was
done in Section 4.1.1 shows that the angle $\theta$ and the tension induced in the filament now
vary as (both dimensionless):

$$\frac{\partial \theta}{\partial t} = \sin(2\theta),$$  \hspace{1cm} (4.16)
$$T(s) = -\frac{\mu}{4c} \cos 2\theta (s^2 - s).$$  \hspace{1cm} (4.17)

The form of tension here (with the opposite sign and when $\theta \sim 0$) is identical to Equation
(4.10) in the extensional regime.
The fixed points of this system are $\theta = n\pi/2$ with odd $n$ representing stable solutions and even ones being unstable (Figure 4.14 (b)). Clearly, a filament in an arbitrary initial orientation moves towards the nearest stable solution.

Along this path, if the case be that the thrusting force from tension ($\sim \mu \gamma L^2/\ln(1/\epsilon^2 e)$) balances the restoring elastic force ($\sim A/L^2$), a ‘stretch-coil’ transition is seen. This is complementary to the widely studied ‘coil-stretch’ transition of flexible polymers [8]. At critical values of this tension [4, 20], the buckling amplitude corresponding to a higher eigenvalue grows with the mean filament angle, until the filament reaches the extensional quadrant where the (now positive) tension tries to extend and align it with the axis. Filament shapes as obtained from simulations are shown in Figure 4.15, and qualitatively match recent experimental observations [4]. The filament buckles into a ‘U’ shape (Figure 4.15(a)) for the first unstable mode, followed by ‘S’ (Figure 4.15(b)) and ‘W’ (Figure 4.15(c)) shapes and then superpositions of the same as the tensile force increases. It has been shown [4, 20] that the critical points corresponding to the onset of the U, S and W shapes have magnitudes
Figure 4.15: The stretch-coil transition: (a) ‘U’ modes at $\tilde{\Sigma} = 2.5$, (b) ‘S’ modes at $\tilde{\Sigma} = 10.0$ and (c) ‘W’ and higher modes at $\tilde{\Sigma} = 40.97$. The transition is rounded by thermal fluctuations but the thresholds are seen to be quite consistent with analytical predictions.
\( \tilde{\Sigma} = 0.3932, 1.9876 \) and \( 4.9555 \) respectively.

As indicators of the extent of buckling, we use two measures. Fractional compression is measured using the end-to-end displacement. This value drops from the initial condition to a minimum at the point of maximum compression, and then grows back to close to unity as the filament is extended along the extensional axis. This minimum value \( \mathcal{L} \) is made dimensionless as the fractional compression \( 1 - \mathcal{L}/L \), where \( L \) is the contour length of the filament. Figure 4.16(a) shows this measure for the entire range of \( \tilde{\Sigma} \) that was simulated. Another measure is the elastic energy in the filament, which is high for high curvatures that may result from heavy buckling. This measure has been used previously to quantify buckling of non-Brownian rods in shear flow [3]. Figure 4.16(b) shows the growth of dimensionless elastic energy with \( \tilde{\Sigma} \), clearly indicating more prominent buckling. In both the measures, it should be noted that the values shown are ensemble averages over many runs and the variance remains high, especially for larger values of \( \tilde{\Sigma} \). This is due to the fact that even in cases where the filament can take the ‘W’ shapes, the compression might force the filament to bend into a lower mode (a simple ‘U’ for instance) in which case the fractional compression as measured by \( \mathcal{L} \) is far from that corresponding to a ‘W’ or an ‘S’ shape. This renders this value widely disparate.

A quantitative treatment of this transition accounting for thermal fluctuations is an open problem, and one that is a future avenue for this work. One approach along the lines of a previous work on elastic rods [51] is to expand Equation 4.8 in terms of the angle \( \theta \), and by manipulations of the first few terms of the expansion (which are the ones that matter the most at the onset of instability), a Ginzburg-Landau-type theory governing the stability can be obtained. This treatment is yet to be pursued, and might quantitatively reveal how thermal fluctuations round the stretch-coil transition.
Figure 4.16: Indicators of buckling instability: (a) Fractional compression measured by the end-to-end displacement $L$ and (b) Elastic energy in the filament
4.2.3 An Application - Cellular Hyperbolic flows

An interesting application of the buckling instability as modulators of microscale transport is cellular flow. Actin filaments have been observed to be propelled along myosin coated surfaces [52] or in arrayed flows where motor proteins buckle microtubules [48]. The dynamics of bio-polymers in such flows can help design, for instance, assaying techniques.

For our simulations, we define the ratio of filament length to cell size as $\alpha = L/W$ [20]. A filament is initially placed at the origin and then the array of hyperbolic flows causes the filament to meander between them, buckling and extending at junctions, to eventually get trapped in one of the cells - ‘buckled in translation’ as Wandersman et al. [47] chose to call it! Figure 4.17 shows a typical trajectory. For our results presented here, we set $\ell_p/L = 99$ so that the filament is relatively rigid to thermal fluctuations so as to minimize thermal rounding of the transitions.

Two key points arise out of applying our algorithm to this example: the effect of effective viscosity $\bar{\mu}$ and that of the cell size $\alpha$. Young & Shelley showed that an elastic non-Brownian filament meanders among the cells like a random walker, and characterized the diffusivity associated with different values of $\bar{\mu}$. They predicted higher diffusivity associated with increasing $\bar{\mu}$ till a critical value at which the filament remains trapped in one of the cells, a result consistent with our simulations. Furthermore, higher $\bar{\mu}$ is seen to lead the filament to diffuse faster, though to a shorter distance away from its initial position (Figure 4.18).

Cell size also affects transport properties. For $\alpha = 1/\pi$ (Figure 4.18 (a)), the filaments diffuse over much fewer cells that for $\alpha = 1/2\pi$ (Figure 4.18 (b)). This suggests that in the case of larger cells, the filament takes more time in its transit between junctions to align with the axis and this reduces its chances of getting trapped in a cell.

These observations are key to deciphering how filament flexibility can change transport properties in cellular flows. Brownian forces will introduce altogether new dynamics, which will become more predominant as the persistence length gets smaller. As was seen with
Figure 4.17: Typical trajectory of a filament placed in a cellular flow field. Red indicates positions along the axes where the filament is translated, and green are positions where the filament is seen to be trapped. Trajectory of the center of mass of the filament over time is shown in cyan.

...polymer tumbling, thermal fluctuations can cause filaments to align off the axis and may thus increase the chances of filament trapping. Our preliminary results indicate this, but the diffusivity and related properties need to be addressed - a topic left as a future direction.
Figure 4.18: Center of mass trajectory of a meandering filament over the same time period for $\bar{\mu} = 20000$ (blue), 40000 (red) and 80000 (green) for (a) $\alpha = 1/\pi$ and (b) $\alpha = 1/2\pi$.
4.3 Concluding Remarks

In this chapter, we applied our validated model from Chapters 2 and 3 to single semiflexible filaments in background flows. We particularly focused on flows that are commonly seen in microfluidic devices.

We started with the simple case of a non-Brownian straight rod for which an analytical solution is straightforward: the filament tends to align itself with the shearing axis which we saw is a stable fixed point (Section 4.1.1). In the numerical simulations of fibers, it is seen that the trajectory is identical to the analytical case when the filament is rigid. Furthermore, flexible fibers show interesting buckling phenomena which are ascribed to the non-uniform tension that is generated in the filament. Even in this case, however, the filament approaches the stable solution by aligning with the axis.

When Brownian motion is introduced, the dynamics is different. It was shown how the Brownian terms introduce a bifurcation leading to a stable and unstable branch, with the unstable branch corresponding to a position where the shear can now drive the filament over an entire half period to align with the axis. This led us to study polymer tumbling (Section 4.1.2) in shear flows, where the tumbling frequency is found to be consistent with previous experimental findings.

Section 4.2 introduced the applications and recent literature on the dynamics of semiflexible filaments near hyperbolic stagnation points. Using a variational method and assuming small-amplitude fluctuations away from the axis, we were able to derive the eigenfunctions for the shape of a filament when placed along the extensional axis (Section 4.2.1 and Appendix A). The variance of fluctuations away from the axis is predicted to be suppressed as the rate of strain increases, and our simulations reproduced this excellently. This is attributed to the tensile force generated in the filament that tries to extend it thereby flattening out the fluctuations. The mean orientation is also seen to be suppressed with increasing rate of extension.
In the case when the filament is along with the compressional manifold (Section 4.2.2) the tension is negative, causing the filament to be pulled inward towards itself. Previous literature has shown how this can lead to a buckling instability beyond a critical value of tension, giving rise to higher mode shapes as the tension (or the rate of extension that drives this tension) increases. Our simulations are able to consistently reproduce this instability.

Lastly, we applied the simulation to a topic of recent interest: that of cellular flows. Our preliminary results agree with recent results in the literature regarding transport of filaments across an array of hyperbolic flows (Section 4.2.3). It is seen that relative cell size and filament flexibility affects transport properties, in a way consistent with experimental observations.

Among the many contexts in which filament occur in linear shear or hyperbolic flows include biological processes (locomotion, ciliary streaming) and experimental techniques (DNA trap and observation devices, assaying techniques). A firm understanding of the complex phenomena that occur due to the interplay of viscous, elastic and Brownian forces is necessary to fully appreciate the flow physics in these scenarios, and possibly design microfluidic devices with better capabilities.
Chapter 5

Conclusion and Future Work

5.1 Conclusion

We have presented a model based on slender body theory for hydrodynamics to describe free single semiflexible polymers in flow. Such polymers, with length of the order of the persistence length, are commonly seen in a myriad of applications ranging from biology (actin, microtubules, DNA, cilia) to chemical/biomolecular-engineering (DNA/RNA experiments) to industrial applications (single carbon nanotubes). This model has relative benefits over the more widely used bead-rod and bead-spring models in the way that its is easily extensible to capture interactions, wall effects and detailed internal dynamics.

The single filament model developed in Chapter 2 does not include hydrodynamic interactions between different parts of the polymer, which are assumed to be small under the purview of this work. Viscous drag, which is a leading order effect, is accounted for by a mobility operator that captures drag anisotropy due to the slenderness. Euler-Bernoulli elasticity along with a fluctuation dissipation theorem define the forces acting on the filament: the tensile force that keeps the filament inextensible, elastic forces that actively try to resist buckling and Brownian forces that are random and satisfy required statistical properties. It was seen that the inextensibility condition gives rise to a tension equation which is coupled with the centerline equation of the filament and is solved numerically using a semi-implicit time marching algorithm.

We first validated our model against equilibrium properties and scalings available in the literature in the absence of background flow. In Chapter 3, end-to-end distance, radius
of gyration, relaxation time and the mean-square displacement of the end-to-end distance (MSD) were studied in detail and it was seen that the model performs very well to reproduce the time-dependent and equilibrium statistics due to thermal fluctuations. Particularly, our simulations were able to reproduce the $t^{3/4}$ sub-diffusive growth followed by saturation of MSD as previously predicted analytically and proven experimentally. We also looked at the short and long-time diffusivities of the filament center of mass, and saw how more flexible chains are more diffusive. The short-time diffusivity in the direction parallel to current filament orientation was found to be more than that in a perpendicular direction by a factor very close to the approximation for a straight filament.

We then turned to the main applications of the current work in Chapter 4: that of the dynamics of free semiflexible polymers in linear shear and hyperbolic flows. An analytical solution and analogous dynamical argument show how a non-Brownian straight filament aligns with the $x$-axis. The numerical solution followed this, and allowed us to study the more difficult case of flexible filaments. In the non-Brownian case, these filament rotations showed interesting buckling patterns that match previous studies, and they too orient along the $x$-axis with time. The buckling was attributed to the non-uniform tension induced in the filament to keep it locally inextensible. In the case when Brownian forces are included, the axis is no longer a stable solution as thermal fluctuations can dislodge the filament easily from that position and shear can cause it to move out of it in one direction. In fact, this has been previously reported to result in characteristic tumbling. Our simulations show that the characteristic frequency of this tumbling varies as $Wi^{2/3}$ where $Wi$ is the Weissenberg number, a scaling that has been previously seen in experiments.

Semiflexible filaments show interesting non-linear behavior in the vicinity of hyperbolic stagnation points, and the second half of Chapter 4 was devoted to this. Two interesting phenomena are observed in such flows - firstly, when the filament is aligned with the extensional axis, thermal fluctuations are suppressed with increasing rate of extension. We quantified the ratio of tensile force (due to the extensional strain) to elastic forces that resist
filament bending by a non-dimensional parameter $\tilde{\Sigma}$. The variance of amplitude fluctuations away from the axis is shown to be well approximated by an analytical formulation obtained under the assumption of small amplitude fluctuations. Furthermore, this variance and the mean filament angle away from the axis are seen to be suppressed with increasing $\tilde{\Sigma}$.

The second phenomenon is a buckling instability when the filament is initially placed in the compressional manifold. The tension, which is now negative, tends to buckle the filament beyond a critical value (directed by the magnitude of $\tilde{\Sigma}$). It has been previously noted that there are threshold values of $\tilde{\Sigma}$ at which the filament buckles into higher modal shapes - our simulations follow these transitions quite well, though the boundaries are heavily rounded by thermal fluctuations. The fractional compression (measured with respect to the end-to-end displacement) and elastic energy of the filament are seen to increase with higher $\tilde{\Sigma}$ indicating more severe bending.

Finally, the transport of semiflexible fibers across arrays of hyperbolic stagnation points was studied. Our preliminary results indicate that transport properties are heavily affected by filament flexibility (flexibility here with respect to viscous forces). Higher strain rates led to filament being trapped inside cells more easily, while lower strain rates would render the filament less diffusive. Cell size also plays a key role, especially with Brownian fluctuations as the filament gets longer time to align with the axis and that reduces the chance of trapping. Brownian fluctuations also tend to round these transitions and this is a topic yet to be explored, as we focused on cases were the filament was relatively rigid to Brownian fluctuations.

To conclude, the model works very well to capture hydrodynamics of semiflexible filaments in complex flow patterns. Given that the slender body equations are extensible to capture other effects, this promises to be a detailed and efficient simulation method for solutions of such polymer flows.
5.2 The Road Ahead

There are many avenues along which the current work is planned to be extended, some of which are mentioned below. A complete model would include Brownian motion, intra-chain hydrodynamic interactions, chain-chain hydrodynamic interactions, steric and hydrodynamic interactions with boundaries, and external flows.

- **Interactions and Non-local rheology:** We have yet so far only accounted for the modified local mobility operator. The integral operator in Equation (1.8) was ignored under the assumption that effects of intra-chain interactions are minimal as compared to leading order effects. Including this is a numerically challenging task, as the operator is singular and particular care has to be taken to regularize this [3]. The extension to multiple filaments will follow this. Including interactions will allow us to study the contribution of the filaments to the background stress tensor, which renders the bulk fluid non-Newtonian [2, 3]. This study will complement previous work on rigid rods and flexible polymers by considering the case of highly confined semiflexible chains.

- **Confinement and Cross-streamline migration:** Models of confined polymers oftentimes altogether neglect hydrodynamic interactions with boundaries, and only include steric interactions. Hydrodynamic interactions are however crucial in pressure-driven flows, as they can lead to cross-streamline migration [53, 15]. Most previous simulations that account for hydrodynamic interactions rely on Green’s functions for the Stokes equations, which are known analytically in simple geometries [15] or can be calculated numerically in more complex settings [33]. These Green’s functions are however highly complex and are not compatible with the use of fast algorithms. More recently, a new approach based on a periodic solution, which is subsequently corrected by an auxiliary solution to satisfy the correct boundary condition was proposed [34] and holds scope to be applied to the current model because of its efficient implementation and flexibility of handling arbitrary geometries. Such cross-streamline migration has
been well characterized in the case of long-chain flexible polymers, rigid rods, and short flexible polymers, but has not been studied in the case of semiflexible polymers under strong confinement. An extended model will enable one to solve for such cases, and also study in detail the effect of inter-chain interactions.

- **Electrokinetic transport:** The model holds the capability to be extended to study electrokinetic transport of charged polymers in nanochannels [11, 5]. This will require coupling the equations described in this work to a Laplace solver for the electric potential inside the channels, and inclusion of an additional electric force acting on the polymer chains. This extension of the algorithm can be applied to study electrophoretic separation of short-chain flexible polymers, such as DNA fragments, which has been reported in experiments but has yet to be fully explained theoretically. Other potential applications of this work will include polymer translocation through pores.

- **Analytical formulation of the buckling instability:** The fractional compression due to buckling near hyperbolic stagnation points was mentioned to be strongly rounded due to thermal fluctuations. A rigorous approach on the lines of thermal fluctuations in the Euler buckling problem [51] will enable us to predict this transition, and compare results from simulation. This is a variational approach where the energy is expanded in terms of the angle it makes with the axis, and then manipulated to obtain a Ginzburg-Landau-like theory, which governs the stability.

- **Biolocomotion:** Throughout this work, we set the flow field around the filament, and evaluate forces and position that the filament takes. The reverse problem is of equal interest, where the forces (or location) is specified and the flow field is to be found. This is the case in flagellar or ciliary propulsion. There are many factors that come in here, including the choice of filament shapes [21] and optimal forcing for maximum swimming efficiency.
Appendix A

The $D_{\Sigma}$ Operator

The Eigenvalue Problem

We first derive the eigenvalue problem that was widely used in the context of suppression of fluctuations in Chapter 4, abbreviated here as $D_{\Sigma}W^{(n)} = \Lambda_n W^{(n)}$. Consider a filament aligned very close to the $x$-axis due the extensional flow $u_0 = (\dot{\gamma}x, -\dot{\gamma}y)$ between $-L/2$ and $L/2$ with its center at the stagnation point at $x = (0, 0)$. Following Equation (4.8), we have the (potential) energy of the filament due to elasticity and induced tension for small amplitude fluctuations $h(x)$ away from the $x$-axis as

$$E = \frac{1}{2} \int_{-L/2}^{L/2} \left[ Ah_{xx}^2 + T(x) h_x^2 \right] dx, \quad (A.1)$$

where the tension was derived to be (Equation (4.11))

$$T(x) = \frac{2\pi \mu \dot{\gamma}}{\ln(1/\epsilon^2 e)} \left[ \frac{L^2}{4} - x^2 \right]. \quad (A.2)$$

Now, the Euler-Lagrange equations that minimizes $E$ for $h(x)$ is

$$\frac{\partial E}{\partial x} - \frac{\partial}{\partial s} \left( \frac{\partial E}{\partial h_s} \right) + \frac{\partial^2}{\partial s^2} \left( \frac{\partial E}{\partial h_{ss}} \right) = 0. \quad (A.3)$$
Substituting Equation (A.2) in the Euler-Lagrange equation gives us the governing equation for the energetically most favorable positions \( h(x) \) that satisfy

\[
Ah_{xxxx} - (T(x)h_x)_x = f(x),
\]

(A.4)

where subscripts denote differentiation with respect to \( x \), and \( f(x) \) is a force distribution per unit length that causes the filament to assume this shape. Using Equation (A.1) for \( T(x) \) gives

\[
Ah_{xxxx} - \frac{2\pi \mu \dot{\gamma}}{\ln(1/\epsilon^2 e)} \left[ \left( \frac{L^2}{4} - x^2 \right) h_x \right]_x = f(x),
\]

(A.5)

which is a linear fourth-order differential equation for \( h(x) \). This admits the eigenvalue problem with eigenfunctions \( W^{(n)}(x) \) and corresponding eigenvalues \( \lambda_n \):

\[
AW^{(n)}_{xxxx} - \frac{2\pi \mu \dot{\gamma}}{\ln(1/\epsilon^2 e)} \left[ \left( \frac{L^2}{4} - x^2 \right) W^{(n)}_x \right]_x = \lambda_n W^{(n)},
\]

(A.6)

with the conditions of force-free and moment-free ends, \( W^{(n)}_{xx}(\pm L/2) = W^{(n)}_{xxx}(\pm L/2) = 0 \).

A convenient rescaling is \( \xi = \pi x/L \) such that now \( \xi \in [-\pi/2, \pi/2] \). The system then becomes

\[
W^{(n)}_{\xi\xi\xi\xi} - \tilde{\Sigma} \left[ \left( \frac{\pi^2}{4} - \xi^2 \right) W^{(n)}_\xi \right]_\xi = \Lambda_n W^{(n)}
\]

(A.7)

or

\[
D_{\xi\xi} W^{(n)} = \Lambda_n W^{(n)},
\]

where \( \tilde{\Sigma} \) is a dimensionless ratio of the tensile force causing the filament to extend (or buckle if the strain were in the opposite direction) to elastic force, defined as

\[
\tilde{\Sigma} = \frac{2\mu \dot{\gamma} L^4}{\pi^3 A \ln(1/\epsilon^2 e)},
\]

(A.8)

and \( \Lambda_n \) are the rescaled eigenvalues \( \Lambda_n = L^4 \lambda_n / \pi^4 A \). Equation (A.7) along with the bound-
ary conditions define the basis that represents positions that the filament may realize.

**Energy and Variance**

From Equation (A.1), we have by repeated integration by parts

\[ \mathcal{E} = \frac{1}{2} \int_{-L/2}^{L/2} \left[ Ah_{xx}^2 + T(x)h_x^2 \right] \, dx \]  
(A.9)

\[ = \frac{1}{2} \left[ (Ah_{xx}h_x)|_{-L/2}^{L/2} - \int_{-L/2}^{L/2} h_{xxx}h_x \, dx + (Th_x h)|_{-L/2}^{L/2} - \int_{-L/2}^{L/2} (Th_x x h) \, dx \right] \]  
(A.10)

\[ = \frac{1}{2} \left[ -A \left\{ (h_{xxx}h_x)|_{-L/2}^{L/2} - \int_{-L/2}^{L/2} h_{xxxx}h_x \, dx \right\} - \int_{-L/2}^{L/2} (Th_x x h) \, dx \right] \]  
(A.11)

\[ = \frac{1}{2} \int_{-L/2}^{L/2} \left[ (Ah_{xxxx} - (Th_x x) h) \right] \, dx, \]  
(A.12)

where all boundary terms (in Equations (A.10) and (A.11)) are zero due to the boundary conditions and the fact that tension is zero at the ends by definition. Now, since \( h(x) \) is projected onto the \( \{W^{(n)}(x)\} \) basis, we may write

\[ h(x) = \sum_{n=1}^{\infty} a_n W^{(n)}(x). \]  
(A.13)

This then leads to

\[ \mathcal{E} = \frac{1}{2} \int_{-L/2}^{L/2} \left\{ A \sum_{n=1}^{\infty} a_n W^{(n)}_{xxx} - \left( T \sum_{n=1}^{\infty} a_n W^{(n)}_x \right) \right\} \left( \sum_{n=1}^{\infty} a_n W^{(n)} \right) \, dx \]  
(A.14)

\[ = \frac{1}{2} \int_{-L/2}^{L/2} \left( \sum_{n=1}^{\infty} \left\{ AW^{(n)}_{xxx} - (TW^{(n)}_x) \right\} a_n \right) \left( \sum_{n=1}^{\infty} a_n W^{(n)} \right) \, dx \]  
(A.15)

\[ = \frac{1}{2} \int_{-L/2}^{L/2} \left( \sum_{n=1}^{\infty} a_n \lambda_n W^{(n)} \right) \left( \sum_{n=1}^{\infty} a_n W^{(n)} \right) \, dx, \]  
(A.16)
where we have used the expansion for tension and Equation (A.6). Now, defining the or-
thogonality condition of the \{W^{(n)}(x)\} basis to be

\[ \frac{1}{L} \int_{-L/2}^{L/2} W^{(m)}(x)W^{(n)}(x)dx = \delta_{mn}, \]  

(A.17)

Equation (A.16) simplifies to

\[ \mathcal{E} = \frac{L}{2} \sum_{n=1}^{\infty} a_n^2 \lambda_n. \]  

(A.18)

This tells us that the energy decomposes into a sum of contributions from independent
modes. It then follows from the the equipartition principle that each of these independent
contributions \( \langle a_n^2 \lambda_n L/2 \rangle \) must equal \( k_B T/2 \). In other words, emphasising the independence
of contributions from different modes, we may write

\[ \langle a_m a_n \rangle = \delta_{mn} \frac{k_B T}{\lambda_n L}. \]  

(A.19)

Using the rescaled eigenvalue \( \Lambda_n = \lambda_n L^4 / \pi^4 A \) and the definition of the persistence length
\( \ell_p = A/k_B T \), this simplifies to

\[ \langle a_m a_n \rangle = \delta_{mn} \frac{L^3}{\Lambda_n \pi^4 \ell_p}. \]  

(A.20)

We now define the variance of amplitude fluctuations as

\[ V(x) = \langle [h(x) - \bar{h}]^2 \rangle, \]  

(A.21)

where \( \bar{h} \) is the mean filament amplitude. When aligned approximately with the \( x \)-axis, we
can set \( \langle a_n \rangle = 0 \) and so \( \bar{h} = 0 \). This also follows from the variance of the mean filament

angle from the $x$-axis being very small. Then using Equation (A.20),

$$V(x) = \langle h(x)^2 \rangle$$

\[= \left\langle \left[ \sum_{n=1}^{\infty} a_n W^{(n)}(x) \right]^2 \right\rangle \quad \text{(A.22)}\]

\[= \sum_{n=1}^{\infty} \frac{L^3}{\Lambda_n \pi^4 \ell_p} W^{(n)}(x)^2 \quad \text{(A.23)}\]

\[\Rightarrow V(x; \tilde{\Sigma}) = \frac{L^3}{\ell_p \pi^4} \sum_{n=1}^{\infty} \frac{W^{(n)}(x; \tilde{\Sigma})^2}{\Lambda_n(\tilde{\Sigma})}. \quad \text{(A.24)}\]

Equation (A.25) appears in Chapter 4 as Equation (4.15).

**Solving for the Eigenfunctions**

In the special case of $\tilde{\Sigma} = 0$, the operator $D_{\tilde{\Sigma}}$ reduces to a one-dimensional biharmonic equation; Equation (A.6) reduces to

$$\nabla^4 W^{(n)} = k_n^4 W^{(n)}.$$  \quad \text{(A.26)}

We solve the system for in the range $x \in [0, L]$ as the solution is relatively simpler when shifted to this range. $W^{(n)}(x)$ then admits solutions of the form:

$$W^{(n)}(x) = A \sin k_n x + B \cos k_n x + C \sinh k_n x + D \cosh k_n x.$$  \quad \text{(A.27)}

Clearly, the boundary conditions $W^{(n)}_{xx}(0) = W^{(n)}_{xxx}(0) = 0$ yields $A = D$ and $B = E$. The conditions $W^{(n)}_{xx}(L) = W^{(n)}_{xxx}(L) = 0$ then has

$$\frac{A}{B} = \frac{\sin k_n L + \sinh k_n L}{\cos k_n L - \cosh k_n L}.$$  \quad \text{(A.28)}
This is subject to a solvability condition on the wavevectors $k_n^\dagger$ which for the free-free boundary conditions are
\begin{equation}
\cos k_n L \cosh k_n L = 1,
\end{equation}
with $k_0 = 0$ (corresponding to the constant solution $W^{(0)} = 1$) and $k_n L \simeq (n + 1/2)\pi$ for $n \geq 1$. Since $k_n^4 = \lambda_n / A = \Lambda_n \pi^4 / L^4$, we can immediately see that $\Lambda_n \simeq (n + 1/2)^4$. This fact was used in Section 4.2.1 to justify the resemblance of the variance profile to the contribution from fundamental mode: $V(x, \tilde{\Sigma})$ in Equation (A.25) is dominated by the first term. The

![Figure A.1: First few eigenfunctions $W^{(n)}(x)$ of the biharmonic operator (solid lines), and corresponding eigenfunctions of the $D_{100}$ operator (dashed line).](image)

\footnote{The interested reader is directed to Problems 4 through 6 in section 25 of Landau & Lifshitz [46] or Appendix B of Wiggins et al. [22] for a comprehensive treatment of the solvability conditions and eigenfunctions for not just the free end boundaries but a wide range of possible scenarios including clamped ends, hinged ends and combinations thereof.}
eigenfunctions are of the form

\[
W^{(n)}(x) = A \{(\sin k_n L + \sinh k_n L)(\sin k_n x + \sinh k_n x) \\
+ (\cos k_n L - \cosh k_n L)(\cos k_n x + \cosh k_n x)\}.
\] (A.30)

The shapes of these eigenfunctions (normalized) are plotted in Figure A.1. Eigenfunctions of \( D_{\tilde{\Sigma}} \) when \( \tilde{\Sigma} \neq 0 \) cannot be determined analytically but a numerical solution is relatively straightforward, and the shapes are seen to be strikingly similar to the \( \tilde{\Sigma} = 0 \) case.
References


