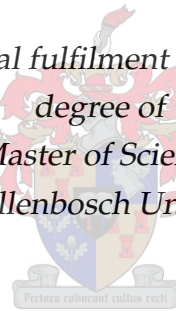# Dynamics of an active crosslinker on a chain and aspects of the dynamics of polymer networks

by

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at Stellenbosch University

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Faculty of Science

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Declaration

By submitting this thesis electronically, I declare that the entirety of the work contained therein is my own, original work, that I am the owner of the copyright thereof (unless to the extent explicitly otherwise stated) and that I have not previously in its entirety or in part submitted it for obtaining any qualification.

December 2011
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i

Abstract

Active materials are a subset of soft matter that is constantly being driven out of an equilibrium state due to the energy input from internal processes such as the hydrolysis of adenosine triphosphate (ATP) to adenosine diphosphate (ADP), as found in biological systems.

Firstly, we construct and study a simple model of a flexible filament with an active crosslinker/molecular motor. We treat the system on a mesoscopic scale using a Langevin equation approach, which we analyse via a functional integral approach using the Martin-Siggia-Rose formalism. We characterise the steady state behaviour of the system up to first order in the motor force and also the autocorrelation of fluctuations of the position of the active crosslink on the filament. We find that this autocorrelation function does not depend on the motor force up to first order for the case where the crosslinker is located in the middle of the contour length of the filament. Properties that characterise the elastic response of the system are studied and found to scale with the autocorrelation of fluctuations of the active crosslink position.

Secondly, we give a brief overview of the current state of dynamical polymer network theory and then propose two dynamical network models based on a Cayley-tree topology. Our first model takes a renormalisation approach and derive recurrence relations for the coupling constants of the system. The second model builds on the ideas of an Edwards type network theory where Wick's theorem is employed to enforce the constraint conditions. Both models are examined using a functional integral approach.

Opsomming

Aktiewe stelsels is 'n subveld van sagte materie fisika wat handel oor sisteme wat uit ekwilibruim gedryf word deur middel van interne prossesse, soos wat gevind word in biologiese stelsels.

Eerstens konstruëer en bestudeer ons 'n model vir 'n buigbare filament met 'n aktiewe kruisskakelaar of molekulêre motor. Ons formuleer die stelsel op 'n mesoskopiese skaal deur gebruik te maak van 'n Langevin vergelyking formalisme en bestudeer die stelsel deur gebruik te maak van funksionaal integraal metodes deur middel van die Martin-Siggia-Rose formalisme. Dit laat ons in staat om die tydonafhankle gedrag van die stelsel te bestudeer tot op eerste orde in die motorkrag. Ons is ook in staat om die outokorrelasie fluktuasies van die posisie van die aktiewe kruisskakelaar te karakteriseer. Ons vind dat die outokorrelasie onafhanklink is van die motorkrag tot eerste orde in die geval waar die kruisskakelaar in die middel van die filament geleë is. Die elastiese eienksappe van die sisteem word ook ondersoek en gevind dat die skaleer soos die outokorrelasie van die fluktuasies van die aktiewe kruisskakelaar posisie.

Tweedens gee ons 'n vlugtige oorsig van die huidige toestand van dinamiese polimeer netwerk teorie en stel dan ons eie twee modelle voor wat gebasseer is op 'n Caylee-boom topologie. Ons eerste model maak gebruik van 'n hernormering beginsel en dit laat ons toe om rekurrensierelasies vir die koppelingskonstates te verkry. Die tweede model bou op idees van 'n Edwards tipe netwerk teorie waar Wick se teorema ingespan word om die beperkingskondisies af te dwing. Beide modelle word met funksionaal integraal metodes bestudeer.

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I am most grateful for the bursary awarded to me by the National Institute for Theoretical Physics during my B.Sc. Hons and M.Sc. studies. Without their financial support I would not have been able to successfully complete my research according to a standard that I hold myself to.

I would then like to thank some of the students in the department for their valuable insights and friendship. I would like to single out M.J. Mateyisi, C.M. Rowher and H.W. Groenewald. Talks with M.J. Mateyisi led to greater insight into the physical nature of my research. C.M. Rohwer was perhaps the best soundboard for my frustrations regarding my research and provided advice that led to the successful completion of this work. H.W. Groenewald has been a friend to me since my first year and his great mathematical insight and the friendly competitive behaviour between us has been invaluable to further my research.

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Contents

Contents   vi

List of Figures

Chapter 1

Introduction

1.1 Active Materials

The *cytoskeleton* is the backbone of a biological cell and is responsible for the dominant mechanical properties of the cell[1]. The cytoskeleton is known to contain biopolymer networks mainly consisting of protein filaments known as actin, tubulin and vimetin. These biopolymer networks all have various levels of rigidity, but are also known to have the property of dynamical flexibility due to the way the filaments are crosslinked. Biopolymer networks are further known to play a role in cell motility and cell division.

Soft matter physics[2] is a subfield of condensed matter physics that deals with materials that are easily deformed under the application of mechanical forces or thermal fluctuations. Polymer networks, such as vulcanised rubber used to construct tyres, provide an example of soft matter. The important effects of these systems can be classified classically, i.e. quantum effects are generally not taken into consideration seeing as the energy scales of these systems are comparable to room temperature thermal energy.

Active materials are a subset of soft matter that is constantly being driven out of an equilibrium state due to the energy input from the hydrolysis of adenosine triphosphate (ATP) to adenosine diphosphate (ADP), as found in biological systems[3]. In this thesis we will generally treat these systems on a *mesoscopic* scale, i.e. on a scale larger than the microscopic constituents of the system, but smaller than the macroscopic scale of classical continuum mechanics.

Traditional polymer networks are permanently crosslinked, whereas biopolymer

networks generally contain active crosslinks as well. These reversible, i.e. attachable and detachable, crosslinks are enforced by so called *molecular motors* that are tethered to the filaments. It is these molecular machines that consume the energy provided by adenosine triphosphate to perform mechanical work. These motors operate on energy scales where the thermal fluctuations from the surrounding environment become a significant factor. Examples of cytoskeletal motors include myosin and kinesin. Myosin is a protein that plays a role in muscle contraction along with actin filaments. Kinesin is involved with the intracellular transport of material away from the cell nucleus via microtubules. Microtubules are rope-like structures in the cytoskeleton that are made up of tubulin that can grow up to 25 micrometres long[4].

Due to the possibility of network reorganisation as a result of active crosslinks, the mechanical properties of these active networks will generally be very different than those of traditional polymer networks. Understanding the mechanical properties of active materials may enable one to construct better biocompatible materials.

The main goal of this thesis is to develop dynamical mesoscopic models that will give insight into understanding the effect of motor activity and crosslinking on the elastic properties of active networks such as those found in biological cells.

The mechanical work in an active system is performed in an environment where there is effectively no heat reservoir, such as in a biological system which is mostly at a constant temperature. This is in contrast to most mechanical engines that operate on a Carnot cycle. These type of work generating motors have been explored by Jülicher, Prost and Ajdari[5] in detail using so called Brownian ratchet models. We will not be concerned with this issue and will neglect the scale on which the internal dynamics of these molecular motors contribute to the dynamical behaviour of the systems we want to study. We will thus take the induced motion of a molecular motor for granted.

1.2   Elastic properties of polymer networks and active gels

The experimental work related to the theoretical models that we will present in this thesis can be divided into the study of the elastic properties of classical semiflexible biopolymer networks and the study of how the addition of molecular motors affects the elastic properties of biopolymer networks. Dilute active crosslinked biopolymer

networks are also known as active gels.

Extensive in vitro study has been done on the viscoelastic properties of biopolymer networks by Käs[6] amongst others. This is done using micro- and macrorheological techniques and very detailed results can be found with modern experimental apparatus such as optical tweezers. Experimentalists in this field want to know how the stored elastic energy of a network is related to the amount of filaments in a solution. They are able to measure the storage modulus[1] as a function of the actin concentration.

Active gels have recently received great experimental attention. Mizuno, Schmidt, MacKintosh[1] and others have successfully measured the effects of activity by the addition of myosin on a biopolymer network. One of the remarkable properties that has been discovered is that the shear modulus[2] of the network increases hundredfold when the myosin motors are activated by the addition of ATP to the system. The additional active crosslinking constraints and force generation of the molecular motors on the filaments are responsible for this stiffening process.

1.3   Polymer Theory

The active systems we would like to analyse are constructed out of polymers and molecular motors. In this thesis the terms *polymer*, *filament*, *chain* and *strand* will be used interchangeably. For our theoretical purposes, polymers can be divided into three groups based on their rigidity: flexible, semiflexible, and stiff polymers. To quantify these terms we first have to introduce the concept of the persistence length[7] l_p of a polymer. Simply stated, the persistence length is the length scale at which the orientation of segments of a polymer become uncorrelated and is thus a measure of stiffness. One should keep in mind that segments are not necessarily the microscopic components of the polymer, but rather the coarse grained mesoscopic components. The length of a single coarse grained component for a flexible polymer is called the *Kuhn length*. If we denote the contour length of a polymer by L, then we can classify polymers as flexible, semiflexible or stiff based on how L relates to the persistence length.

For a polymer where the contour length is much longer than the persistence

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[1]The storage modulus is a measure of the stored energy in a network due to to the elastic properties of the network.

[2]The shear modulus is defined as the ratio between the shear stress and the shear strain of a material.

length, i.e. $L \gg l_p$, the equilibrium conformation of the polymer can be explained statistically by a Gaussian distribution if we assume that there is no hydrodynamic interaction and no excluded volume interaction, i.e. the polymer has no real topology in the sense of entanglement. The mesoscopic segments of this model thus perform ordinary Brownian motion. This is known as the phantom chain model for a flexible polymer. One may think of a phantom chain as a random walk in the spatial domain. Flexible polymers are generally easier to deal with theoretically because the mathematical structures arising from their Gaussian nature are relatively straightforward and well worked out. Gaussian approximations are found in various subfields of physics such as quantum field theory and this there is a great body of work that hints towards solving these type of problems. Due to the lack of topology, the filaments may even be found in configurations where every filament segment occupies the same space. This is of course not a realistic scenario, but introducing an excluded volume effect leads to a great increase in mathematical complexity that we will want to avoid.

If a polymer has a contour length comparable to the persistence length, i.e. $L \simeq l_p$ then the polymer is classified as semiflexible. Semiflexible polymers have no extensibility property and only bending degrees of freedom[8]. The bending rigidity, i.e. how much energy it costs for the filament to bend is a function of l_p. The inextensibility condition makes this case more difficult to handle theoretically compared to the flexible case. Real biopolymers tend to be semiflexible and thus one would have to deal with these difficulties if one were to construct a successful theory with application to biological systems. F-actin is an example of a biopolymer with persistence length on the same scale as the contour length of the filament. The persistence length of F-actin is about 10 micrometres[4] which is also about the dimensions of a cell.

Polymers in the overstretched regime where $L \ll l_p$ can effectively be viewed as stiff rods.

In all real systems such as those found in biological cells, the hydrodynamical effects of the surrounding fluid should be taken into account. This can be done by introducing the so called *Oseen tensor*[7]. For the purpose of this thesis we will assume that the effects we are studying will take place on length scales shorter than that where the hydrodynamic interaction becomes important.

1.4   Current Theoretical Models of Biopolymer Networks

The current trend of modeling and studying the elastic response of biopolymer networks and active gels is to consider length and timescales where one could apply formalisms based on continuum or collective dynamics theories. Joanny, Jülicher and Kruse[9; 10] amongst others have been successful in building such theories where they take the symmetries of the system into account to write down their models. These models introduce quantities that are difficult to relate to the underlying microscopic properties of the system. The other alternative would be to measure these quantities experimentally, but this is unsatisfactory if one wants to understand the underlying microscopic mechanisms of the model. For biopolymer networks without activity in terms of molecular motors, Frey and Kroy[11; 12] have presented phenomenological models for studying the viscoelastic properties from a statistical point of view. These models are not easily generalised to theories where one can include the effect of activity of the network. Rubinstein and Panyukov[13] have also developed models for the elasticity of polymer networks with more relation to the microscopic constituents of the network, but still limited to the equilibrium properties of networks.

Liverpool et al.[14] want to quantify the effect that the force generation of molecular motors have on an active gel. They take a different approach where they start with a dynamical and more local analysis, i.e. the properties of pairs of crosslinked filaments, to study the non-equilibrium behaviour of active gels. They formulate an effective theory for analysing and understanding the shear modulus of such a system by considering the force balance of the system. Their model includes the thermal fluctuations of the filaments but implements the active crosslink as a constraint force without its own dynamics. We will study a similar physical model as Liverpool et al., but we will introduce the active crosslink position as a quantity with its own set of dynamics.

For more information, the reader is referred to short review by Joanny et al.[15]

1.5   Mesoscopic Formalism

As stated before, the aim of this thesis is to present a mesoscopic approach to modeling and analysing the dynamical elastic behaviour of active materials. Elastic properties are experimentally measurable and thus a theoretical treatment of the

problem is important to explain the experimental results. We will focus on the non-equilibrium statistical physics behaviour of the mechanical properties of these systems. Active systems are by definition non-equilibrium systems and furthermore, studying these systems might lead to greater insight regarding non-equilibrium statistical physics in general. Specifically we want to study how the elastic properties of the system are related to fundamental quantities such as the noise, drag and motor force. This is of course a very ambitious task and generally mathematically more complicated than building a more effective theory using continuum mechanics theory. We do not claim that this method is in any way superior to the current body of work found in the literature, but that there might be alternative methods to calculate the elastic properties of active systems. Our hope is that by treating a system on this scale that we will not have to introduce quantities to the model where the physical interpretation will be difficult or where said quantities cannot be expressed in terms of fundamental properties of the constituent components of the system.

The methods we will use allow us to fully parametrise the system in terms of quantities that have clear physical meaning. We hope that by doing so that we may gain a better understanding of the mechanism of how an active network stiffens when the molecular motors are activated. Furthermore we hope that by treating the crosslinking problem in a rigorous manner, that we will be able to characterise the emergent dynamical phenomena due to crosslinking.

1.6   Thesis organization

The thesis is divided into the following parts:

- Chapter 2 presents a dynamical model for a single actively crosslinked flexible filament.

- Chapter 3 provides analytical and numerical results for the model introduced in Chapter 2.

- Chapter 4 presents two Cayley-tree network models in order to study the constraint problem in a dynamical formalism.

- Chapter 5 provides the conclusion and outlook of this thesis.

In more detail, the models we study in this thesis can be divided into the following parts:

- First we will study a model of a single flexible filament with an active crosslink in order to understand some properties that characterise the elastic response of the system. We successfully formulate this model using a Langevin equation approach and analyse it via functional integral methods. While the resulting mathematical expressions are lengthy, we are able to calculate said expressions analytically. Specifically, we analyse the dependence of the autocorrelation of the fluctuations of the position of the active crosslink/motor on the motor force. The motor force is a force that provides the molecular motor with a preferential direction to move in. Calculating up to first order in the motor force indicates that there is no timescale dependence of said autocorrelation function on the motor force to first order. We also show that the properties characterising the elastic response of the system are proportional to the autocorrelation function as stated above. While the quantity we examine is not directly related to the elastic properties as studied by Liverpool et al., we provide a discussion on the similarities of our results.

- We then move over from single filament models to dynamical network models so that we may gain a deeper understanding of how the network constraints lead to new complex dynamical behaviour. We only treat traditional polymer networks, i.e. not active, in this thesis due to the already complicated problems arising in this case. We first present a model inspired by the work of Jones and Ball[16] who employed a renormalisation approach to study the force constants in a fixed network of stiff rods. We are able to derive recurrence relations for the drag and localisation behaviour of a Cayley-tree network consisting of polymers modeled as springs.

- We present an alternative dynamical network formalism by considering an Edwards type theory for the dynamical evolution of a Cayley-tree network. We introduce the idea of a generalised density function that is velocity and time dependent. An argument is presented why this quantity might solve a time ordering problem when applying Wick's theorem to this type of theory in a non-equilibrium scenario.

There are many degrees of freedom associated with real biological systems. Our models can only incorporate a limited number of these degrees of freedoms and should thus be viewed as mathematical models inspired by biological systems.

Chapter 2

Motor on a Flexible Chain — Model

2.1   Motivation

It may be wise to consider a simplified version of an active network. We have to figure out how to construct a model for the dynamics of the elements of a network before we can start thinking about assembling these filaments into a fixed network. Considering a full network requires that we deal with the constraint problem of how to link up all the various filaments in such a way that a real network is formed. We may consider the system of two filaments that are crosslinked by a molecular motor. The inspiration for studying these systems comes from Liverpool, Marchetti, Joanny and Prost[14] who studied such a system from a force balance approach. They were able to show that the ground state deformation of such an active gel scales with the square of the motor force f_s and that at high frequencies the effect of activity tends to stiffen the gel. The stiffening of the gel is also proportional to f_s^2. They neglect the effect of thermal fluctuations on the crosslinking position, which we will include in our model.

This symmetrical case may be simplified even further if we just consider a single filament and then fix the point that would have been on the other filament to a point in space. Of course it may be better to do a disorder average over this point in space such as to capture the dynamics. This will increase the mathematical complexity of the problem and we do not expect the results to greatly effect the quantities we will consider. Real biopolymers such as F-actin[14; 17] are semiflexible polymers which

8

means they do no extend, but only bend. The mathematics of semiflexible polymers is usually more complicated compared to the mathematics for a flexible polymer, which is just a random walk in the spatial domain. Even though the flexible case does not directly correspond to a biological system, we hope that our detailed study may still provide valuable insight into how these active systems behave themselves. After studying the flexible model we will briefly discuss aspects of the semiflexible version of this model.

2.2 Model

In this section we look at a dynamical model for the most simplified version of a network of flexible filaments with active crosslinkers. This is the model of a single filament with a molecular motor attached to it, which is in turn anchored to a fixed point in space. Propose the following Hamiltonian for the system,

$$\mathcal{H} = \mathcal{H}_E + \mathcal{H}_K$$
$$= \frac{3k_B T}{2l} \int_0^L ds \left(\frac{\partial r(s,t)}{\partial s} \right)^2 + \frac{k}{2} \left(r(\sigma(t), t) - X \right)^2 \tag{2.1}$$

where $\mathcal{H}_E$ describes the behaviour of the flexible filament of length L and inter-monomer distance l. The filament spatial conformation at any time t is given by $r(s,t)$, parametrised in terms of the arc length s, i.e. $0 \leq s \leq L$. We note that $\mathcal{H}_E$ contains a Wiener measure that describes a random walk in the spatial domain,
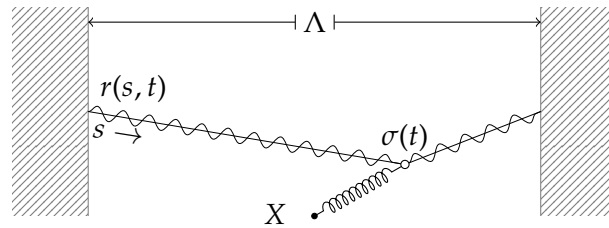
Figure 2.1: A flexible filament with a cross linking molecular motor attached to it. The motor is also anchored at position X via a harmonic interaction. The end points of the filament is kept a distance Λ apart. The filament is parametrised by $r(s,t)$ where the s coordinate runs along the filament and $0 \leq s \leq L$. The position coordinate of the motor or active crosslink is indicated by $\sigma(t)$ and also runs along the filament. The straight line indicates the conformation of the steady state of the filament and the curvy lines the fluctuations around this point. Note that there are no hard boundaries i.e they do not exclude the polymer.

where the entropic contribution is visible in the thermal-dependent prefactor $\frac{3k_BT}{2l}$.
The hydrodynamic interaction between the filament and a surrounding fluid is
neglected and the filament does not interact with itself, i.e. there is no excluded
volume effect. This model is known as the Rouse model[7]. A flexible polymer
can thus be viewed as an entropic spring. Furthermore we impose the following
boundary conditions

$$r(0, t) = 0 \tag{2.2}$$

$$r(L, t) = \Lambda \tag{2.3}$$

and thus fix the endpoints of the filament. The second part of the Hamiltonian
$\mathcal{H}_K$ describes the energetic contribution of a spring with spring constant k that is
attached to the motor crosslink, where the arc length along the filament, where
the crosslink is attached, is parametrised by $\sigma(t)$, and the anchoring point X. Since
we are considering a one-dimensional model, it is necessary for the attachment
point to lie between 0 and Λ, i.e. $0 \leq X \leq \Lambda$. The parameter Λ will be taken as
a free parameter in our system. The position coordinate of the motor runs along
the filament, i.e. $0 \leq \sigma(t) \leq L$. The parameter t indicates a time dependency and
indicates that the position coordinate of the motor has its own dynamics. We are
now in a position to formulate the dynamics of this system in terms of a set of
Langevin equations. The two dynamical quantities in our system, $r(s, t)$ and $\sigma(t)$,
will be regarded as having slower dynamics than the surrounding system (noise),
hence justifying writing down the following coupled set of Langevin equations

$$\gamma_r \frac{\partial r(s, t)}{\partial t} = -\frac{\delta H}{\delta r(s, t)} + f_r(s, t)$$

$$\gamma_\sigma \frac{\partial \sigma(t)}{\partial t} = -\frac{\delta H}{\delta \sigma(t)} + f_\sigma(t) + f_s,$$

where $\frac{\delta H}{\delta r(s,t)}$ and $\frac{\delta H}{\delta \sigma(t)}$ are the functional derivatives of the Hamiltonian with respect
to the dynamical quantities of the system. See Appendix A for the definition and
details of the functional derivative. A motor force f_s is added to the equation of the
dynamics of motor attachment such that the motor attachment point will have a
preferential direction to move in. This force f_s is not time or spatially dependent
so that the model remains as simple as possible. The drag coefficients are given
by γ_r and γ_σ. Both the filament and the motor attachment point on the filament
undergo thermal fluctuating forces as a result from the environment. To keep the

mathematics as simple as possible, white noise is used and the stochastic forces can be characterised by

$$\langle f_r(s,t) \rangle = 0$$
$$\langle f_\sigma(t) \rangle = 0$$
$$\langle f_r(s,t) f_r(s',t') \rangle = \lambda_r \delta(s-s') \delta(t-t')$$
$$\langle f_\sigma(t) f_\sigma(t') \rangle = \lambda_\sigma \delta(t-t') ,$$

where the parameters λ_r and λ_σ control the strength of the respective thermal noises. These quantities are related to the drag coefficients γ_r and γ_σ via the fluctuation-dissipation theorem as

$$\lambda_r = 2\gamma_r k_B T$$
$$\lambda_\sigma = 2\gamma_\sigma k_B T$$

because we are neglecting the effect that the internal dynamics of a motor molecule might have on the surrounding environment. The stochastic forces take on a Gaussian probability distribution, neglecting normalisation, given by the following functional form:

$$P[f_r(s,t)] = \int \mathcal{D}f_r \, e^{-\frac{\lambda_r}{2} \int ds \, dt f_r^2(s,t)}$$
$$P[f_\sigma(t)] = \int \mathcal{D}f_\sigma \, e^{-\frac{\lambda_r}{2} \int dt f_\sigma^2(t)} .$$

(2.4)

Performing the functional derivatives leads to the following set of coupled nonlinear Langevin equations:

$$\gamma_r \frac{\partial r(s,t)}{\partial t} = \frac{3k_B T}{l} \frac{\partial^2 r(s,t)}{\partial s^2} - k\left(r(s,t) - X\right) \delta(s - \sigma(t)) + f_r \tag{2.5}$$

$$\gamma_\sigma \frac{\partial \sigma(t)}{\partial t} = -k\left(r(\sigma(t),t) - X\right) \left.\frac{\partial r(s,t)}{\partial s}\right|_{s=\sigma(t)} + f_\sigma + f_s . \tag{2.6}$$

Details of the derivation can be found in Appendix A.

Let us briefly examine these equations to see if they describe sensible dynamics for our system. Equation 2.5 describes the flexible filament and contains a second spatial derivative of the parametrised curve. The existence of this term can be explained by looking at the continuum limit of the discretised description of a polymer and is expanded upon in Appendix B. The harmonic interaction term can only affect the conformation of the filament at the point where the motor attaches to the filament. The Dirac Delta thus enforces this condition. When we perform dimensional analysis of this equation, in particular the terms derived from the

functional derivative, then we find that it has the units of force per length. Thus for this to be a force balance equation we have to multiply it by a length scale, for instance the average inter-monomer distance l of the polymer. This will aid us in interpreting the drag term γ_r and the noise term f_r. First consider the expression for Stokes drag coefficient

$$\zeta = 6\pi\eta a \, ,$$

where η is the viscosity of the surrounding fluid and a the finite radius of a spherical particle that is experiencing the drag. In the Rouse model the monomer radius a and average bond length l need not be the same. If we consider the quantity

$$\frac{\gamma_r}{l} = 6\pi\eta\frac{a}{l} \, ,$$

where $\frac{a}{l}$ is a dimensionless quantity, then the interpretation of γ_r is clear. Similarly the stochastic force term f_r is a force density where after multiplying with the appropriate length scale, say l, results in the normal stochastic force. The fluctuation-dissipation theorem should also continue to hold as both the drag and the noise strength parameter λ_r need to be scaled with a single length scale. Later in the dynamical calculation we will note that γ_r and λ_r always couple to a length scale. The second equation that describes the dynamics of the molecular motor also contains the harmonic interaction term, which is evaluated at the position of the motor. One should again note that the position of the motor $\sigma(t)$ is a coordinate that runs along the filament. Seeing as the filament is fully flexible, this path length is fixed but the walk can be stretched or compressed. Thus the step length of the molecular motor has to be variable. This dynamic is encoded in the factor $\left.\frac{\partial r(s,t)}{\partial s}\right|_{s=\sigma(t)}$ that describes the local stretching of the filament where the motor attaches to it.

A further assumption we would like to make is that the filament and the position of the motor performs small fluctuations around some steady state solution in the long time limit. This will simplify the mathematics later on and make the problem more analytically tractable. The following functional form of the parametrised filament and position of the motor is proposed,

$$r(s, t) = r_\infty(s) + \rho(s, t) \tag{2.7}$$

$$\sigma(t) = \sigma_\infty + \Delta(t) \, , \tag{2.8}$$

where $r_\infty(s)$ and σ_∞ denote the steady state solutions of the conformation of the

filament and the position of the crosslink respectively and are both time-independent. This means that there can be no fluctuations of the filament at the end points i.e.

$$\rho(0, t) = 0$$
$$\rho(L, t) = 0 \,,$$

which corresponds with the assumed boundary conditions of our model. The steady state solutions can now be found by solving a set of polynomial equations as seen in the next section. Therefore the only quantities that need to be dealt with in a dynamical formalism are that of the fluctuations $\rho(s, t)$ and $\Delta(t)$.

2.3   Steady State

In this section we explore the steady state solution of our system consisting of a molecular motor on a strand. The steady state differential equations without fluctuations are given by

$$0 = \frac{3k_B T}{l} \frac{d^2 r_\infty}{ds^2} - k \left(r_\infty(s) - X \right) \delta(s - \sigma) \tag{2.9}$$

$$0 = -k \left(r_\infty(\sigma_\infty) - X \right) \left. \frac{dr_\infty}{ds} \right|_{s=\sigma_\infty} + f_s \,. \tag{2.10}$$

It is clear that in the steady case that the strand should take on the form of a piecewise linear function

$$r_\infty(s) = \begin{cases} \alpha s & 0 \le s < \sigma_\infty \\ \beta s + \delta & \sigma_\infty \le s \le L \end{cases} \,,$$

with constants α, β and δ that we have to determine. One can now substitute in the boundary conditions. The position of the filament at its end point should be equal to the position where it is tethered to and is given by

$$r_\infty(L) = \beta L + \delta$$
$$= \Lambda \quad \text{(from equation 2.3)}$$
$$\Rightarrow \delta = \Lambda - \beta L \,.$$

The position of the molecular motor can also be expressed in terms of the gradients α and β as follows, noting that $r_\infty(s)$ has to be continuous,

$$r_\infty(\sigma_\infty) = \alpha\sigma_\infty \tag{2.11}$$

$$= \beta\sigma_\infty + \delta$$

$$= \Lambda + \beta(\sigma_\infty - L)$$

$$\Rightarrow \sigma_\infty = \frac{\Lambda - \beta L}{\alpha - \beta} \tag{2.12}$$

which in turn allows one to solve the displacement of the filament at the position where the motor attaches to it,

$$r_\infty(\sigma_\infty) = \frac{\alpha}{\alpha - \beta}\left(\Lambda - \beta L\right) .$$

We now turn to writing down equations that will aid us in solving for the gradients α and β. To do so, consider a set of discretised equations around the point of motor attachment $s = \sigma_\infty$,

$$0 = \frac{3k_B T}{l^2}\left(r_{\infty,+1} - 2r_\infty + r_{\infty,-1}\right) - k\left(r_\infty(\sigma_\infty) - X\right) \tag{2.13}$$

$$0 = -k\left(r_\infty(\sigma_\infty) - X\right)\left(\frac{r_\infty(\sigma_\infty)_{+1} - r_\infty(\sigma_\infty)}{2l} + \frac{r_\infty(\sigma_\infty) - r_\infty(\sigma_\infty)_{-1}}{2l}\right) + f_s \tag{2.14}$$

and notice that we can we can replace the divided differences by the average gradients. We should also keep in mind that the differential equation was a force density equation and thus we must have an addition factor of l when looking at a specific point in space i.e. a force balance equation. Substituting the gradients from our ansatz (equations 2.7 and 2.8) leads to

$$0 = \frac{3k_B T}{l}(\beta - \alpha) - k\left(\frac{\alpha}{\alpha - \beta}(\Lambda - \beta L) - X\right) \tag{2.15}$$

$$0 = -k\left(\frac{\alpha}{\alpha - \beta}(\Lambda - \beta L) - X\right)\frac{\alpha + \beta}{2} + f_s . \tag{2.16}$$

It is not mathematically tractable to exactly solve the above set of algebraic equations, as it reduces to solving a fourth order polynomial. The problem can still be dealt with perturbatively as shown in the next section. We can also show that the same type of equations may be derived from a model with less degrees of freedom, i.e. a model where we exclude the polymer degrees of freedom.

2.3.1 Small Motor Force

If one turns off the motor force, i.e. set $f_s = 0$, then the solution becomes trivial. There are two solutions but only one corresponds to the minimum energy state. Seeing as we are working with a one dimensional system, it is required that the signs of α and β are equal. While the other solution with opposite signs is also valid, it does not correspond to the minimum energy state. Thus the chosen solution is $\alpha = \beta$. The expressions for α and β are easily derived from,

$$
\begin{aligned}
r_\infty(\sigma_\infty) &= \alpha\sigma_\infty \\
&= \beta\sigma_\infty + \Lambda - \beta L \\
\Rightarrow \beta\sigma_\infty &= \beta\sigma_\infty + \Lambda - \beta L \\
\Rightarrow \beta &= \frac{\Lambda}{L} \, .
\end{aligned}
$$

The position of the molecular motor can also be easily derived from equation 2.10 and it follows that

$$
\begin{aligned}
r_\infty(\sigma_\infty) &= X \\
\Rightarrow \sigma_\infty &= \frac{X}{\alpha} \\
&= \frac{XL}{\Lambda} \, .
\end{aligned}
$$

If we place a restriction on the motor force f_s such that it is small, then it is possible to find perturbed solutions for α and β. First one can rewrite the equations 2.15 and 2.16 as

$$
0 = \frac{3k_B T}{l}(\beta - \alpha) - \frac{2f_s}{\alpha + \beta} \tag{2.17}
$$

$$
0 = -k\left(\frac{\alpha}{\alpha - \beta}(\Lambda - \beta L) - X\right)\frac{\alpha + \beta}{2} + f_s \tag{2.18}
$$

where it is now convenient to make the change of variables,

$$
\begin{aligned}
\epsilon &= \beta - \alpha \\
\eta &= \frac{\alpha + \beta}{2}
\end{aligned}
$$

or equivalently,

$$\alpha = \frac{2\eta - \epsilon}{2}$$

$$\beta = \frac{2\eta + \epsilon}{2}$$

leading to the following set of equations

$$0 = \frac{3k_B T}{l}\epsilon - \frac{f_s}{\eta} \tag{2.19}$$

$$0 = -k\left(\frac{\epsilon - 2\eta}{2\epsilon}\left(\Lambda - \frac{2\eta + \epsilon}{2}L\right) - X\right)\eta + f_s, \tag{2.20}$$

which are equivalent to the original equations. Equation 2.12 for the position of the motor can also be rewritten using the same substitution which results in

$$\epsilon\sigma_\infty = \Lambda - \frac{2\eta + \epsilon}{2}L. \tag{2.21}$$

One can now make the perturbation ansatz

$$\epsilon = \epsilon_0 + \epsilon_1 f_s$$

$$\eta = \eta_0 + \eta_1 f_s$$

where ϵ_0 and η_0 are the solutions to the system without any motor force and can be substituted into the above equations to give

$$\epsilon = \epsilon_1 f_s$$

$$\eta = \frac{\Lambda}{L} + \eta_1 f_s.$$

Substituting this into equation 2.19 and keeping up to first order in f_s results in

$$f_s\left(\frac{3k_B T}{l}\epsilon_1 - \frac{L}{\Lambda}\right) = 0,$$

where solving for ϵ_1 leads to

$$\epsilon_1 = \frac{Ll}{3\Lambda k_B T}$$

which can now be substituted into the equation 2.20 and again working up to first order in f_s:

$$\frac{kX\Lambda}{L} - \frac{k\Lambda^2}{2L} + \frac{3kk_BT\eta_1\Lambda^3}{lL^2} = 0$$

where solving for η_1 leads to

$$\eta_1 = \frac{lL(2X - \Lambda)}{6k_BT\Lambda^2} .$$

It is now possible to express the gradients α and β as linear functions of the motor force f_s with the result given by

$$\alpha = \frac{\Lambda}{L} + f_s \left(\frac{lL(X - \Lambda)}{3k_BT\Lambda^2} \right) \tag{2.22}$$

$$\beta = \frac{\Lambda}{L} + f_s \left(\frac{lLX}{3k_BT\Lambda^2} \right) . \tag{2.23}$$

It should be noted that the first order corrections in f_s to the gradients do not depend on the spring constant that connects the motor to an anchoring point at X. Similarly one can apply the same procedure to calculate first order perturbation to the position of the molecular motor. Making a similar ansatz

$$\sigma = \sigma_0 + \sigma_1 f_s$$

one can write by using equation 2.21 that

$$\left(\epsilon_1 f_s + \epsilon_2 f_s^2 \right) \left(\sigma_0 + \sigma_1 f_s \right) = \Lambda - \frac{L}{2} \left(2\eta_0 + 2\eta_1 f_s + 2\eta_2 f_s^2 + \epsilon_1 f_s + \epsilon_2 f_s^2 \right) ,$$

where one now has to solve for σ_1 to first order in f_s, resulting in

$$\sigma_1 = -\frac{\frac{L}{2}\epsilon_2 + L\eta_2 + \epsilon_2\sigma_0}{\epsilon_1} , \tag{2.24}$$

noticing that the first order correction for the position of the motor depends on the second order corrections of η and ϵ. Doing the same as before, propose the ansatz

$$\epsilon = \epsilon_0 + \epsilon_1 f_s + \epsilon_2 f_s^2$$

$$\eta = \eta_0 + \eta_1 f_s + \eta_2 f_s^2 .$$

Substituting ϵ into equation 2.19 as before, and also substituting the solutions for ϵ_0 and ϵ_1, one finds to second order in f_s that

$$0 = f_s^2 \left(\frac{3k_B T \epsilon_2}{l} + \frac{lL^3 X}{3k_B T \Lambda^4} - \frac{lL^3}{6k_B T \Lambda^3} \right)$$

where solving for ϵ_2 leads to

$$\epsilon_2 = -\frac{l^2 L^3 (2X - \Lambda)}{18 k_B^2 T^2 \Lambda^4} .$$

One can in turn solve for η_2 by substituting the solutions for ϵ_0, ϵ_1, η_1 into equation 2.20 as before, leading to the following relation up to second order in f_s:

$$0 = f^2 \left(1 + \frac{klL}{12k_B T} + \frac{2klLX^2}{3k_B T \Lambda^2} - \frac{2klLX}{3k_B T \Lambda} + \frac{3kk_B T \eta_2 \Lambda^3}{lL^2} \right)$$

where solving for η_2 leads to

$$\eta_2 = -\frac{lL^2 \left(8klLX^2 - 8klLX\Lambda + klL\Lambda^2 + 12k_B T \Lambda^2 \right)}{36 k k_B^2 T^2 \Lambda^5} .$$

One is now able to solve for σ_1 by substituting in the solutions obtained thus far into equation 2.24 which leads to

$$\sigma_1 = \frac{L^2 \left(3k_B T \Lambda^2 + klLX(-3X + 2\Lambda) \right)}{3kk_B T \Lambda^4} .$$

Thus the position of the molecular motor up to first order in the motor force is given by

$$\sigma_\infty = \frac{XL}{\Lambda} + f_s \frac{L^2 \left(3k_B T \Lambda^2 + klLX(-3X + 2\Lambda) \right)}{3kk_B T \Lambda^4} . \tag{2.25}$$

Whereas the gradients did not depend on the spring constant k in the first order corrections, the first order correction for the position of the motor does depend on it. The displacement of the filament at the point where the motor attaches to it is now straightforward to calculate, keeping in mind that one is only working up to first

order in f_s,

$$
\begin{aligned}
r_\infty(\sigma_\infty) &= \alpha\sigma_\infty \\
&= \frac{2\eta - \epsilon}{2}\sigma_\infty \\
&= \left(-\frac{1}{2}\epsilon_1 f_s + \eta_0 + \eta_1 f_s\right)(\sigma_0 + \sigma_1 f_s) \\
&= -\frac{1}{2}\epsilon_1\sigma_0 f_s + \frac{1}{2}\cancel{\epsilon_1\sigma_1 f_s^2} + \eta_0\sigma_0 + \eta_0\sigma_1 f_s + \eta_1\sigma_0 f_s + \cancel{\eta_1\sigma_1 f_s^2} \\
&= X + \frac{L\left(klLX(4X - 3\Lambda) - 3k_BT\Lambda^2\right)}{3kk_BT\Lambda^3}f_s,
\end{aligned}
\tag{2.26}
$$

where the second order terms in f_s are neglected because we are only working up to first order in f_s. The first and second derivatives up to first order in f_s of the filament at the point where the motor attaches to it can now be written as

$$
\left.\frac{\partial r_\infty}{\partial s}\right|_{\sigma_\infty} = \frac{\Lambda}{L} + f_s\frac{lL(2X - \Lambda)}{6k_BT\Lambda^2}
\tag{2.27}
$$

$$
\left.\frac{\partial^2 r_\infty}{\partial s^2}\right|_{\sigma_\infty} = \frac{L}{3k_BT\Lambda}f_s.
\tag{2.28}
$$

For the symmetric case where the anchoring point of the motor sits in the middle, $X = \frac{\Lambda}{2}$, we find that the first derivative of the filament at the point where the motor attaches to the filament

$$
\left.\frac{\partial r_\infty}{\partial s}\right|_{\sigma_\infty} = \frac{\Lambda}{L}
$$

to be independent of the motor force to first order. We may note that this ratio indicates the stretching of the filament:

$$
\frac{\Lambda}{L} = \begin{cases} 1 & \text{if } \sqrt{\langle\mathcal{R}^2\rangle} \simeq \Lambda \\ > 1 & \text{if } \sqrt{\langle\mathcal{R}^2\rangle} > \Lambda \\ < 1 & \text{if } \sqrt{\langle\mathcal{R}^2\rangle} < \Lambda, \end{cases}
$$

where $\sqrt{\langle\mathcal{R}^2\rangle}$ is the average end-to-end distance of the free polymer.

2.3.2 Network Deformation

We would like to briefly explore the behaviour of the position of the motor when we stretch the system, i.e. when we change the value of Λ. First let us consider the case

where the anchoring point X is kept fixed as we change the width Λ:

$$\frac{\partial \sigma_\infty}{\partial \Lambda} = f_s \left(-\frac{4lL^3X^2}{3k_BT\Lambda^5} + \frac{2lL^3X}{k_BT\Lambda^4} - \frac{2L^2}{k\Lambda^3} - \frac{lL^3}{3k_BT\Lambda^3} \right) - \frac{LX}{\Lambda^2} \,.$$

We notice that if we turn off the motor force, i.e. $f_s = 0$ and set the anchoring point $X = \frac{\Lambda}{2}$, that

$$\left. \frac{\partial \sigma_\infty}{\partial \Lambda} \right|_{f_s=0,\, X=\Lambda/2} = -\frac{L}{2\Lambda} \tag{2.29}$$

which indicates that the position of the motor is dependent on how much the filament is stretched. In the case where the filament forms part of a bigger network, the anchoring point will also shift as one stretches the network. Thus let us suppose the affine transformation[1] $X \to \chi X$ and $\Lambda \to \chi \Lambda$ as the network is stretched by a factor χ. We would now like to see how the motor's position is affected as we change χ. Consider the expression

$$\frac{\partial \sigma_\infty(\chi)}{\partial \chi} = f_s \frac{2L^2 \left(klLX(3X - 2\Lambda) - 3k_BT\Lambda^2 \right)}{3kk_BT\Lambda^4\chi^3}$$

and note that when we turn off the motor force that

$$\left. \frac{\partial \sigma_\infty(\chi)}{\partial \chi} \right|_{f_s=0} = 0 \,.$$

This is a sensible result because we do not expect the position of the motor to change if the relative displacement between the anchoring point X and the total width Λ is unchanged.

2.3.3   Large Motor Force

We would like to briefly examine the case where we are dealing with a large motor force. We are not able to get the same type of analytical results as for the small force approximation, but the idea presented in this section might still provide additional insight into the steady state solutions. Suppose that we have a strong motor force to the right that causes the filament to the left of the motor to be relaxed and in turn very stretched to the right of the motor. If we follow the same convention of denoting the gradient of the filament to the left by α and to the right by β, then we

---

[1]An affine transformation is a transformation that preserves parallel lines and collinearity of points.

propose that $\xi \equiv \frac{\alpha}{\beta} \ll 1$. Using this to eliminate α in equations 2.17 and 2.18 leads to

$$0 = \frac{3k_B T}{l} \left(\beta - \xi\beta \right) - \frac{2f_s}{\beta + \xi\beta} \tag{2.30}$$

$$0 = -k \left(\frac{\xi\beta}{\xi\beta - \beta} \left(\Lambda - \beta L \right) - X \right) \frac{\xi\beta + \beta}{2} + f_s . \tag{2.31}$$

We can now rewrite equation 2.30 as follows

$$\begin{aligned}
0 &= \frac{3k_B T}{l} \left(\beta - \xi\beta \right) \left(\beta + \xi\beta \right) - 2f_s \\
&= \frac{3k_B T}{l} \left(\beta^2 - \cancel{\xi^2 \beta^2} \right) - 2f_s ,
\end{aligned}$$

where we neglect higher order term of ϕ. This is admittedly not a very rigorous exercise seeing that β has to be kept finite as we send the ratio $\frac{\alpha}{\beta}$ to zero. Unfortunately we cannot provide a better analysis at this time. If we continue with this idea, then we can show that

$$f_s \sim \frac{3k_B T}{l} \beta^2$$

as an upper limit for the large force.

2.4 Dynamical Calculation

Solving the dynamical equations 2.5 and 2.6 exactly is not feasible and a strategy has to be devised to deal with the mathematical complexity of the problem at hand. The mathematical formalism should allow for straightforward and clear approximations. A technique we will employ is to rewrite the system as a functional integral problem. This technique was first proposed in operator form by Martin, Siggia and Rose[18] and later in the functional integral form by Jouvet, Phythian[19] and Jensen[20]. The advantage of the functional integral formalism is that in general approximation schemes are easy to understand. In particular we shall choose a Gaussian approximation for non-linear terms seeing as the resulting integral will be fairly straightforward to calculate.

A basic outline of the technique and calculation will now be discussed. First the Langevin equations are cast into generating functional form by making use of a Dirac Delta functional and the functional Fourier transformation. The generating functional now depends on all the dynamical quantities of the system as defined via the Langevin equations and additional auxiliary fields for every dynamical

variable. The auxiliary fields have their origin in the functional Fourier transformation. By taking functional derivatives with respect to source[2] terms, various dynamical correlation functions can be obtained. More details about this technique can be founded in Appendix C. The main part of this calculation is to integrate out dynamical quantities in the generation functional except for those quantities which one wishes to obtain correlation functions from. One of the important quantities we wish to analyse in this model is the autocorrelation function of fluctuations of the position of the molecular motor. In this calculation we will see that while it is possible to analytically take all vibrational modes of the filament into account when analysing the system, that it becomes mathematically intractable to do so. Arguments will be given for why we can neglect higher vibrational modes in the long time limit. The generating functional that will be used to derive correlation functions is given by

$$
\mathcal{Z} = \int \mathcal{D}r(s,t)\mathcal{D}\sigma(t)
$$
$$
\times \delta\left[\gamma_r\frac{\partial r(s,t)}{\partial t} - \frac{3k_BT}{l}\frac{\partial^2 r(s,t)}{\partial s^2} + k\left(r(s,t) - X\right)\delta(s-\sigma(t)) + f_r(s,t)\right]
$$
$$
\times \delta\left[\gamma_\sigma\frac{\partial \sigma(t)}{\partial t} + k\left(r(\sigma(t),t) - X\right)\left.\frac{\partial r(s,t)}{\partial s}\right|_{s=\sigma(t)} + f_s + f_\sigma(t)\right]
$$
$$
\times \exp\left(\int dsdt\, h(s,t)r(s,t) + \int dt\, g(t)\sigma(t)\right),
$$

with the source terms given by $h(s,t)$ and $g(t)$. This form of generating functional is valid if we assume that the system has a unique solution. We may introduce the functional Fourier transformation to raise the arguments of the functional Dirac delta functions into the exponent. We can also introduce the probability distribution for the stochastic forces from equation 2.4 to arrive at

$$
\mathcal{Z} = \int \mathcal{D}r(s,t)\mathcal{D}\sigma(t)\mathcal{D}\hat{r}(s,t)\mathcal{D}\hat{\sigma}(t)\mathcal{D}f_r(s,t)\mathcal{D}f_\sigma(t)
$$
$$
\times \exp\left\{i\int_{s,t}\hat{r}(s,t)\left[\gamma_r\frac{\partial r(s,t)}{\partial t} - \frac{3k_BT}{l}\frac{\partial^2 r(s,t)}{\partial s^2} + k\left(r(s,t) - X\right)\delta(s-\sigma(t))\right.\right.
$$
$$
\left.\left. + f_r(s,t)\right]\right\} \times \exp\left\{i\int_t\hat{\sigma}(t)\left[\gamma_\sigma\frac{\partial \sigma(t)}{\partial t} + k\left(r(\sigma(t),t) - X\right)\left.\frac{\partial r(s,t)}{\partial s}\right|_{s=\sigma(t)} + f_s + f_\sigma(t)\right]\right\}
$$
$$
\times \exp\left\{-\frac{1}{2\lambda_r}\int_{s,t}f_r(s,t)^2 - \frac{1}{2\lambda_\sigma}\int_t f_\sigma(t)^2\right\},
$$

---

[2]Given a quantity x whose statistical average is to be obtained with respect to some distribution, $\langle x\rangle = \int dx\, xp(x)$, then one can rewrite this in terms of a generating function with the aid of a source term h as follows: $\langle x\rangle = \frac{\partial}{\partial h}\left(\int dx\, p(x)e^{hx}\right)\big|_{h=0}$. This generalises to the case of functionals and functional integrals.

where the shorthand $\int_{\mathbb{R}} ds\, dt = \int_{s,t}$ will be used from now on. Note that the source terms are suppressed in the above and this convention will be followed through in this thesis. Second order autocorrelations are given by the inverse of the matrix associated with the quadratic term of said quantity as shown in Appendix C. Integrating over all realisations of the stochastic forces $f_r(s,t)$ and $f_\sigma(t)$ results in the following generating functional,

$$
\langle \mathcal{Z} \rangle = \int \mathcal{D}r(s,t)\mathcal{D}\sigma(t)\mathcal{D}\hat{r}(s,t)\mathcal{D}\hat{\sigma}(t)
$$

$$
\times \exp \left\{ -\frac{\lambda_r}{2} \int_{s,t} \hat{r}^2(s,t) \right.
$$

$$
\left. + i \int_{s,t} \hat{r}(s,t) \left[\gamma_r \frac{\partial r(s,t)}{\partial t} - \frac{3k_B T}{l} \frac{\partial^2 r(s,t)}{\partial s^2} + k\left(r(s,t) - X\right)\delta(s - \sigma(t)) \right] \right\}
$$

$$
\times \exp \left\{ -\frac{\lambda_\sigma}{2} \int_t \hat{\sigma}^2(t) + i \int_t \hat{\sigma}(t) \left[\gamma_\sigma \frac{\partial \sigma(t)}{\partial t} + k\left(r(\sigma(t),t) - X\right) \frac{\partial r(s,t)}{\partial s}\bigg|_{s=\sigma(t)} + f_s \right] \right\},
$$

where the dynamical quantities $r(s,t)$ and $\sigma(t)$ are now coupled to their respective Gaussian fluctuating conjugate fields. The thermal average is indicated by $\langle \dots \rangle$. In theory it is now possible to integrate out the auxiliary fields $\hat{r}(s,t)$ and $\hat{\sigma}(t)$ but this will leave us with non-Gaussian functional integrals which are not mathematically feasible to solve. Thus our aim is now to first linearise the argument of the exponential terms so that after integrating over the auxiliary fields we are left with something quadratic in the exponential. The idea of writing our dynamical quantities in terms of steady state solutions and fluctuation terms will be useful here. We only want to work to lowest order in the fluctuating terms, thus terms containing products of the fluctuation terms of the position of the motor and filament respectively will be ignored. First consider the expression

$$
\gamma_\sigma \frac{\partial \sigma(t)}{\partial t} + k\left(r(\sigma(t),t) - X\right)\frac{\partial r(s,t)}{\partial s}\bigg|_{s=\sigma(t)}
$$

where one can now rewrite the spatial derivative by introducing a Dirac Delta function and a spatial integral as follows,

$$
\gamma_\sigma \frac{\partial \sigma(t)}{\partial t} + k\left(r(\sigma(t),t) - X\right)\int ds\, \frac{\partial r(s,t)}{\partial s}\delta(s - \sigma(t)) .
$$

Suppressing the integral notation for now and substituting in expressions for the

fluctuations of the dynamical quantities (equations 2.7 and 2.8) leads to

$$\gamma_\sigma \frac{\partial \Delta(t)}{\partial t} + k \left[r_\infty(\sigma_\infty + \Delta(t), t) + \rho_\infty(\sigma_\infty + \Delta(t), t) - X) \right] \tag{2.32}$$

$$\times \left(\frac{\partial r_\infty(s)}{\partial s} + \frac{\partial \rho_\infty(s, t)}{\partial s} \right) \delta(s - \sigma_\infty - \Delta(t)) \tag{2.33}$$

where it should be noted that the steady state solution of the position of the molecular motor is time independent and thus the derivative with respect to time is zero. To correctly work up to first order in the fluctuations $\rho(s, t)$ and $\Delta(t)$ the following Taylor series expansions around the steady state solutions to first order have to be made:

$$r_\infty(\sigma_\infty + \Delta(t), t) = r_\infty(\sigma_\infty) + \Delta(t) \frac{\partial r_\infty(s)}{\partial s} \bigg|_{s=\sigma_\infty} + \mathcal{O}\left(\Delta(t)^2 \right) \tag{2.34}$$

$$\rho(\sigma_\infty + \Delta(t), t) = \rho(\sigma_\infty) + \Delta(t) \frac{\partial \rho(s, t)}{\partial s} \bigg|_{s=\sigma_\infty} + \mathcal{O}\left(\Delta(t)^2 \right) \tag{2.35}$$

$$\delta(s - \sigma_\infty - \Delta(t)) = \delta(s - \sigma_\infty) - \Delta(t)\delta'(s - \sigma_\infty) + \mathcal{O}\left(\Delta(t)^2 \right), \tag{2.36}$$

noting from equation 2.35 that the first derivative of the fluctuations of the conformation of the filament around the steady state is multiplied by the fluctuation of the motor term and thus the resulting expression is already second order and must thus be neglected in our calculation. Substituting the above into equation 2.32 results in the following expression:

$$\gamma_\sigma \frac{\partial \Delta(t)}{\partial t} + k \int_s \left(r_\infty(\sigma_\infty) + \Delta(t) \frac{\partial r_\infty(s)}{\partial s} \bigg|_{s=\sigma_\infty} + \rho(\sigma_\infty) - X \right)$$

$$+ k \int_s \left(r_\infty(\sigma_\infty) - X \right) \frac{\partial \rho(s, t)}{\partial t} \delta(s - \sigma_\infty)$$

$$- k \int_s \Delta(t) \left(r_\infty(\sigma_\infty) - X \right) \frac{\partial r_\infty(s)}{\partial s} \delta'(s - \sigma_\infty).$$

One can apply the same technique to the remaining part of the exponential of our generating functional. Doing so results in

$$\gamma_r \frac{\partial r(s, t)}{\partial t} - \frac{3k_B T}{l} \frac{\partial^2 r(s, t)}{\partial s^2} + k \left(r(s, t) - X \right) \delta(s - \sigma(t))$$

$$= \gamma_r \frac{\partial \rho(s, t)}{\partial t}(s, t) - \frac{3k_B T}{l} \frac{\partial^2 r_\infty(s)}{\partial s^2} - \frac{3k_B T}{l} \frac{\partial^2 \rho(s, t)}{\partial s^2} + k \left(r_\infty(s) + \rho(s, t) - X \right) \delta(s - \sigma_\infty)$$

$$- k\Delta(t)((r_\infty(s) - X) \delta'(s - \sigma_\infty) + \mathcal{O}\left(\left(\rho(s, t) \right)^2, \left(\Delta(t) \right)^2 \right),$$

where details of this calculation can be found in Appendix D.1.

Dealing with the spatial and time derivatives in the exponential of the functional integral is tricky and a change of basis can greatly simplify the mathematical complexity of this problem. The first technique we will apply is to expand the filament in its Fourier modes, also referred to as the Rouse modes of the polymer. Noting that we split up the filament in a steady state solution and a fluctuation term, we only need to expand the fluctuation term in its Rouse modes. The general expansion for a polymer of length L in terms of this new basis is given by

$$\rho(s, t) = \sum_{m=0}^{\infty} \left(a_m(t) \sin \frac{\pi m s}{L} + c_m(t) \cos \frac{\pi m s}{L} \right) , \qquad (2.37)$$

where one can now impose the boundary conditions $\rho(0, t) = \rho(L, t) = 0$ and the fact that the for the end points it must hold that the first derivatives of the fluctuations are zero, i.e.

$$\left. \frac{\partial \rho(s, t)}{\partial t} \right|_{s=0} = 0$$
$$\left. \frac{\partial \rho(s, t)}{\partial t} \right|_{s=L} = 0 .$$

Making use of the above and of the fact that the Fourier basis forms a complete orthogonal basis, the correct expansion for the fluctuations of the filament is given by

$$\rho(s, t) = \sum_{m=0}^{\infty} a_m(t) \sin \frac{\pi m s}{L} .$$

We would like to expand the auxiliary field $\hat{r}(s, t)$ in this same basis. Because we are working with an infinite dimensional basis, the following expansion is sufficient,

$$\hat{r}(s, t) = \sum_{m=0}^{\infty} b_m(t) \sin \frac{\pi m s}{L} .$$

The flexible polymer model we are using is based on the continuum limit (see Appendix B for details) of a discrete model of a filament length L with inter monomer distance l. All vibrational modes above $m = L/l$ can thus be neglected, but care should be taken to differentiate between a finite series and truncating an infinite series. It should now be clear that by working in this basis that the dynamical information of the filament and its auxiliary field is encoded in the expansion coefficients $a_m(t)$ and $b_m(t)$. Thus all spatial derivatives only work in on the basis vectors of our expansion and we do not have to integrate over quantities involving

spatial derivatives.

The complexity of time derivatives in our generating functional is easily handled by rather working in frequency space. To do so we introduce the continuous Fourier transform (up to a normalisation constant) for all quantities with a time dependency,

$$\tilde{f}(\omega) = \int_{\mathbb{R}} dt\, f(t) e^{i\omega t}\,.$$

This allows time derivative terms to be rewritten as follows

$$\int_{\mathbb{R}} dt\, \frac{\partial f(\omega)}{\partial t} e^{i\omega t} = i\omega \tilde{f}(t)\,.$$

Note that we assume that f is a square integrable function. See Appendix D.2 for details on how various terms of our generating functional transform under the Fourier transformation. In our new basis there are now no spatial or time derivatives of the dynamical quantities. The resulting generating functional where the thermal averages have been taken is given by

$$\langle \mathcal{Z} \rangle = \int \mathcal{D}\tilde{\Delta}(\omega)\mathcal{D}\hat{\tilde{\sigma}}(\omega) \prod_m \mathcal{D}\tilde{a}_m(\omega) \prod_m \mathcal{D}\tilde{b}_m(\omega)$$

$$\times \exp\Bigg\{ -\frac{\lambda_r}{2} \int_{s,\omega} \sum_{m,m'}^{\infty} \tilde{b}_m(\omega)\tilde{b}_{m'}(-\omega) \sin\frac{\pi m s}{L} \sin\frac{\pi m' s}{L}$$

$$+ i \int_{s,\omega} \sum_m^{\infty} \tilde{b}_m(-\omega)\sin\frac{\pi m s}{L} \left[\begin{array}{l} -i\omega\gamma_r \sum_m^{\infty} \tilde{a}_m(\omega)\sin\frac{\pi m s}{L} \\[2ex] + \dfrac{3k_B T}{l}\dfrac{\pi^2}{L^2}\sum_m^{\infty} m^2 \tilde{a}_m(\omega)\sin\frac{\pi m s}{L} \\[2ex] + k\delta(s-\sigma_\infty)\sum_m^{\infty}\tilde{a}_m(\omega)\sin\frac{\pi m s}{L} \\[2ex] - k\tilde{\Delta}(r_\infty - X)\delta'(s-\sigma_\infty) \end{array} \right]$$

$$- \frac{\lambda_\sigma}{2} \int_\omega \hat{\tilde{\sigma}}(\omega)\hat{\tilde{\sigma}}(-\omega)$$

$$+ i \int_\omega \hat{\tilde{\sigma}}(-\omega) \left[\begin{array}{l} -i\gamma_\sigma\omega\tilde{\Delta}(\omega) + k\int_s \tilde{\Delta}(\omega)\left(\dfrac{\partial r_\infty(s)}{\partial s}\bigg|_{s=\sigma_\infty}\right)^2 \delta(s-\sigma_\infty) \\[2ex] + k\int_s \dfrac{\partial r_\infty(s)}{\partial s}\delta(s-\sigma_\infty)\sum_m^{\infty}\tilde{a}_m(\omega)\sin\frac{\pi m s}{L} \\[2ex] + k\int_s (r_\infty - X)\dfrac{\pi}{L}\delta(s-\sigma_\infty)\sum_m^{\infty} m\cos\frac{\pi m s}{L}\tilde{a}_m(\omega) \\[2ex] - k\int_s \tilde{\Delta}(\omega)(r_\infty - X)\dfrac{\partial r_\infty(s)}{\partial s}\delta'(s-\sigma_\infty) \end{array} \right] \Bigg\}\,.$$

The dynamical quantities are independent of the spatial variable s and thus we can now perform the integrals over s. Note that after applying the Fourier transform from the time to frequency domain that the dependence on the motor force is now only via the steady state solutions $r_\infty(s)$ and σ_∞. Orthogonality relations between the $\sin \frac{\pi m s}{L}$ and $\cos \frac{\pi m s}{L}$ basis vectors can be exploited and integrating over the distributional derivative $\delta'(s - \sigma_\infty)$ shifts the derivative to the function it is composed with. Details of this calculation is given in Appendix D.4 and the result is

$$
\langle \mathcal{Z} \rangle = \int \mathcal{D}\tilde{\Delta}(\omega)\mathcal{D}\hat{\tilde{\sigma}}(\omega) \prod_m \mathcal{D}\tilde{a}_m(\omega) \prod_m \mathcal{D}\tilde{b}_m(\omega)
$$

$$
\times \exp\Bigg\{ -\frac{\lambda_r L}{4} \int_\omega \sum_m^\infty \tilde{b}_m^2(\omega)
$$

$$
+ i \int_\omega \sum_m^\infty \tilde{b}_m(\omega)
\begin{bmatrix}
-i\omega\gamma_r \dfrac{L}{2}\tilde{a}_m(\omega) + \dfrac{3k_B T}{l}\dfrac{\pi^2}{L^2}m^2\tilde{a}_m(\omega)\dfrac{L}{2} \\[2mm]
+ k\sin\dfrac{\pi m \sigma_\infty}{L} \displaystyle\sum_{m'}^\infty \tilde{a}_{m'}(\omega)\sin\dfrac{\pi m' s}{L} \\[2mm]
+ k\tilde{\Delta}(\omega)\Big((r_\infty(\sigma_\infty) - X)\dfrac{\pi}{L}m\cos\dfrac{\pi m \sigma_\infty}{L} \\[2mm]
\qquad + \dfrac{\partial r_\infty(s)}{\partial s}\Big|_{s=\sigma_\infty}\sin\dfrac{\pi m \sigma_\infty}{L}\Big)
\end{bmatrix}
$$

$$
- \frac{\lambda_\sigma}{2}\int_\omega \hat{\tilde{\sigma}}^2(\omega)
$$

$$
+ i \int_\omega \hat{\tilde{\sigma}}(\omega)
\begin{bmatrix}
-i\gamma_\sigma \omega \tilde{\Delta}(\omega) + k\tilde{\Delta}(\omega)\left(\dfrac{\partial r_\infty(s)}{\partial s}\Big|_{s=\sigma_\infty}\right)^2 \\[2mm]
+ k\dfrac{\partial r_\infty(s)}{\partial s}\Big|_{s=\sigma_\infty} \displaystyle\sum_m^\infty \tilde{a}_m(\omega)\sin\dfrac{\pi m \sigma_\infty}{L} \\[2mm]
+ k(r_\infty(\sigma_\infty) - X)\dfrac{\pi}{L}\displaystyle\sum_m^\infty m\cos\dfrac{\pi m \sigma_\infty}{L}\tilde{a}_m(\omega) \\[2mm]
+ k\tilde{\Delta}(\omega)(r_\infty(\sigma_\infty) - X)\dfrac{\partial^2 r_\infty(s)}{\partial s^2}\Big|_{s=\sigma_\infty}
\end{bmatrix}
\Bigg\},
$$

(2.38)

where the shorthand notation $\hat{\tilde{\sigma}}^2(\omega) = \hat{\tilde{\sigma}}(\omega)\hat{\tilde{\sigma}}(-\omega)$ etc. will be used from now on. The integrals dependent on ω run over the entire real line and thus all functions dependent on the frequency are invariant under sign change of ω i.e. $\int_\omega f(\omega) = \int_\omega f(-\omega)$. To simplify the appearance of the equations we introduce the following

shorthand notation

$$\alpha_m = \sin \frac{\pi m \sigma_\infty}{L}$$
$$\beta_m = \cos \frac{\pi m \sigma_\infty}{L}$$

and also

$$\phi_m = (r_\infty(\sigma_\infty) - X)\frac{\pi}{L}m \cos \frac{\pi m \sigma_\infty}{L} + \frac{\partial r_\infty(s)}{\partial s}\bigg|_{s=\sigma_\infty} \sin \frac{\pi m \sigma_\infty}{L}\,.$$

We are now in the position to integrate over the auxiliary fields $\tilde{b}_m(\omega)$ and $\hat{\sigma}(\omega)$. The algebra is straightforward and the expression for the generating functional after the auxiliary fields have been integrated is given by

$$\langle \mathcal{Z} \rangle = \int \prod_m \mathcal{D}\tilde{a}_m(\omega)\mathcal{D}\tilde{\Delta}(\omega)$$

$$\times \exp \Bigg\{ -\frac{1}{\lambda_r L}\int_\omega \sum_m \tilde{a}_m^2 \left[\omega^2 \gamma_r^2 \frac{L^2}{4} + \left(\frac{3k_B T}{l}\right)^2 \frac{\pi^4 m^4}{4L^2} \right]$$

$$-\frac{1}{2}\int_\omega \tilde{\Delta}^2 \left[\begin{array}{l} \dfrac{\omega^2 \gamma_\sigma^2}{\lambda_\sigma} + \dfrac{2k^2}{\lambda_r L}\sum_m \phi_m^2 \\[2ex] + \dfrac{k^2}{\lambda_\sigma}\left(\left(\dfrac{\partial r_\infty(s)}{\partial s}\bigg|_{s=\sigma_\infty}\right)^2 + (r_\infty(\sigma_\infty)-X)\dfrac{\partial^2 r_\infty(s)}{\partial s^2}\bigg|_{s=\sigma_\infty}\right)^2 \end{array} \right]$$

$$-\int_\omega \sum_m \tilde{a}_m \tilde{\Delta} \left[\begin{array}{l} \dfrac{k^2}{\lambda_\sigma}\left(\left(\dfrac{\partial r_\infty(s)}{\partial s}\bigg|_{s=\sigma_\infty}\right)^2 + (r_\infty(\sigma_\infty)-X)\dfrac{\partial^2 r_\infty(s)}{\partial s^2}\bigg|_{s=\sigma_\infty}\right)\phi_m \\[2ex] + k\dfrac{1}{\lambda_r L}\dfrac{3k_B T}{l}\dfrac{\pi^2 m^2}{L}\phi_m + \dfrac{1}{\lambda_r L}k^2\left(\sum_{m'}\alpha_{m'}\phi_{m'}\right) \end{array} \right]$$

$$-\frac{1}{\lambda_r L}\int_\omega \left[k^2\left(\sum_{m'}\alpha_{m'}^2\right)\left(\sum_m \alpha_m \tilde{a}_m\right)^2 + k\frac{3k_B T}{l}\frac{\pi^2}{L}\sum_m m^2 \alpha_m \tilde{a}_m \sum_{m'}\alpha_{m'}\tilde{a}_{m'} \right]$$

$$-\frac{1}{2\lambda_\sigma}\int_\omega k^2\left(\sum_m \tilde{a}_m \phi_m\right)^2 \Bigg\}\,.$$

$$(2.39)$$

The last two terms in the above expression appear to be non-linear in the Rouse modes $\tilde{a}_m$. One may introduce a Hubbard-Stratonovich transformation[3] to lin-

---

[3] Given a field ϕ, one can introduce an additional auxiliary field ψ (up to a normalisation constant) as follows:

$$\int \prod_m \mathcal{D}\phi_m\, e^{-\int (\sum_m \phi_m)^2} = \int \prod_m \mathcal{D}\phi_m \mathcal{D}\psi\, e^{-\frac{1}{2}\int \psi^2 + i\int \psi(\sum_m \phi_m)}\,,$$

earise these terms by introducing additional auxiliary fields. Steps for doing this calculation is outlined in Appendix D.4.

The rest of this calculation will follow a different approach because of the mathematical complexity introduced by these additional fields. Instead we will approximate our system by only considering the lowest vibrational mode $m = 1$. To motivate this argument[7] consider the following expression for the correlation function of the end-to-end vector of a flexible polymer

$$\langle \vec{\mathcal{R}}(t) \cdot \vec{\mathcal{R}}(0) \rangle \sim \sum_{m=1,3,\dots} \frac{1}{m^2} \exp\left(\frac{-tm^2}{\tau_1} \right),$$

where τ_1 is some timescale related to the parameters of the system and the index m refers to the m'th mode of our system, i.e. $\tilde{a}_m$. It is clear from the above expression that for every successive term in the summation dependent on the value of m that the decay rate is much faster than the previous term. Thus while there are higher order effects in our system, we will make the assumption that the first mode contribution will dominate the behaviour of the system. The zeroth mode is also neglected because it is usually related to the center of mass of the system and will not influence the dynamical quantities that we want to examine. By making the first mode contribution approximation $m = 1$ we get the following expression for the generating functional:

$$\langle \mathcal{Z} \rangle = \int \mathcal{D}\tilde{a}(\omega) \mathcal{D}\tilde{\Delta}(\omega)$$

$$\times \exp\left\{ -\int_\omega \tilde{a}^2 \left[\begin{array}{c} \dfrac{L}{4\lambda_r}\omega^2\gamma_r^2 + \dfrac{1}{\lambda_r L}\left(\dfrac{3k_BT}{l}\right)^2 \dfrac{\pi^2}{4L^2} \\[2mm] + \dfrac{1}{\lambda_r L}k^2\alpha_1^4 + \dfrac{k}{\lambda_r L}\dfrac{3k_BT}{l}\dfrac{\pi^2}{L}\alpha_1^2 + \dfrac{1}{2\lambda_\sigma}k^2\phi_1^2 \end{array} \right] \right.$$

$$- \int_\omega \tilde{\Delta}^2 \left[\begin{array}{c} \dfrac{1}{\lambda_\sigma}\omega^2\gamma_\sigma^2 + \dfrac{2}{\lambda_r L}k^2\phi_1^2 \\[2mm] + \dfrac{k^2}{\lambda_\sigma}\left(\left(\dfrac{\partial r_\infty(s)}{\partial s}\Big|_{s=\sigma_\infty}\right)^2 + (r_\infty(\sigma_\infty) - X)\dfrac{\partial^2 r_\infty(s)}{\partial s^2}\Big|_{s=\sigma_\infty} \right)^2 \end{array} \right]$$

$$\left. - \int_w \tilde{\Delta}\tilde{a} \left[\begin{array}{c} \dfrac{1}{\lambda_\sigma}k^2\left(\left(\dfrac{\partial r_\infty(s)}{\partial s}\Big|_{s=\sigma_\infty}\right)^2 + (r_\infty(\sigma_\infty) - X)\dfrac{\partial^2 r_\infty(s)}{\partial s^2}\Big|_{s=\sigma_\infty} \right)\phi_1 \\[2mm] + \dfrac{1}{\lambda_r L}\phi_1\left(k^2\alpha_1^2 + k\dfrac{3k_BT}{l}\dfrac{\pi^2}{L} \right) \end{array} \right] \right\}.$$

This is only a good approximation if we assume that the motor crosslink position is

where one can now do the integral over ϕ in the system and then over the auxiliary field ψ.

around the middle of the filament and not close to the end of the filament. We may view the entire filament as two filaments that are joined together at the crosslink position and thus the total lowest vibrational mode is just the sum of the lowest vibrational modes of each segment respectively. If the crosslink position is near the end of the filament, then the vibrational behaviour of the two filament segments will not be the same, as the vibrational behaviour of the shorter segment will definitely have more higher order vibrational mode contributions.

The convention $\tilde{a} \equiv \tilde{a}_1$ will be used for the rest of the discussion.

2.4.1 Symmetrical approximation

We can simplify our model for the symmetric case where the attachment point of the motor spring is located at the middle i.e. $X = \frac{\Lambda}{2}$ and the steady state position of the motor on the filament is approximately where $\sigma_\infty = \frac{L}{2}$. We will only handle the small force approximation in this case and thus we do not expect the motor to drift far from the steady state solution for the case where the product of the spring constant k and extension $r_\infty(\sigma_\infty) - X$ is relatively large compared to the motor force f_s. We will now calculate a rough approximation of the timescale τ. Remembering that we wrote $\sigma_\infty = \sigma_0 + \sigma_1 f_s$, the correct way to deal with these terms would be to perform a series expansion around $\sigma_\infty = \frac{L}{2}$ for small $\sigma_1 f_s$ and keep terms up to the first order in f_s. Calculating this expansion around $\sigma_0 = \frac{L}{2}$ results in

$$\sin \frac{\pi \sigma_\infty}{L} = 1 - \frac{\pi^2 \sigma_1^2 f_s^2}{2L^2} \tag{2.40}$$

$$\cos \frac{\pi \sigma_\infty}{L} = -\frac{\pi \sigma_1 f_s}{L} + \mathcal{O}\left(\sigma_1^2 f_s^2\right) . \tag{2.41}$$

We can thus set all powers of α_1 equal to unity and powers of β_1 above one can be neglected, i.e. $\beta_1^n \sim 0 \quad \forall n \geq 2$. Consider the expression

$$\phi_1 = (r_\infty(\sigma_\infty) - X)\frac{\pi}{L} \cos \frac{\pi \sigma_\infty}{L} + \frac{\partial r_\infty(s)}{\partial s}\bigg|_{s=\sigma_\infty} \sin \frac{\pi \sigma_\infty}{L} ,$$

where substituting equations 2.40, 2.41, 2.27 and 2.26 results in

$$\phi_1 = -\frac{\pi}{L}\left(\frac{L\left(3k_B T\Lambda^2 + klLX(-2X+\Lambda)\right)}{3kk_B T\Lambda^3}\right)\frac{\pi\sigma_1 f_s}{L} f_s^2 + \frac{\Lambda}{L} - f_s \frac{lL(2X-\Lambda)}{6k_B T\Lambda^2} .$$

Furthermore if we require that the spring anchoring point is at $X = \frac{\Lambda}{2}$, then

$$\phi_1 = \frac{\Lambda}{L} \, .$$
(2.42)

Consider the expression

$$\Gamma \equiv \left(\left. \frac{\partial r_\infty(s)}{\partial s} \right|_{s=\sigma_\infty} \right)^2 + (r_\infty(\sigma_\infty) - X) \left. \frac{\partial^2 r_\infty(s)}{\partial s^2} \right|_{s=\sigma_\infty}$$

and substitute equations 2.27 and 2.28 which leads to

$$\Gamma = \frac{\Lambda^2}{L^2} + \mathcal{O}\left(f_s^2 \right) \, .$$

Using the approximations above, the model is now in a form where we can sensibly analyse the dynamical behaviour of the system for the case where the position of the crosslink is located in the middle of the contour length of the filament. This will be explored in the next chapter.

Chapter 3

Motor on a Flexible Chain — Dynamical Results

3.1   Introduction

In this chapter we would like analyse some of the dynamical behaviour of the model presented in the previous chapter. We will analyse the stability of the steady state solutions, the autocorrelation of the fluctuations of the position of the crosslink and the fluctuations of the force that tethers the crosslink position $\sigma(t)$ to the anchoring point X, i.e. $k\left(r(\sigma(t), t) - X\right)$. The latter quantity is not directly related to the elastic response of the filament, but may have the same scaling behaviour in terms of the motor force f_s. We will also briefly discuss how the results may change when modifying the model to include a curvature dependence.

3.2   Stability of the Steady State

In this section we would like to explore the stability of our system around its equilibrium solutions or steady state solutions. We can represent our generating functional at this point without the small motor force approximation as

$$\langle \mathcal{Z} \rangle = \int \mathcal{D}\vec{x}\,\exp\left(-\vec{x}^T \mathbb{A}\vec{x}\right),$$

where $\vec{x} = \begin{pmatrix} \tilde{a}(\omega) \\ \tilde{\Delta}(\omega) \end{pmatrix}$ and the matrix $\mathbb{A}$ has the form

$$\mathbb{A} = \begin{pmatrix} A & \frac{1}{2}C \\ \frac{1}{2}C & B \end{pmatrix} \tag{3.1}$$

with

$$
\begin{aligned}
A(\omega) &= \frac{L}{4\lambda_r}\omega^2\gamma_r^2 + \frac{1}{\lambda_r L}\left(\frac{3k_B T}{l}\right)^2 \frac{\pi^2}{4L^2} \\
&\quad + \frac{1}{\lambda_r L}k^2\alpha_1^4 + \frac{k}{\lambda_r L}\frac{3k_B T}{l}\frac{\pi^2}{L}\alpha_1^2 + \frac{1}{2\lambda_\sigma}k^2\phi_1^2 \\
B(\omega) &= \frac{1}{\lambda_\sigma}\omega^2\gamma_\sigma^2 + \frac{2}{\lambda_r L}k^2\phi_1^2 \\
&\quad + \frac{k^2}{\lambda_\sigma}\left(\left(\frac{\partial r_\infty(s)}{\partial s}\bigg|_{s=\sigma_\infty}\right)^2 + (r_\infty(\sigma_\infty) - X)\frac{\partial^2 r_\infty(s)}{\partial s^2}\bigg|_{s=\sigma_\infty}\right)^2
\end{aligned}
$$

and

$$
\begin{aligned}
C &= \frac{1}{\lambda_\sigma}k^2\left(\left(\frac{\partial r_\infty(s)}{\partial s}\bigg|_{s=\sigma_\infty}\right)^2 + (r_\infty(\sigma_\infty) - X)\frac{\partial^2 r_\infty(s)}{\partial s^2}\bigg|_{s=\sigma_\infty}\right)\phi_1 \\
&\quad + \frac{1}{\lambda_r L}\phi_1\left(k^2\alpha_1^2 + k\frac{3k_B T}{l}\frac{\pi^2}{L}\right) .
\end{aligned}
$$

We require the eigenvalues to be real numbers, because the matrix $\mathbb{A}$ is symmetric and must thus always have real eigenvalues. Furthermore $\mathbb{A}$ has to be positive definite for the functional integral to converge. It should be noted that we require that the real part of the eigenvalues to be strictly greater than zero i.e. $\lambda_i > 0$ so that an inverse for $\mathbb{A}$ exists. This places a restriction of the parameters of our system. The eigenvalues for $\mathbb{A}$ are given by

$$\lambda_1 = \frac{1}{2}\left(A + B - \sqrt{(A - B)^2 + C^2}\right)$$

and

$$\lambda_2 = \frac{1}{2}\left(A + B + \sqrt{(A - B)^2 + C^2}\right) .$$

The discriminant $(A - B)^2 + C^2$ is the sum of squares and is thus always positive because there are no complex or pure imaginary quantities in the matrix $\mathbb{A}$ and we

require eigenvalues to be real numbers. Also if we consider the expression for A and B then we see that they both only contain squares of real numbers and thus A and B must be positive and real. From this we can already conclude that the one eigenvalue has to be strictly positive i.e. $\lambda_2 > 0 \quad \forall A, B, C \neq 0$. Consider the determinant of the matrix $\mathbb{A}$

$$\det(\mathbb{A}) = AB - \frac{C^2}{4}$$

and recall that this has to be equal to the product of the eigenvalues of $\mathbb{A}$ i.e. $\det(\mathbb{A}) = \lambda_1 \lambda_2$. The determinant of a positive definite matrix has to be positive and because we know that the one eigenvalue $\lambda_2 > 0$, finding restrictions on the parameters of the system to satisfy $\lambda_1 > 0$ is equivalent to looking at the case where $\det(\mathbb{A}) > 0$. So we now have to examine the inequality

$$AB - \frac{C^2}{4} > 0 \,.$$

Our system contains numerous free parameters where we have to fix some of the parameters to perform numerical analysis.
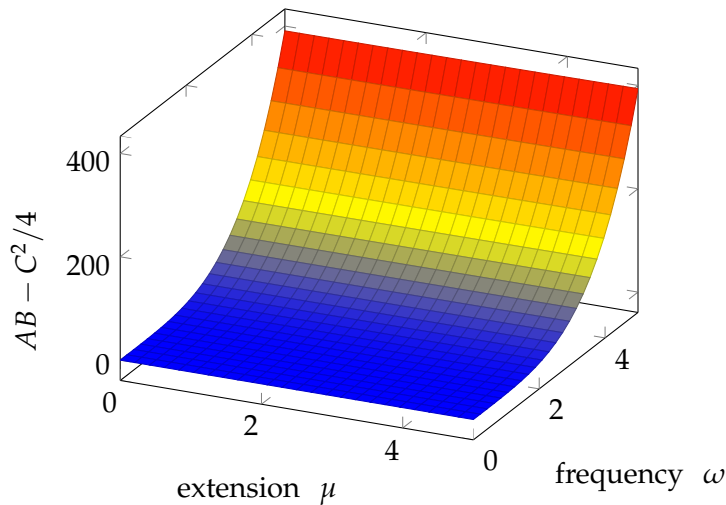
Figure 3.1: Surface plot of the stability function of the system where all the parameters are fixed, except for the frequency ω and the extension $\mu \equiv \frac{l}{\Lambda}$ of the polymer. The chosen parameters are $k_B T = 1$, $l = 1$, $\Lambda = 10$, $\gamma_r = 1$ and $\gamma_\sigma = 1$. The units are arbitrary. The surface is smooth and for the chosen parameters we find that $AB - C^2/4 \geq 0$ and thus do not expect any strange behaviour except maybe where $\omega \to 0$.

If we consider the symmetrical case with a small motor force approximation as explained in section 2.4.1 and fix all the parameters of the system, except for the frequency ω and the extension $\mu \equiv \frac{L}{\Lambda}$ of the polymer, then the system is well behaved as seen in figure 3.1. For the parameters that were selected, $AB - C^2/4 \geq 0$ and we do not expect strange behaviour except maybe for the case where $\omega \to 0$.

3.3 Motor Fluctuation Timescale

We are interested in determining the autocorrelation function of the fluctuations of the position of the active crosslinker i.e. $\langle \tilde{\Delta}^2(\omega) \rangle$. To do so we have to integrate over the remaining vibrational mode $\tilde{a}_1(\omega)$ and then take a functional derivative with respect to the source term (suppressed in our calculation) that couples to $\tilde{\Delta}(\omega)$. This result, up to a normalisation constant, reduces to taking the inverse of the matrix $\mathbb{A}$ associated with the quadratic term, i.e. $\int_\omega \tilde{\Delta}(\omega)\mathbb{A}(\omega)\tilde{\Delta}(-\omega)$ where in our case the matrix will be diagonal and there are no complicated problems associated with finding an inverse and determinant seeing as they are both trivial. First let us integrate over $\tilde{a}_m(\omega)$. Doing so results in

$$\langle \mathcal{Z} \rangle = \int \mathcal{D}\tilde{\Delta}(\omega)$$

$$\times \exp \int_\omega \tilde{\Delta}^2 \left\{ \left[\frac{1}{\lambda_r L}\left(\omega^2\gamma_r^2\frac{L^2}{4} + \left(\frac{3k_BT}{l}\right)^2\frac{\pi^4}{4L^2} + k^2\alpha_1^4 + k\frac{3k_BT}{l}\frac{\pi^2}{L}\alpha_1^2 \right) \right. \right.$$

$$\left. + \frac{1}{2\lambda_\sigma}k^2\phi_1^2 \right]^{-1} \times \left[\frac{1}{\lambda_r L}\phi_1\left(k\frac{3k_BT}{l}\frac{\pi^2}{L} + k^2\alpha_1^2 \right) \right.$$

$$\left. + \frac{1}{\lambda_\sigma}k^2\phi_1\left(\left(\frac{\partial r_\infty(\sigma_\infty)}{\partial s}\right)^2 + (r_\infty(\sigma_\infty) - X)\frac{\partial^2 r_\infty(\sigma_\infty)}{\partial s^2} \right) \right]^2$$

$$\left. - \frac{1}{2\lambda_\sigma}\left(\omega^2\gamma_\sigma^2 + k^2\left(\left(\frac{\partial r_\infty(\sigma_\infty)}{\partial s}\right)^2 + (r_\infty(\sigma_\infty) - X)\frac{\partial^2 r_\infty(\sigma_\infty)}{\partial s^2} \right)^2 \right) + \frac{1}{\lambda_r L}k^2\phi_1^2 \right\}.$$

From the above equation one can derive the expression for the inverse of the motor position fluctuation autocorrelation function $\left[\langle \tilde{\Delta}(\omega)\tilde{\Delta}(-\omega)\rangle\right]^{-1}$ by just reading off the coefficient of $\tilde{\Delta}^2$, i.e. what stands between $\{\dots\}$. To make sense of this quantity, let us consider

$$\left[\langle \tilde{\Delta}(\omega)\tilde{\Delta}(-\omega)\rangle\right]^{-1} = A\omega^2 + B + \frac{C}{D\omega^2 + E} \tag{3.2}$$

where

$$A = \frac{\gamma_\sigma^2}{2\lambda_\sigma}$$

$$B = \frac{k^2}{2\lambda_\sigma} \left(\left(\frac{\partial r_\infty(\sigma_\infty)}{\partial s} \right)^2 + (r_\infty(\sigma_\infty) - X)\frac{\partial^2 r_\infty(\sigma_\infty)}{\partial s^2} \right)^2 + \frac{k^2}{\lambda_r L}\phi_1^2$$

$$C = \left[\frac{1}{\lambda_r L}\phi_1 \left(k\frac{3k_B T}{l}\frac{\pi^2}{L} + k^2\alpha_1^2 \right) + \right.$$

$$\left. \frac{1}{\lambda_\sigma}k^2\phi_1 \left(\left(\frac{\partial r_\infty(\sigma_\infty)}{\partial s} \right)^2 + (r_\infty(\sigma_\infty) - X)\frac{\partial^2 r_\infty(\sigma_\infty)}{\partial s^2} \right) \right]^2$$

$$D = \frac{L\gamma_r^2}{4\lambda_r}$$

and

$$E = \frac{1}{\lambda_r L} \left(\left(\frac{3k_B T}{l} \right)^2 \frac{\pi^4}{4L^2} + k^2\alpha_1^4 + k\frac{3k_B T}{l}\frac{\pi^2}{L}\alpha_1^2 \right) + \frac{1}{2\lambda_\sigma}k^2\phi_1^2 \,.$$

After some algebraic manipulation of equation 3.2 we end up with

$$\left[\langle \tilde{\Delta}(\omega)\tilde{\Delta}(-\omega) \rangle \right]^{-1} = \frac{\cancel{AD\omega^4} + \omega^2(AE + BD) + BE + C}{D\omega^2 + E}$$

where the higher order term ω^4 is neglected because the long time limit that we are considering throughout this problem corresponds to the case where $\omega \to 0$. Taking the inverse leads to

$$\langle \tilde{\Delta}(\omega)\tilde{\Delta}(-\omega) \rangle = \frac{D\omega^2 + E}{\omega^2(AE + BD) + BE + C} \tag{3.3}$$

where the Fourier transformation $\mathcal{F}$ of the above equation from the frequency to time domain will have the form of an exponential decay process at some timescale τ we have to determine i.e.

$$\mathcal{F}\left\{ \frac{\omega^2}{\frac{1}{\tau^2} + \omega^2} \right\} \sim e^{-t/\tau} \,.$$

This makes sense because we do not expect the fluctuations of the position of the motor to be correlated over a long time. Extracting leading order behaviour of equation 3.3 and doing some algebraic manipulation we find that

$$\langle \tilde{\Delta}(\omega)\tilde{\Delta}(-\omega) \rangle \sim \frac{\omega^2}{\omega^2 + \frac{BE+C}{AE+BD}} \tag{3.4}$$

where the timescale is given by $\tau^2 = \frac{AE+BD}{BE+C}$. This results in a complicated analytical expression where making use of the approximations outlined in section 2.4.1 we

find that

$$\tau \sim \text{const.} + \mathcal{O}\left(f_s^2\right)$$

and thus the timescale does not depend linearly on the motor force. This result is sensible because in the symmetric case we do not expect the direction of the motor force, which can be positive or negative, to have an effect on the timescale. The factor const. is a complicated function of the parameters of the system.

3.3.1   Numerical Results

We shall now present a brief numerical analysis of the timescale τ as calculated. Arbitrary units will be used throughout this discussion. Let us consider the ratio
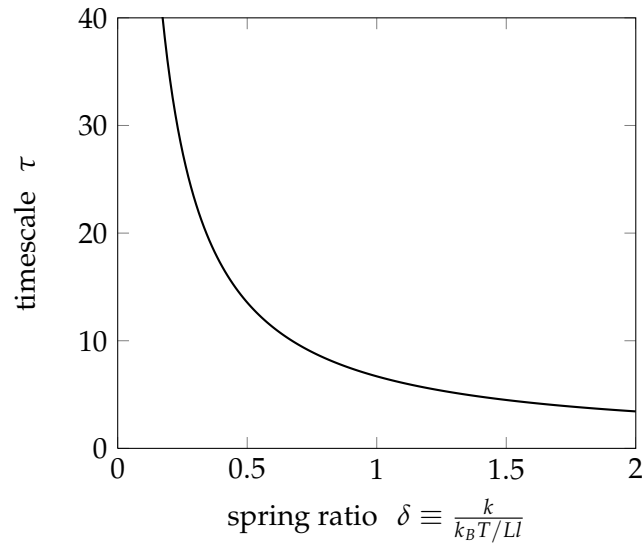

Figure 3.2: Dependence of the motor position fluctuation timescale t on the ratio of the spring constants $\delta \equiv \frac{k}{k_B T/Ll}$. The units are arbitrary. The parameters $k_B T = 1$, $\gamma_r = 1$, $\gamma_\sigma = 1$, $l = 1$, $L = 10$ and $\Lambda = 10$ were used. When the spring constant that anchors the motor becomes large relative to the entropic spring behaviour of the polymer, the timescale t decreases. This is a sensible result, because the larger spring constant enforces a stronger localisation of the position of the motor. For small values of δ the localisation of the position of the motor becomes negligible and τ diverges. This is in the regime where our model approximations do not hold anymore, as the position of the motor is free to be anywhere on the filament.

$\delta = \frac{k}{k_B T/Ll}$ of the spring constant k and the entropic spring constant from the polymer $\frac{k_B T}{lL}$ and fix the parameters $k_B T = 1$, $\gamma_r = 1$, $\gamma_\sigma = 1$, $l = 1$, $L = 10$ and $\Lambda = 10$. When δ becomes large, then we find that the timescale τ decreases as seen in figure 3.2. This

is equivalent to stating that the spring constant that is responsible for anchoring the position of the motor becomes large in comparison to the entropic spring behaviour of the polymer. This is a sensible result because the localisation of the position of the motor will increase as δ grows and thus correlation times decrease. We are able to explicitly calculate the limit $\delta \to \infty$ and we find that $\tau(\delta) \to 0$.

For the case where where δ becomes small, the spring constant k becomes negligible in comparison to $\frac{k_B T}{Ll}$ and thus the motor is effectively decoupled from the anchoring point $X = \frac{\Lambda}{2}$ and τ diverges. We should mention that our approximations up to now relied on the fact that the position of the motor is located somewhere near the middle of the contour length of the polymer, i.e $\sigma \approx \frac{L}{2}$. Thus if we remove the anchoring of the position of the motor then the position is free to take on all values on the contour $[0, L]$. This is thus an unreliable result in the scope of our approximations.
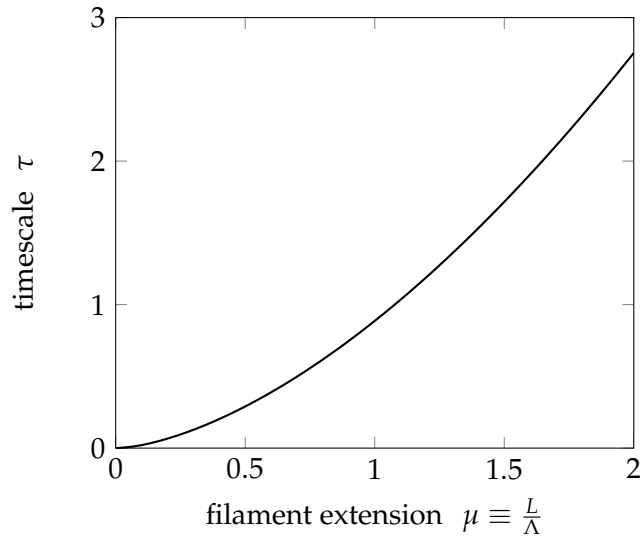
Figure 3.3: Dependence of the motor position fluctuation timescale on the filament extension $\mu \equiv \frac{L}{\Lambda}$. The units are arbitrary. The parameters $k_B T = 1$, $\gamma_r = 1$, $\gamma_\sigma = 1$, $l = 1$, $k = 1$ and $\Lambda = 10$ were used. We notice that the timescale τ increases as the contour length of the polymer increases. Extending the polymer increases the walk length and thus the increase in the timescale is sensible.

Now also considering the extension of the polymer i.e. the ratio of the contour length of the polymer and the displacement between the endpoints of the polymer, has on the timescale τ. The parameters of the system are fixed to $k_B T = 1$, $\gamma_r = 1$,

$\gamma_\sigma = 1$, $l = 1$, $k = 1$ and $\Lambda = 10$ and the units are taken as arbitrary. We find that the timescale τ increases as the polymer extension μ grows. Increasing the polymer extension increases the walk length and thus an increase in the time taken for the motor position autocorrelation to decay is expected.

3.4   Spring force fluctuation

We would like to briefly explore the elastic properties of our model. Calculating the tension in the filament at the endpoints of the filament is difficult with our current model and we will rather explore the fluctuations of the spring force that anchors the motor around the steady state solution, i.e.

$$\mathfrak{F}(t) \equiv k^2 \left\langle \left[(r(\sigma(t), t) - X) - (r_\infty(\sigma_\infty) - X) \right]^2 \right\rangle . \tag{3.5}$$

Making use of equations 2.7 and 2.8, we can perform a series expansion to first order in the small quantities $\Delta(t)$ and $\rho(s, t)$ to find that

$$r(\sigma(t), t) = r_\infty(\sigma_\infty) + \rho(\sigma_\infty, t) + \Delta(t) \left. \frac{\partial r_\infty(s)}{\partial s} \right|_{s=\sigma_\infty} . \tag{3.6}$$

Furthermore using the lowest vibrational mode approximation and equation 2.40, we may write that

$$\rho(\sigma_\infty, t) = a_1(t) . \tag{3.7}$$

Substituting the above into equation 3.5 results in

$$\mathfrak{F}(t) = k^2 \left\langle \left[a_1(t) + \Delta(t) \left. \frac{\partial r_\infty(s)}{\partial s} \right|_{s=\sigma_\infty} \right]^2 \right\rangle , \tag{3.8}$$

where it is sufficient to study the Fourier transformation of $\mathfrak{F}(t)$ given by

$$\tilde{\mathfrak{F}}(\omega) = k^2 \left\langle \left[\tilde{a}(\omega) + \tilde{\Delta}(\omega) \left. \frac{\partial r_\infty(s)}{\partial s} \right|_{s=\sigma_\infty} \right]^2 \right\rangle \tag{3.9}$$

$$= k^2 \left\langle \tilde{a}^2(\omega) \right\rangle + k^2 \left(\left. \frac{\partial r_\infty(s)}{\partial s} \right|_{s=\sigma_\infty} \right)^2 \left\langle \tilde{\Delta}^2(\omega) \right\rangle + k^2 \left. \frac{\partial r_\infty(s)}{\partial s} \right|_{s=\sigma_\infty} \left\langle \tilde{\Delta}(\omega)\tilde{a}(\omega) \right\rangle . \tag{3.10}$$

The expression for $\left\langle \tilde{\Delta}^2(\omega) \right\rangle$ is given by equation 3.4. The other two correlation functions on the right hand side of the above equation may be found by considering

the inverse of matrix 3.1 given by

$$\mathbb{A}^{-1} = \begin{pmatrix} \frac{4B}{4AB-C^2} & \frac{2C}{-4AB+C^2} \\ \frac{2C}{-4AB+C^2} & \frac{4A}{4AB-C^2} \end{pmatrix} . \tag{3.11}$$

The respective correlation functions may now we found by reading off the elements that connect the required quantities. Thus the autocorrelation function for the lowest vibrational mode is given by

$$\left\langle \tilde{a}_1^2(\omega) \right\rangle = \mathbb{A}_{0,0}^{-1} \tag{3.12}$$

$$= \frac{4B}{4AB - C^2} \tag{3.13}$$

and the correlation between the lowest vibrational mode and the fluctuation of the motor is given by

$$\left\langle \tilde{\Delta}(\omega)\tilde{a}_1(\omega) \right\rangle = 2\mathbb{A}_{0,1}^{-1} = 2\mathbb{A}_{1,0}^{-1} \tag{3.14}$$

$$= \frac{2C}{-4AB + C^2} . \tag{3.15}$$

Using the above and equation 2.27 we can now express the fluctuation of the spring force by

$$\tilde{\tilde{\mathfrak{F}}}(\omega) = \mathfrak{C} + k^2 \frac{\Lambda}{L} \left\langle \tilde{\Delta}^2(\omega) \right\rangle , \tag{3.16}$$

where $\mathfrak{C}$ is some complicated function of the parameters of the system. The fluctuations of the spring force are thus proportional to the square of the motor force i.e. f_s^2 because $\tilde{\Delta}^2(\omega) \sim f_s^2$.

3.5   Directed Filament

In this section we would like to propose and discuss a modified version of our system where we add a curvature dependent term to the Hamiltonian given by equation 2.1. We will also only consider the case where the polymer is stretched enough so that the conformation of the polymer can be described by a single valued function at all times, i.e. there are no overhangs. This is known as a directed polymer. The resulting Hamiltonian is given by

$$\mathcal{H} = \frac{\theta}{2} \int_0^L ds \left(\frac{\partial^2 r(s,t)}{\partial s^2} \right)^2 + \frac{3k_B T}{2l} \int_0^L ds \left(\frac{\partial r(s,t)}{\partial s} \right)^2 + \frac{k}{2} \left(r(\sigma,t) - X \right)^2 , \tag{3.17}$$

where the parameter θ indicates the bending rigidity, i.e. the energy penalty required to bend the filament.

Similar Hamiltonians were found in the literature to model the transversal component of semiflexible filaments in the weakly bending limit[21; 22], but we will refrain from labeling our model as one that describes a semiflexible polymer due to problems that arise with introduction of a local inflexibility constraint. To briefly explain our concern, consider the local inflexibility constraint for a semiflexible polymer:

$$\left(\frac{\partial r(s,t)}{\partial s}\right)^2 = 1 \quad \forall s, t \,. \tag{3.18}$$

One of the standard ways to describe a semiflexible polymer is by the Kratky-Porod[8] Hamiltonian which is given by

$$\mathcal{H} = \frac{\theta}{2} \int_0^L ds \, \left(\frac{\partial^2 r(s,t)}{\partial s^2}\right)^2 + \int_0^L \Xi(s,t) \left(\left(\frac{\partial r(s,t)}{\partial s}\right)^2 - 1\right) \,, \tag{3.19}$$

where $\Xi(s,t)$ is a functional Lagrange multiplier that enforces the inflexibility constraint for every segment at all times. Dealing with the Lagrange multiplier $\Xi(s,t)$ is difficult because it forces us to introduce another dynamical equation to describe the behaviour of the multiplier. The route that Benetatos and Terentjev[21] takes is to separate the transversal and longitudinal behaviour of the filament, i.e

$$\vec{r}(s,t) = \vec{r}_\perp(s,t) + \left(s - r_\parallel(s,t)\right) \hat{e}_\parallel \,,$$

with $\hat{e}_\parallel$ the unit vector parallel to the contour of the filament. We may now rewrite the inflexibility constraint 3.18 as

$$\left(\frac{\partial r_\perp(s,t)}{\partial s}\right)^2 + \left(1 - \frac{\partial r_\parallel(s,t)}{\partial s}\right)^2 = 1$$

and in the weakly bending limit where $|\partial_s r_\perp(s,t)| \ll 1$ reduces to

$$\frac{\partial r_\parallel(s,t)}{\partial s} \approx \frac{1}{2} \left(\frac{\partial r_\perp(s,t)}{\partial s}\right)^2 \,. \tag{3.20}$$

They now make the assumption that because the parallel component is already

second order in the transversal component, which is very small, that we may write

$$\frac{\partial r_\parallel(s,t)}{\partial s} \approx 0 \,.$$

The leads them to write down a Hamiltonian of the same functional form as the first two terms in our proposed Hamiltonian given by equation 3.17. We have not found a formal method to derive their model based on the given assumption.

Returning to our model, we would like to make a few predictions on the behaviour of the system when introducing the curvature dependence. If we assume the same steady state plus fluctuating behaviour (ansatz 2.7 and 2.8) as for the normal flexible polymer and expand the fluctuation $\rho(s,t)$ into Rouse modes, then we will find that

$$\frac{\partial^4 \rho(s,t)}{\partial s^4} = \sum_m a_m(t) \frac{\pi^4 m^4}{L^4} \sin\frac{\pi m s}{L} \,. \tag{3.21}$$

This will lead to the transformation

$$\frac{3k_B T}{l} \frac{\pi^2}{L^2} m^2 \tilde{a}_m(\omega) \frac{L}{2} \rightarrow \frac{3k_B T}{l} \frac{\pi^2}{L^2} m^2 \tilde{a}_m(\omega) \frac{L}{2} - \theta \frac{\pi^4}{L^4} m^4 \tilde{a}_m(\omega) \frac{L}{2} \tag{3.22}$$

in equation 2.38, which effectively creates a new effective spring constant for the polymer, where one should notice the sign difference between the two terms and might indicates some competition that drastically changes the behaviour of the system at the point where the sum of these quantities changes over from positive to negative. We are only considering the stretched case where the directed property of the polymer holds at all times and thus do not expect strange behaviour where the effective spring constant may become negative.

If we consider equation 2.39 then we will have an additional term proportional to m^8 coupled to $\tilde{a}_m^2$. Integration over $\tilde{a}_m$, assuming we can deal with the apparent non-linearities using a Hubbard-Stratonovich transformation, will produce additional terms proportional to $\frac{1}{m^8}$. These terms will thus decay very rapidly for higher vibrational modes and our approximation of $m = 1$ for the original flexible model should hold as well.

We do not expect any drastic change to the functional form of the motor position fluctuation autocorrelation function given by equation 3.4 due to the addition of the curvature dependence term. The frequency dependence will be the same and we would expect the same type of exponential decay with a modified timescale dependence. The dependence on the motor force should still be proportional to f_s^2

with no linear dependence on the motor force.

Further study is required to see how a real semiflexible model would alter the dynamics presented for the flexible case.

3.6   Remarks and Outlook

In this chapter we saw that it is possible to construct a simple model for a flexible filament with an active crosslinker attached to it. We were also able to extract some properties from this system, even though the analytical feasibility of determining some properties leaves something to be desired. Further study is required to see if one can maybe rewrite this system in such way so that we do not end up with so many free parameters to deal with. On the other hand, the expressions in terms of the fundamental parameters of the system can be determined analytically and thus we have achieved what we set out to do.

Something one might want to study is the two filament version of our model. In our model the anchoring point X is a free parameter, but in the two strand model the coordinate X will also be a dynamical quantity i.e. X will be the crosslink position on the other filament.

An important aspect that should be explored is to see if one could map this onto other models in the literature such as those based on a hydrodynamics formalism. One would most likely have move over to collective variables[23] to achieve this. If one were able to create a type of mapping then the unknown parameters in the hydrodynamic models can be given a microscopic interpretation. Unfortunately this is not a trivial task, because as later discussed in chapter 4, the introduction of constraints to form a fixed network introduces its own set of mathematical complexity and problems.

It would be of great advantage if a controlled experiment could measure the time scale dependence on the motor force f_s so that we may see if our result is realistic. While it makes sense that $\tau \sim f_s^2$, it would be good to get a confirmation. In the work by Liverpool et al. [14] for the static response it was found that the ground state deformation of the active gel scales with f_s^2. For the dynamic response of their model, they found that that the stiffening of the active gel is also proportional to f_s^2. While not the same quantity, we were able to show in the dynamic case that the spring force that anchors the motor also scales with f_s^2. The active crosslinker is in turn pulling on the filament and thus it might not be so far fetched to believe that

the elastic properties of the filament will also have the same scaling behaviour.

Our approximations are only applicable to the domain where the active crosslinker is located near the middle of the contour length of the filament. A different set of approximations is required to study the extreme case where the active crosslinker is located near the end points of the filament, as different physics will arise in these cases.

Chapter 4

Network Models

4.1 Motivation

In the preceding chapters we looked at single strand models which are the most simplified elements of active networks. While these models give insight into understanding active materials, they still cannot describe complex behaviour that arises from the collective dynamics of many strands with molecular motors all interacting with each other and the crosslinking constraints. We must first try and understand the dynamical behaviour of a normal polymer network before we can even begin to consider the dynamics of a polymer network with active cross linkers. The equilibrium aspects of polymer networks have been thoroughly examined using the powerful functional integral approach of Edwards[24; 25]. Unfortunately this technique does not easily translate to the non-equilibrium case for a network with fixed cross linkers. This chapter will briefly touch upon some ideas found in the literature that have been considered about the dynamics of polymer networks. First will also then present a very simple toy model for a network that follows a different analytical approach than what we have mostly found in the literature. Keeping to the theme of the work in this thesis, we will try to formulate it from a mesoscopic framework. While our model also has its own set of problems, it might lead to being able to form an effective theory using similar arguments. Alternatively we will also introduce an Edwards type theory for the dynamics of a polymer network where we generalise to time and velocity dependent fields. We will also introduce the concept of a generalised density function in the framework of this theory.

4.2   Graph-Theoretical Models

In this section we would like to briefly cover the graph-theoretical models that have been found in the literature. The lineage of this work traces back to Forsman[26] who first presented this idea for a linear chain and then subsequently expanded upon by Pearson, Raju[27], Eichinger[28], Guenza and Mormino[29] for more complicated geometries. Similar ideas were used by Solf and Vilgis[30] to construct a network theory with hard constraints. Describing the network in a graph-theoretical sense allows one to unify chain dynamics and statistics i.e. the representation of the graph, such as a matrix, can be used to derive statistical quantities such as the mean square radius of gyration[1] and also dynamical quantities such as the relaxation modes of the polymer.

We will follow the same line of discussion as Nitta[31] when sketching the idea of this theory, who gives a lucid description of the theory for tree-like networks, but the ideas generalise to any arbitrary network. Let us first establish some terminology. In a network consisting of polymers, we would have the potentials that keep the monomers of individual polymers connected and then there are different potentials or hard constraints that fix some points on the polymers to points on other polymers. It is these latter constraints that create the network topology. For the purpose of this section we will only consider monomers that are connected to a fixed number of other monomers via a harmonic potential. Thus we are not really looking at a polymer network, but rather a branched polymer. In the language of graph theory we would call the monomers vertices and the lines that show the relationship between the vertices we call edges. Edges for our purpose will be undirected, seeing as there is a symmetric interaction between monomers. There are various matrix representations for the relationship between the vertices and edges. We will use what is called the Kirchoff matrix which is defined as follows

$$
\mathbb{M}_{ij} = \begin{cases} \phi & \text{if } i = j \\ -1 & \text{if there is an edge from vertex } i \text{ to vertex } j \\ 0 & \text{otherwise} \, , \end{cases}
$$

where ϕ is the functionality of the network, i.e. the number of edges that are con-

---

[1]The mean square radius of gyration is a measure of the size of the polymer and is defined by $R_g \equiv \frac{1}{N^2} \sum_{n,m=1}^{N} \overline{(R_n - R_m)^2}$ with R_i being the position of the i'th monomer and $\overline{\dots}$ indicates an ensemble average.

nected to every vertex. Vertices that are directly connected by edges are known as adjacent vertices. It would be more general to consider that every vertex can have its own functionality, but we will restrict ourselves to a network where the functionality is uniform. We also assume that there are no loops in the network. Of course the properties of a graph should not depend on on a labeling scheme and thus the determinant of the Kirchoff matrix is invariant under change of representation. The following properties[32] hold for the matrix $\mathbb{M}$ with eigenvalues λ_i:

- $\mathbb{M}$ is always positive semidefinite and thus $\lambda_0 = 0$ and $\lambda_i \geq 0 \, \forall i = 1, \ldots, n-1$.

- The multiplicity of λ_0 indicates the number of connected components in the graph, i.e. subnetworks that are not linked. We assume the network has no loops and thus it is not possible for there to be any disconnected subnetworks. The multiplicity will thus always be equal to unity.

- $\mathbb{M}$ has no inverse due to $\lambda_0 = 0$.

The matrix $\mathbb{M}$ is also a matrix representation of the discrete negative Laplacian operator which may be viewed as a discrete approximation of the usual continuous Laplacian operator. We will now briefly discuss how one may represent the basic Rouse model as explained in Appendix B using this language. For a polymer of N monomers we know that

$$\gamma \frac{\partial R_n(t)}{\partial t} = \frac{3k_B T}{l^2} \left(R_{n+1}(t) - 2R_n(t) + R_{n-1}(t) \right) + f_n(t)$$

holds for all $n = 2, \ldots, N-1$. This can be rewritten as the following matrix equation:

$$\partial t \vec{R}(t) = \frac{3k_B T}{l^2} \mathbb{M}_R \vec{R} + \vec{f}(t)$$

where

$$\vec{R}(t) = \begin{pmatrix} R_2(t) \\ R_3(t) \\ \vdots \\ R_{N-1}(t) \end{pmatrix}, \quad \vec{f}(t) = \begin{pmatrix} f_2(t) \\ f_3(t) \\ \vdots \\ f_{N-1}(t) \end{pmatrix}$$

and the Kirchoff matrix $\mathbb{M}_R$ is given by

$$\mathbb{M}_R = \begin{pmatrix} 2 & -1 & 0 & \cdots & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \cdots & -1 & 2 \end{pmatrix} .$$

The matrix $\mathbb{M}_R$ is not invertible and thus we cannot find exact solutions to $\vec{R}(t)$. We can diagonalise the system by expanding it into Rouse modes and then as mentioned in Doi and Edwards[7], the relaxation timescales for the normal coordinates. Clearly this is the same as diagonalising $\mathbb{M}_R$ and it can be shown that the eigenvalues λ_i for $i > 0$ are related to the timescales presented by Doi and Edwards as follows:

$$\tau_i = \frac{\gamma l^2}{6 k_B T} \frac{1}{\lambda_i} .$$

The lowest eigenvalue $\lambda_0 = 0$ is related to the translation of the centre of mass of the polymer[33] and does not influence its conformational dynamics. One can of course find the spectrum of any Kirchoff matrix for arbitrary network topologies. Determining how the spectrum relates to the relaxation modes of the network is very specific to the topology of the model and not easily generalised[31]. Another problem is that this does not really allow us to extract more information about a specific network.

There is no clear way of how one can introduce activity in terms of motors in this theoretical framework and then see how the effect of activity changes the relaxation spectrum of the network or even how one calculates quantities such as the shear modulus of the network. An additional problem with the formalism is that there are no real polymer degrees of freedom between the cross linked areas, i.e. in a real polymer network there are the degrees of freedom associated with the individual polymers and then the degrees of freedom associated with the crosslinking points where the polymers are connected to each other. In this graph-theoretical formalism the degrees of freedom of the polymers are reduced to that of a springs.

Solf and Vilgis[30; 34] presented a model where the polymer behaviour and

cross linking are separated. Briefly, what they do is propose a Hamiltonian

$$\mathcal{H} = \frac{3k_B T}{l^2} \sum_n^N \left(R_{n+1}(t) - 2R_n(t) + R_{n-1}(t) \right) + \frac{3}{2\varepsilon^2} \sum_e^M \left(R_{n_e}(t) - R_{n'_e}(t) \right)^2$$

for a polymer with N segments and M cross links. We can recover the Edwards[35] type hard constraints of the form $\prod_\varepsilon \left(R_{n_e}(t) - R_{n'_e}(t) \right)$ if we take the limit $\varepsilon \to 0$. The case where $\varepsilon \to \infty$ reduces $\mathcal{H}$ to that of a free flexible chain. One can write down a Langevin equation following the usual approach of taking a derivative of the Hamiltonian with respect to the dynamical quantity. They are then able to describe the diffusive motion of a single cross link based on the Kirchoff matrix for this model. Again, this is a very specific model that is difficult to extend to a model where we would like collective behaviour, i.e. analytical results for more than a single cross link.

4.3   Cayley-Tree Network Model
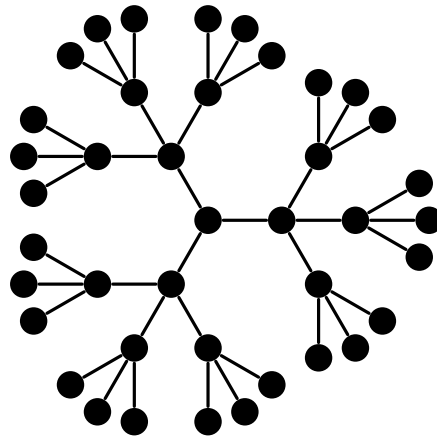
4.3.1   Motivation

Figure 4.1: Cayley-tree of depth 3 and functionality $\phi = 4$. Notice that there is a unique path between any two nodes of the network.

Defining a mesoscopic model is a difficult process if one requires an explicit labelling scheme for the nodes of the network. We will avoid this ambiguity by using a tree-structure which can be uniquely labelled. A Cayley-tree is a tree network where every node has a fixed number of edges connected to it, except for the leaf

nodes, i.e. the outermost nodes in the network, and the central node. This topology is visually represented in figure 4.1. There is only one path one can take between two elements of a tree network. The idea for using a Cayley-tree was used by Jones and Ball[16] who calculated fixed points of force constants of a tree network consisting of rigid rods using a renormalisation process. Our hope is that we might be able to also a apply a type of renormalisation process for flexible chains to study the dynamics of a network with this topology. Of course real polymer networks will have much more complicated topologies than this, but it is possible to synthesise star shaped networks[36] which are almost Cayley-tree like in the small radius approximation.

4.3.2   Model

In this section the idea of a network with a restricted topology will be investigated. The choice of topology would be that of a Cayley-Tree as described in the preceding section and is represented in figure 4.2. First of all, the hope is that this will simplify the mathematics and secondly, experiments have shown that certain filaments do tend to form similar structures[37] in the kinds of systems we are also hoping to understand. We need a sensible model and strategy if we want to set up a renormalisation process. We will consider a very simplified model where we only consider a subnetwork of nodes that are directly coupled to other nodes. These subnetworks can then in turn be in turn linked together to form a full network. We thus neglect the polymer degrees of freedom that might occur on the segments between two cross links and model the polymers by springs. We will also neglect any excluded volume effect and hydrodynamic interaction with the surrounding fluid. The only interaction with the environment will be through a drag force with drag constant γ_0 and a time dependent stochastic force $f(t)$. The idea of this calculation will be to see if it is possible to define a set of Langevin equations for the individual elements of this network and then integrate out degrees of freedom so that we may end up with a renormalised structure with new interaction constants that describes the collective behaviour of the network. The Martin-Siggia-Rose[18] formalism in its functional integral formulation[20] will be employed for this procedure. See Appendix C for a brief description and derivation of this formalism.

Firstly a Hamiltonian of the form

$$\mathcal{H} = \frac{k}{2} \sum_{i=1}^{\phi-1} (r_i(t) - R(t))^2 \tag{4.1}$$

can be defined for the position of the leaf nodes of the tree and the position of the node that they branch from below as is seen in figure 4.2. We denote the position of the free leaf nodes by $r_i(t)$ and we denote the position of the node they branch from by $R(t)$. These nodes all have the same dynamics and this is purely a labelling scheme as to make the mathematics easier to follow.
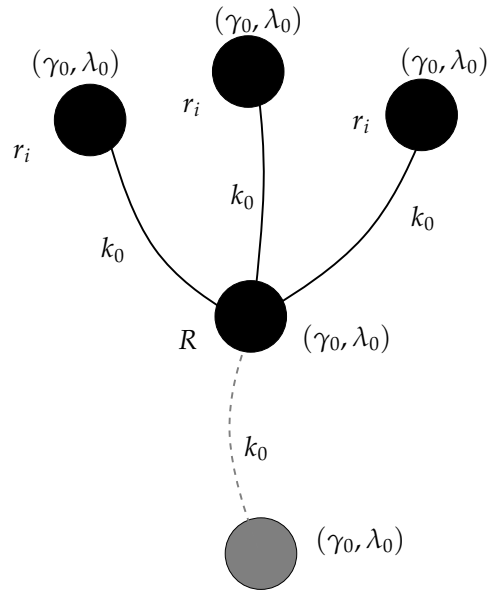

Figure 4.2: Cayley-tree of identical Brownian particles experiencing a drag force with drag coefficient γ_0 and connected with harmonic springs with spring constant k_0. The hydrodynamic interaction and volume excluded effect is neglected. There is no difference between particles r_i and R, this is only for labelling. Their dynamics are exactly the same.

The parameter ϕ indicates the functionality of the network, in other words, the number of edges connected a node, except for the leaf and root nodes. We will form the network coupling by introducing a harmonic interaction, with spring constant k_0, between the nodes. We can now write down a set of Langevin equations that describes the dynamics of the nodes by taking the derivatives with respect to $r_i(t)$ and $R(t)$, i.e.

$$\gamma_0 \frac{\partial r_i(t)}{\partial t} = -k_0 \frac{\partial \mathcal{H}}{\partial r_i(t)} + f(t)$$
$$\gamma_0 \frac{\partial r_i(t)}{\partial t} = -k_0 \frac{\partial \mathcal{H}}{\partial R(t)} + f(t)$$

which leads to

$$\gamma_0 \frac{\partial r_i(t)}{\partial t} = -k_0 \left(r_i(t) - R(t) \right) + f(t) \tag{4.2}$$

$$\gamma_0 \frac{\partial R(t)}{\partial t} = k_0 \sum_i^{\phi-1} \left(r_i(t) - R(t) \right) + f(t) . \tag{4.3}$$

The stochastic noise $f(t)$ is chosen to be delta-correlated and can be characterised by

$$\langle f(t) \rangle = 0$$

$$\langle f(t)f(t') \rangle = \lambda_0 \delta(t - t') ,$$

with the parameter λ controlling the strength of the noise and is related to the drag coefficient γ_0 by the fluctuation-dissipation theorem[38]:

$$\lambda_0 = 2k_B T \gamma_0 . \tag{4.4}$$

The functional probability distribution, up to a normalisation constant, for the noise is given by

$$P\left[f(t) \right] = \int \mathcal{D}f(t) e^{-\frac{1}{2\lambda_0} \int dt\, f(t)^2} . \tag{4.5}$$

4.3.3   Dynamical Calculation

As stated before, in order to integrate out the leaf nodes r_i, it is first convenient to convert this into a functional integral problem using the Martin-Siggia-Rose formalism. First it will prove convenient to introduce the coordinate transformation

$$\rho_i(t) = r_i(t) - R(t) ,$$

where the Jacobian of this transformation is clearly trivial. Equations 4.2 and 4.3 can now be rewritten as

$$\gamma_0 \frac{\partial \rho_i(t)}{\partial t} = -\gamma_0 \frac{\partial R(t)}{\partial t} - k_0 \rho_i(t) + f(t)$$

$$\gamma_0 \frac{\partial R(t)}{\partial t} = k_0 \sum_{i=1}^{\phi-1} \rho_i(t) + f(t) .$$

One can now define a generating functional where the resulting expression given by

$$\mathcal{Z}\left[h(t), h'(t)\right] = \int \prod_i \mathcal{D}\rho_i(t)\mathcal{D}R(t)\mathcal{D}\hat{\rho}_i(t)\mathcal{D}\hat{R}(t)\mathcal{D}f_r(t)\mathcal{D}f_R(t)$$

$$\times \exp\left\{ +i \int_t \sum_{i=1}^{\phi-1} \hat{\rho}_i(t)\left[\gamma_0\partial_t\rho_i(t) + \gamma_0\partial_t R(t) + k_0\rho_i(t) + f_r(t)\right]\right.$$

$$\left. +i \int_t \hat{R}(t)\left[\gamma_0\partial_t R(s) - k_0\sum_{i=1}^{\phi-1}\rho_i(t) + f_R(t)\right]\right\}$$

$$\times \exp\left\{ \int_t h(t)R(t) + \int_t h'(t)\rho_i(t)\right\}.$$

For the remainder of the calculation the source terms $h(t)$ and $h'(t)$ will be suppressed. We can now take the thermal averages by using equation 4.5 and integrating over the stochastic forces. Doing so leads to

$$\langle \mathcal{Z}\rangle = \int \prod_i \mathcal{D}\rho_i(t)\mathcal{D}R(t)\mathcal{D}\hat{\rho}_i(t)\mathcal{D}\hat{R}(t)$$

$$\times \exp\left\{ -\frac{\lambda_0}{2}\int_t \sum_{i=1}^{\phi-1}\hat{\rho}_i^2(t) \quad +i\int_t \sum_{i=1}^{\phi-1}\hat{\rho}_i(t)\left[\gamma_0\partial_t\rho_i(t) + \gamma_0\partial_t R(t) + k_0\rho_i(t)\right]\right.$$

$$\left. -\frac{\lambda_0}{2}\int_t \hat{R}^2(t) \quad\quad\quad +i\int_t \hat{R}(t)\left[\gamma_0\partial_t R(s) - k_0\sum_{i=1}^{\phi-1}\rho_i(t)\right]\right\}$$

where $\langle\cdots\rangle$ indicates the thermal average. The dynamical quantities $\rho_i(t)$ and $R(t)$ are now coupled to their respective Gaussian fluctuating conjugate fields $\hat{\rho}_i(t)$ and $\hat{R}(t)$. Dealing with the time derivatives in the exponent is not something we would like to do, so a change of basis can be made to turn the differential equations into algebraic equations. It is now convenient to introduce the Fourier transformation, up to a normalisation constant, from the time domain to the frequency domain:

$$\tilde{f}(\omega) = \int dt\, f(t)e^{i\omega t},$$

for $f(t)$ a square integrable function. Time derivative terms will thus now transform as follows,

$$\frac{\partial f(t)}{\partial t} = i\omega\tilde{f}(\omega),$$

by using integration of parts when applying the integral transformation. The resulting generating function where the dynamical quantities are frequency dependent is

now given by

$$\langle \mathcal{Z} \rangle = \int \prod_i \mathcal{D}\tilde{\rho}_i(\omega)\mathcal{D}\tilde{R}(\omega)\mathcal{D}\hat{\tilde{\rho}}_i(\omega)\mathcal{D}\hat{\tilde{R}}(\omega) \tag{4.6}$$

$$\times \exp\left\{ -\frac{\lambda_0}{2} \int_w \sum_{i=1}^{\phi-1} \hat{\tilde{\rho}}_i^2(\omega) + i\int_w \sum_{i=1}^{\phi-1} \hat{\tilde{\rho}}_i(\omega)\left[i\omega\gamma_0\tilde{\rho}_i(\omega) + i\omega\gamma_0\tilde{R}(\omega) + k_0\tilde{\rho}_i(\omega) \right] \right.$$

$$\left. -\frac{\lambda_0}{2} \int_w \hat{\tilde{R}}^2(\omega) + i\int_w \hat{\tilde{R}}(\omega)\left[i\omega\gamma_0\tilde{R}(\omega) - k_0\sum_i \tilde{\rho}_i(\omega) \right] \right\}, \tag{4.7}$$

where the aim is now to try and integrate out the leaf nodes r_i and examine how this will renormalise the coupling constants λ_0 and γ_0. Integrating over the auxiliary field $\hat{\tilde{\rho}}(\omega)$, one finds that

$$\langle \mathcal{Z} \rangle = \int \prod_i \mathcal{D}\tilde{\rho}_i(\omega)\mathcal{D}\tilde{R}(\omega)\mathcal{D}\hat{\tilde{R}}(\omega)$$

$$\times \exp\left\{ -\frac{1}{2\lambda_0} \int_w \sum_i \|i\omega\gamma_0\tilde{\rho}_i + i\omega\gamma_0 + k_0\tilde{\rho}_i\|^2 \right.$$

$$\left. -\frac{\lambda_0}{2} \int_w \hat{\tilde{R}}^2 + i\int_w \hat{\tilde{R}}\left[i\omega\gamma_0\tilde{R} - k_0\sum_i \tilde{\rho}_i \right] \right\},$$

where it is now convenient to define the change of variables $\pi_i(\omega) = \tilde{\rho}_i(\omega) + \frac{i\omega\gamma_0}{i\omega\gamma_0+k_0}\tilde{R}(\omega)$ as to simplify the mathematics of the next integration step. The Jacobian of the transformation is trivial. Doing so one obtains

$$\mathcal{Z} = \int \prod_i \mathcal{D}\pi_i(\omega)\mathcal{D}\tilde{R}(\omega)\hat{\tilde{R}}(\omega) \exp\left\{ -\frac{1}{2\lambda_0} \int_w \sum_{i=1}^{\phi-1} \|\pi_i\|^2 \|i\omega\gamma_0 + k_0\|^2 \right.$$

$$-i\int_w \sum_i k_0\hat{\tilde{R}}\left[\pi_i - \frac{i\omega\gamma_0}{i\omega\gamma_0 + k_0}\tilde{R} \right]$$

$$\left. -\frac{\lambda_0}{2} \int_w \hat{\tilde{R}}^2 + i\int_w \hat{\tilde{R}}\left[i\omega\gamma_0\tilde{R} \right] \right\},$$

where by integrating over the π_i field one obtains the following "renormalised" expression:

$$\mathcal{Z} = \int \mathcal{D}\tilde{R}(\omega)\hat{\tilde{R}}(\omega) \exp\left\{ -\int_w \left[\frac{\lambda_0}{2} + \frac{\lambda_0}{2}\frac{\phi-1}{\omega^2\gamma_0^2 + k_0^2}k_0^2 \right] \hat{\tilde{R}}^2 \right.$$

$$\left. +i\int_w \hat{\tilde{R}}\left[\left(\frac{i\omega\gamma_0}{i\omega\gamma_0 + k_0}k_0(\phi-1) \right)\tilde{R} + i\omega\gamma_0\tilde{R} \right] \right\}.$$

We can now make sense of the new complex coefficient of $\tilde{R}(\omega)$ by decomposing it in to real and imaginary parts. Doing so leads to

$$\frac{i\omega\gamma_0}{i\omega\gamma_0 + k_0}k_0(\phi - 1) = \frac{k_0^2(\phi-1)i\omega\gamma_0}{\omega^2\gamma_0^2 + k_0^2} + \frac{k_0(\phi-1)\omega^2\gamma_0^2}{\omega^2\gamma_0^2 + k_0^2} , \qquad (4.8)$$

where we can see that the imaginary part describes a friction coefficient, because terms that contain the $i\omega$ factor come from the Fourier transform of a time derivative term, i.e. a drag force. The real part describes a new harmonic localisation in the system. One can think of the new spring constant addition to be a localisation to a background medium that the network provides. Formally one can write down the following expressions for the noise, drag and spring constants after one renormalisation step,

$$\lambda_1 = \lambda_0 + \frac{\lambda_0(\phi-1)k_0^2}{\omega^2\gamma_0^2 + k_0^2}$$

$$\gamma_1 = \gamma_0 + \frac{\gamma_0 k_0^2(\phi-1)}{\omega^2\gamma_0^2 + k_0^2}$$

$$k_1 = k_0 + \frac{k_0(\phi-1)\omega^2\gamma_0^2}{\omega^2\gamma_0^2 + k_0^2} .$$

Note that for the spring constant k_1 the term k_0 has to be added by hand seeing as our Hamiltonian did not include the explicit downwards bare coupling to the rest of the tree. The first step of the renormalisation process is represented by figure 4.3 and the grey coloured edge indicates term k_0 that we had to add.

We can now again write down a generating functional for a tree network where the leaf nodes are now the renormalised nodes calculated above. The generating functional is given by

$$\langle \mathcal{Z} \rangle = \int \prod_i \mathcal{D}\rho_i(t)\mathcal{D}R(t)\mathcal{D}\hat{\rho}_i(t)\mathcal{D}\hat{R}(t)$$

$$\times \exp\left\{ -\frac{\lambda_1}{2}\int_t \sum_{i=1}^{\phi-1}\hat{\rho}_i^2(t) \quad +i\int_t\sum_{i=1}^{\phi-1}\hat{\rho}_i(t)\Big[\gamma_1\partial_t\rho_i(t) + \gamma_1\partial_t R(t) + k_1\rho_i(t)\Big]\right.$$

$$\left. -\frac{\lambda_0}{2}\int_t \hat{R}^2(t) \qquad\qquad +i\int_t \hat{R}(t)\left[\gamma_0\partial_t R(s) - k_1\sum_{i=1}^{\phi-1}\rho_i(t)\right]\right\}$$

with the usual definition that $R(t)$ refers to the unrenormalised node at the bottom
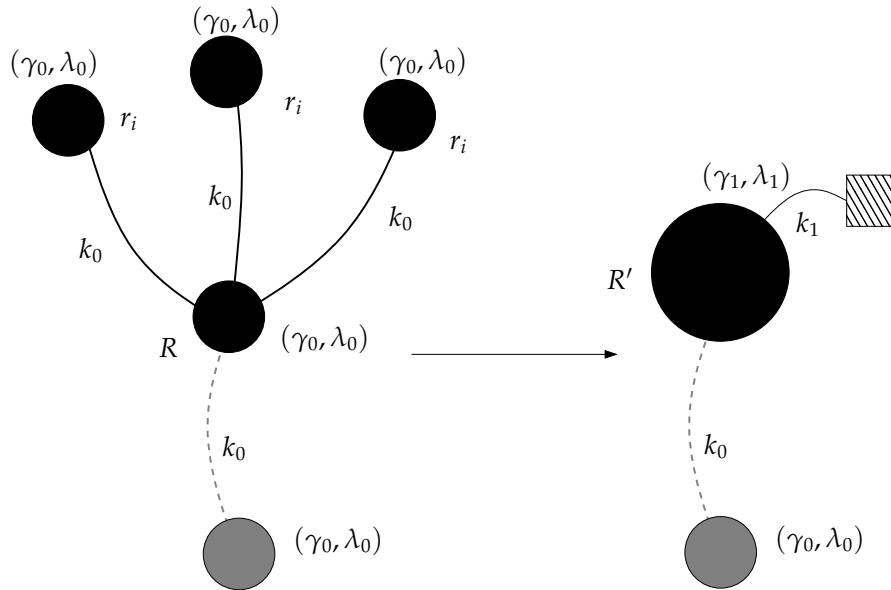
Figure 4.3: Tree subnetwork after one integration step. The leaf nodes and the node they branch from are replaced by a node experiencing a different drag with drag coefficient γ_1 and localised with a new spring constant k_0. We may now use this as the leaf nodes of a new subnetwork and repeat the procedure.

of the sub-tree. We notice that this generating functional has the same functional form as our first generating functional given by equation 4.7. Integrating out the leaf nodes as we did before should then yield

$$\lambda_2 = \lambda_0 + \frac{\lambda_1(\phi - 1)k_1^2}{\omega^2\gamma_1^2 + k_1^2}$$

$$\gamma_2 = \gamma_0 + \frac{\gamma_1 k_1^2(\phi - 1)}{\omega^2\gamma_1^2 + k_1^2}$$

$$k_2 = k_0 + \frac{k_1(\phi - 1)\omega^2\gamma_1^2}{\omega^2\gamma_1^2 + k_1^2} \, ,$$

where we may repeat this process again, i.e. place renormalised nodes with coupling constants γ_2, λ_2 and k_2 at the leaves of the tree and an unrenormalised node at the bottom. We may then integrate out the leave nodes again to find expressions for γ_3, λ_3 and k_3. Without needing to do any formal mathematical induction, we see that after N steps of repeating this procedure, that the following recurrence relations can

be obtained:

$$\lambda_{n+1} = \lambda_0 + \frac{\lambda_n(\phi - 1)k_n^2}{\omega^2\gamma_n^2 + k_n^2} \tag{4.9}$$

$$\gamma_{n+1} = \gamma_0 + \frac{\gamma_n k_n^2(\phi - 1)}{\omega^2\gamma_n^2 + k_n^2} \tag{4.10}$$

$$k_{n+1} = k_0 + \frac{k_n(\phi - 1)\omega^2\gamma_n^2}{\omega^2\gamma_n^2 + k_n^2} \ . \tag{4.11}$$

These three coupled recurrence relations are not independent, because the drag coefficient γ_0 and noise parameter λ_0 are linked by the fluctuation-dissipation theorem as shown in equation 4.4. Thus we only have to study either the set $\{\lambda_n, k_n\}$ or $\{\gamma_n, k_n\}$. This set of coupled recurrence relations is non-linear and unfortunately no closed form solution has been found yet.

If one were to surmise that for large N that the coupling constants reach a fixed point, i.e.

$$\gamma_n \to \gamma_{n+1}$$
$$k_n \to k_{n+1}$$

as $N \to \infty$. Substituting the above into equations 4.10 and 4.11 we would find that

$$\gamma_n = \gamma_0 + \frac{\gamma_n k_n^2(\phi - 1)}{\omega^2\gamma_n^2 + k_n^2}$$
$$k_n = k_0 + \frac{k_n(\phi - 1)\omega^2\gamma_n^2}{\omega^2\gamma_n^2 + k_n^2} \ .$$

where solving for γ_n and k_n analytically is not mathematically tractable.

We may still attempt to solve it in the case where $\omega \to 0$. This results in

$$\gamma_n = -\frac{\gamma_0}{\phi - 2}$$
$$k_n = k_0 \ ,$$

where clearly this cannot be correct seeing as for any value of the functionality greater than two, the friction coefficient becomes negative. Also for the case of a linear chain $\phi = 2$, the friction coefficient diverges. Similar problems arise when dealing with the $\omega \to \infty$ limit. *Thus we find we cannot solve these recurrence relations by assuming the coupling constants converge to a fixed point.*

If we abandon the idea of trying to find a fixed point, we can still learn more about the system by looking at the various extreme limits of our recurrence relations. First one may consider the long time limit or equivalently as $\omega \to 0$. The recurrence relations then reduce to

$$\gamma_{n+1} = \gamma_0 + \gamma_n(\phi - 1)$$
$$k_{n+1} = k_0$$

and does seem to make sense. If we are probing the system at a low frequency, then the drag of the total network should be the sum total of all the individual drag components i.e. if we slowly probe the system then there is enough time for the effect of the entire network to propagate to the point we are examining. Also if we consider the expression for γ_n then we see that the renormalised drag should scale exponentially in the functionality of the network as we integrate out more of the network, i.e. $\gamma_n \sim \gamma_0 \phi^n$. This makes sense seeing as the total number of nodes in a Cayley-tree grows proportional to ϕ^n for each generation n.

On the other extreme end we can consider the $\omega \to \infty$ limit or equivalently looking at a very short time scale. The recurrence relations are then given by

$$\gamma_{n+1} = \gamma_0$$
$$k_{n+1} = k_n(\phi - 1)\,,$$

which implies that on short time scales the drag coefficient does not change and we only see the local drag of the system and not the total drag of the network. This again complies with our intuition as there is not enough time for the effect of the rest of the network to propagate to the point we are probing.

4.3.4   Numerical Analysis

We would like to briefly study the recurrence relations 4.10 and 4.11 from a numerical point of view. For the purpose of our analysis the dimensional units will be suppressed and we chose the functional $\phi = 10$ and the initial conditions as $k_0 = 1$ and $\gamma_0 = 1$. First we consider the behaviour of the spring constant k_n for three renormalisation steps as shown in figure 4.4. We find that the renormalisation processes does not change the spring constant k_n from k_0 in the limit where $\omega \to 0$. For the case where ω grows larger we find that there is an exponential growth
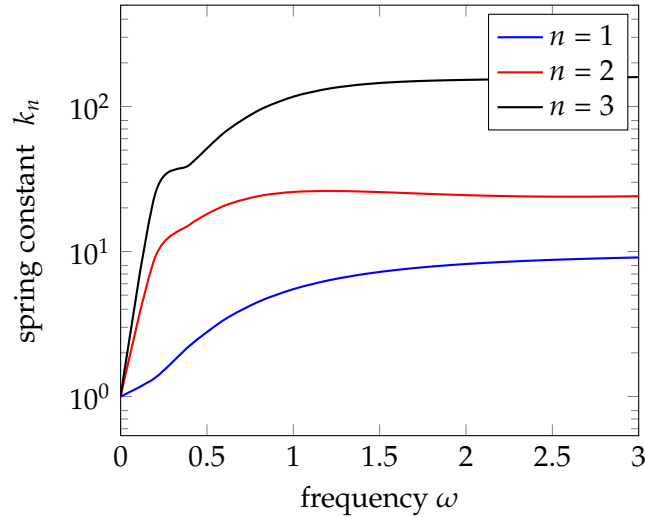
Figure 4.4: First three renormalisation steps of the spring constant k_n. The functionality $\phi = 10$ and the initial conditions $k_0 = 1$ and $\gamma_0 = 1$ are used. The vertical axis is scaled logarithmically. For the case where the frequency $\omega \to 0$, we find that $k_n \to k_0$ in agreement with our theoretical analysis. As the ω grows there is a type of transient behaviour and then exponential growth for k_n which is also in agreement with our theoretical treatment.

for the spring constant. Both of these numerical results are in agreement with our theoretical treatment of the problem.

We now turn to analysing the renormalisation of the drag coefficient γ_n. We consider the first three renormalisation steps. The behaviour of the system for small frequencies ω is depicted in figure 4.5. We find that for small ω that the drag coefficient tends to scale exponentially with functionality of the network, i.e. $\gamma_n \sim \gamma_0 \phi^n$. Figure 4.6 indicates this exponential scaling behaviour for the drag coefficient γ_n where we chose the same parameters for the system as before and set the frequency $\omega = 10$. This is the same behaviour we found using theoretical methods. Lastly we consider the same drag coefficient renormalisation, but in the domain where ω grows larger as shown in figure 4.7. We find that renormalised drag coefficient γ_n tends to the original drag coefficient γ_0 as ω grows. This is also in agreement with our theoretical analysis. We note that that the decay rate $\gamma_n \to \gamma_0$ as a function of the frequency seems to increase substantially for each successive renormalisation step.

In all the cases we discussed we note that there is highly non-linear transient behaviour between the two extreme limits that we could analyse theoretically. Unfortunately this still does not give us insight how to find a closed-form expression
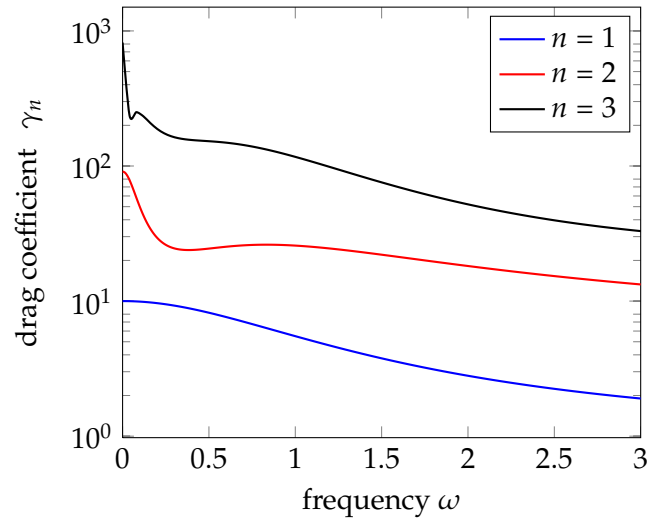
Figure 4.5: First three renormalisation steps of the drag coefficient γ_n. The functionality $\phi = 10$ and the initial conditions $k_0 = 1$ and $\gamma_0 = 1$ are used. The vertical axis is scaled logarithmically. In the limit where $\omega \to 0$ we find that that $\gamma_n \sim \phi^n$ are we found in our theoretical analysis.
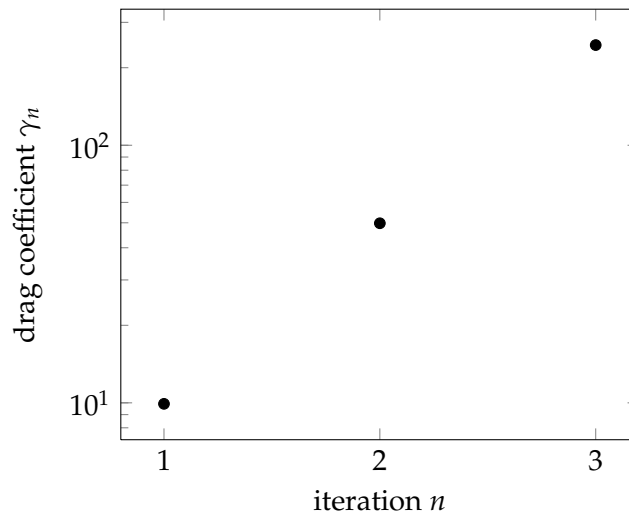
Figure 4.6: Scaling behaviour of the drag coefficient γ_n for the first three renormalisation steps. The functionality $\phi = 10$, frequency $\omega = 10$ and the initial conditions $k_0 = 1$ and $\gamma_0 = 1$ are used. The vertical axis is scaled logarithmically. We find that $\gamma_n \sim \phi^n$ as predicted theoretically.

for the recurrence relations. Of course a closed form expression need not exist and the best we can do is leave the result as is.

Figure 4.7: First three renormalisation steps of the drag coefficient γ_n. The functionality $\phi = 10$ and the initial conditions $k_0 = 1$ and $\gamma_0 = 1$ are used. The vertical axis is scaled logarithmically. In the limit where ω grows large, we see that γ_n decays to γ_0 which ag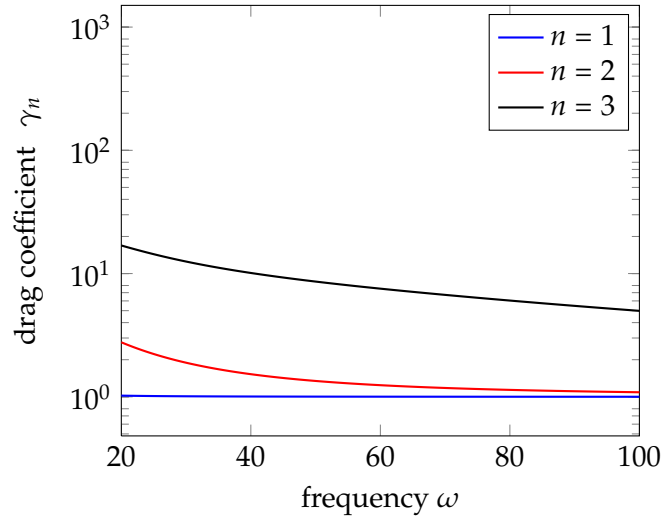rees with our theoretical analysis. The decay rate seems to become much larger for each renormalisation step. The $n = 3$ case does eventually also decay to γ_0 but is not shown in this figure.

4.4   Field-Theoretical Approach

4.4.1   Introduction and Motivation

Edwards[24] has been successful in explaining the equilibrium statistical properties of polymer networks with permanent cross links. This method relies on Wick's theorem to generate all possible cross link configurations for a network. For our purposes we may state Wick's theorem as follows:

Theorem. *Given the Gaussian distributed random variables $\{x_1, x_2, \ldots, x_{2n}\}$ with zero mean, the expectation value*

$$\langle x_1 x_2 \ldots x_{2n} \rangle = \sum_{permutations} \prod_{i<j} \langle x_i x_j \rangle$$

i.e. the n-point correlation function can be decomposed into a sum over all distinct ways one can partition it into 2-point correlation functions. Furthermore, given a set of Gaussian

fluctuation fields

$$\mathcal{K} = \{x(t_1), x(t_2), \ldots, x(t_n), x^\star(t_1)x^\star(t_2), \ldots, x^\star(t_m)\} \,,$$

the n-point correlation function is given by

$$\langle x(t_1), x(t_2), \ldots, x(t_n), x^\star(t_1)x^\star(t_2), \ldots, x^\star(t_m)\rangle = \sum_{permutations} \prod_{i<j} \delta(t_i - t_j) \qquad (4.12)$$

if n = m and one considers the limit where the variance goes to zero.

Proof. We will provide a sketch of the proof along the same lines as how Edwards presents it, which will be sufficient for our purposes. Consider the integral

$$N \int dx \, x^2 \exp\left(-\frac{1}{2a}x^2\right) = a$$

where N is a normalisation constant. We may generalise this to matrices as follows

$$N \int d\vec{x} \, x_i x_j \exp\left(-\frac{1}{2}\vec{x}\mathbb{A}^{-1}\vec{x}\right) = A_{ij}$$

where $\mathbb{A}$ is a positive definite matrix. We may generalise this even further if we assume that we can take the limit as the number of indices goes to infinity. The integral is then replaced by a functional integral of the form

$$N \int \mathcal{D}x \, x(t)x(t') \exp\left(-\frac{1}{2}\int_{t,t'} x(t)\mathcal{A}^{-1}(t, t')x(t')\right) = \mathcal{A}(t, t') \,,$$

where $\langle x(t)x(t')\rangle = \delta(t - t')$ when $\mathcal{A}$ is taken as the continuum limit of the identity matrix. If we now transform to the complex fields $x(t) = \chi_1(t) + i\chi_2(t)$ and $x^\star(t) = \chi_1(t) - i\chi_2(t)$ then we can show that

$$N \int \mathcal{D}x(t)\mathcal{D}x^\star(t) \, x(t)x(t') \exp\left(-\frac{1}{2}\int_{t,t'} x(t)x^\star(t)\right) = 0$$

$$N \int \mathcal{D}x(t)\mathcal{D}x^\star(t) \, x(t)x^\star(t') \exp\left(-\frac{1}{2}\int_{t,t'} x(t)x^\star(t)\right) = \delta(t - t') \,.$$

We may now consider the set of fields

$$\mathcal{K} = \{x(t_1), x(t_2), \ldots, x(t_n), x^\star(t_1)x^\star(t_2), \ldots, x^\star(t_m)\}$$

and then we find that

$$N \int \mathcal{D}x(t)\mathcal{D}x^\star(t') \, \mathcal{K} \exp\left(-\frac{1}{2} \int_{t,t'} x(t)x^\star(t') \right) = \begin{cases} \sum \prod_{i<j} \delta(t_i - t_j) & \text{if } m = n \\ 0 & \text{otherwise} \end{cases}.$$

□

4.4.2 Dynamical Formulation

We can thus use a field and its complex conjugate to represent the head and tail respectively of the components of a network. When calculating the expectation value of all the fields, we get all possible ways to form a network. Of course we might get loops and defects in the network, but Edwards has argued that the number of these configurations is small compared to the number of fully cross linked configurations. Figure 4.8 provides a visual representation of the components of a Cayley-tree network and its associated fields. We would now like to write down a dynamical
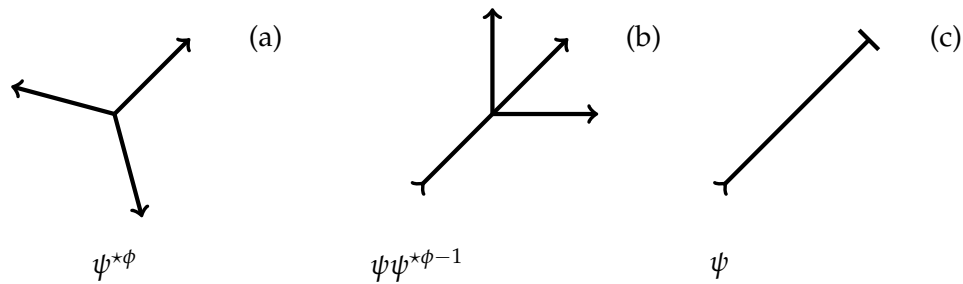

(a) $\psi^{\star\phi}$

(b) $\psi\psi^{\star\phi-1}$

(c) ψ

Figure 4.8: Fundamental components of a Cayley-tree network. The field ψ is associated with a head ⟶ and the field $\psi^\star$ is associated with the tail ⟩— . The network is terminated at some finite depth via the ⟩⊢ components. Heads may only link up with tails. To form a complete tree network without defects of depth N and functionality ϕ, we require that there is one component of type (a), $\sum_{n=1}^{N-1} \phi(\phi-1)^{n-1}$ of type (b) and $\phi(\phi-1)^{N-1}$ of type (c).

theory for an end-linked Cayley-tree network where the linking constraints will be enforced via Wick's theorem using the components presented in figure 4.8. The result from Wick's theorem will be zero unless there are enough components in the system such that all pairs match up. For a single tree of depth N it is required that there is one central component of type (a), $\sum_{n=1}^{N-1} \phi(\phi-1)^{n-1}$ components of type (b) and $\phi(\phi-1)^{N-1}$ components of type (c). We will assume that the central component is fixed in space and carries no dynamics. The dynamics of the polymers

in components type (b) and type (c) will be described by Langevin equations of the form

$$\mathcal{L} \equiv \mathcal{L}(r_1(t), r_2(t)) \, ,$$

where the Langevin equations only explicitly depend on the end-points $r_1(t)$ and $r_2(t)$ of the polymer. We may now introduce a Martin-Siggia-Rose (see Appendix C) generating functional with Edwards style constraints as follows

$$
\begin{aligned}
\mathcal{Z} = \int \mathcal{D}\psi\,(r, v, t)\, \mathcal{D}\psi^\star\,(r, v, t) \exp\left(-\int_{r,t} \psi\psi^\star\right) \prod_t \psi^{\star\phi}(0, 0, t) \\
\times \left\{ \int \mathcal{D}r_1(t)\mathcal{D}r_2(t)\, \delta\left[\mathcal{L}(r_1, r_2)\right] \prod_t \psi\psi^{\star\phi-1} \right\}^{\sum_{n=1}^{N-1} \phi(\phi-1)^{n-1}} \\
\times \left\{ \int \mathcal{D}r_1(t)\mathcal{D}r_2(t)\, \delta\left[\mathcal{L}'(r_1, r_2)\right] \prod_t \psi \right\}^{\phi(\phi-1)^{N-1}} \, ,
\end{aligned}
$$ (4.13)

where the fields ψ and $\psi^\star$ that will enforce the constraints are given explicit velocity v and time t dependence. The reason for doing so is that in the formalism we provided, the ordering of time evolution and spatial reconfiguration is switched around. For this theory to be sound, we require a specific network configuration is generated via Wick's theorem and then evolved through time, then a next configuration and so forth. As it stands here, our theory provides every possible network configuration at every time step. It is still not clear if it is possible to rewrite our generating functional to overcome this problem. We hope that by providing an explicit velocity dependence, that mostly the same network configurations will be present at every time step if we assume that the cross links have a low velocity. At this point it is difficult to state if this provides the desired result.

To continue analysing our model, we can now raise the time product terms into the exponential by making use of the logarithm. For example consider

$$\prod_t \psi^{\star\phi} = \exp\left(\log \prod_t \psi^{\star\phi}\right)$$ (4.14)

$$= \exp\left(\sum_t \log \psi^{\star\phi}\right)$$ (4.15)

and by taking the continuous time limit $\sum_t \to \int_t$

$$= \exp\left(\int_t \log \psi^{\star\phi}\right) \, .$$ (4.16)

Let us now define a "generalised density" function of the form

$$\rho(r, v, t) = \sum_i \delta(r - r_i)\delta(v - \frac{dr_i}{dt})$$

which we can use to rewrite equation 4.16, the result being

$$\exp\left(\int_t \log \psi^{\star\phi}\right) = \exp\left(\int_{r,v,t} \rho(r, v, t) \log \psi^{\star\phi}\right) .$$

Following the same type of argument as Fantoni and Müller-Nedebock[39], we introduce the generalised density for the other time product terms, where we may rewrite equation 4.13 as

$$\mathcal{Z} = \int \mathcal{D}\psi(r, v, t)\, \mathcal{D}\psi^\star(r, v, t) \exp\left(-\int_{r,v,t} \psi\psi^\star\right) \exp\left(\int_{r,v,t} \rho_0 \log \psi^{\star\phi}(0, 0, t)\right)$$
$$\times \left\{\int \mathcal{D}r_1(t)\mathcal{D}r_2(t)\, \delta\left[\mathcal{L}(r_1, r_2)\right] \exp\left(\int_{r,v,t} \rho_1 \log \psi\right.\right.$$
$$\left.\left. + \int_{r,v,t} \rho_2 \log \psi^{\star\phi-1}\right)\right\}^{\sum_{n=1}^{N-1} \phi(\phi-1)^{n-1}}$$
$$\times \left\{\int \mathcal{D}r_1(t)\mathcal{D}r_2(t)\, \delta\left[\mathcal{L}'(r_1, r_2)\right] \exp\left(\int_{r,v,t} \rho_3 \log \psi\right)\right\}^{\phi(\phi-1)^{N-1}}$$

where the generalised density terms have different subscripts so that the theory remains as general as possible. This field theory is highly non-linear and our only hope of finding analytical results would be by examining the saddle point approximation. The saddle point solutions are given by

$$\left.\frac{\delta\mathcal{F}}{\delta\psi}\right|_{\overline{\psi},\overline{\psi}^\star} = 0 \qquad \text{and} \qquad \left.\frac{\delta\mathcal{F}}{\delta\psi^\star}\right|_{\overline{\psi},\overline{\psi}^\star} = 0 .$$

where $\mathcal{F}$ indicates the sum of all the arguments in the exponential functions. We may rewrite our generating functional as

$$\mathcal{Z} = \int \mathcal{D}\psi(r, v, t)\, \mathcal{D}\psi^\star(r, v, t) \exp\left(-\int_{r,v,t} \psi\psi^\star\right) \exp\left(\int_{r,v,t} \rho_0 \log \psi^{\star\phi}(0, 0, t)\right)$$
$$\times \prod_{\alpha=1}^{M'} \int \mathcal{D}r_1^{(\alpha)}\mathcal{D}r_2^{(\alpha)}\, \delta^{(\alpha)}\left[\mathcal{L}^{(\alpha)}\left(r_1^{(\alpha)}, r_2^{(\alpha)}\right)\right] \exp\left(\sum_{\alpha=1}^{M'} \int_{r,v,t} \left[\rho_1^{(\alpha)} \log \psi\right.\right.$$
$$\left.\left. + \rho_2^{(\alpha)} \log \psi^{\star\phi-1}\right]\right)$$
$$\times \prod_{\alpha=1}^{N'} \int \mathcal{D}r_1^{(\alpha)}\mathcal{D}r_2^{(\alpha)}\, \delta^{(\alpha)}\left[\mathcal{L}^{(\alpha)}\left(r_1^{(\alpha)}, r_2^{(\alpha)}\right)\right] \exp\left(\sum_{\alpha=1}^{M'} \int_{r,v,t} \rho_1^{(\alpha)} \log \psi\right) ,$$

where $M' = \sum_{n=1}^{N-1} \phi(\phi-1)^{n-1}$ and $N' = \phi(\phi-1)^{N-1}$. Explicitly calculating the saddle point solutions leads to

$$\frac{\delta \mathcal{F}}{\delta \psi}\bigg|_{\overline{\psi},\overline{\psi}^\star} = 0$$

$$= -\overline{\psi}^\star + \overline{\psi}^{-1} \sum_{\alpha=1}^{M'} \rho_1^{(\alpha)} + \overline{\psi}^{-1} \sum_{\alpha=1}^{N'} \rho_3^{(\alpha)}$$

$$\frac{\delta \mathcal{F}}{\delta \psi^\star}\bigg|_{\overline{\psi},\overline{\psi}^\star} = 0$$

$$= -\overline{\psi} + \frac{\rho_0(-\phi)\overline{\psi}^{\star\phi-1}}{\psi^{\star\phi}}\delta(r)\delta(v) + \sum_{\alpha=1}^{M'} \frac{\rho_2^{(\alpha)}}{\psi^{\star\phi-1}}(\psi-1)\overline{\psi}^{\star\phi-2}$$

$$= -\overline{\psi} + \frac{\rho_0\phi}{\psi^\star}\delta(r)\delta(v) + \sum_{\alpha=1}^{M'} \frac{\rho_2^{(\alpha)}}{\overline{\psi}^\star}(\psi-1)\overline{\psi}^{\star\phi-1}$$

where if we define

$$P_i = \sum_{\alpha=1} \rho_i^{(\alpha)}$$

we may rewrite the saddle point solutions as

$$0 = -\overline{\psi}^\star + \frac{P_1}{\overline{\psi}} + \frac{P_3}{\overline{\psi}}$$

$$0 = -\overline{\psi} + \frac{\rho_0\phi}{\overline{\psi}^\star}\delta(r)\delta(v) + \frac{P_2(\phi-1)}{\overline{\psi}^\star} .$$

Combining the these solutions we find that

$$0 = -\overline{\psi} + \overline{\psi}\frac{\rho_0\phi}{P_1+P_3}\delta(r)\delta(v) + \overline{\psi}\frac{P_2\phi}{P1+P3}$$

and for the case where the solution $\overline{\psi}$ is non-zero we may divide by $\overline{\psi}$ to get the relation

$$0 = -1 + \frac{\rho_0\phi}{P_1+P_3}\delta(r)\delta(v) + \frac{P_2\phi}{P_1+P_3} . \tag{4.17}$$

Unfortunately we cannot directly obtain useful properties of the network from equation 4.17 as it only provides information on how the various generalised densities are related. Further study is required to see if one can obtain a useful result from the given information.

4.4.3   Generalised density-density correlation

In this section we would like to examine the meaning of the generalised density-density correlation function given by

$$\langle \rho(r, v, t) \rho(r', v', t') \rangle .$$

We will restrict our study to a minimalistic system of a Brownian particle in a harmonic potential as in figure 4.9. The overdamped Langevin equation that describes
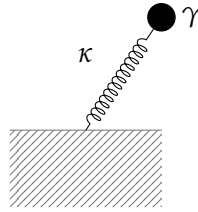

Figure 4.9: Brownian particle in a harmonic potential with spring constant k, coefficient γ and noise strength parameter λ. Note that the barrier does not exclude the particle.

this system is given by

$$\gamma \frac{\partial r(t)}{\partial t} = -\kappa r(t) ,$$

where $r(t)$ indicates the position of the particle, γ the drag coefficient and κ the spring constant. We can apply the time Fourier transformation to rewrite this in a frequency basis which leads to

$$-i\gamma \omega \tilde{r}(\omega) = \kappa \tilde{r}(\omega).$$

The Martin-Siggia-Rose generating functional for this system is given by

$$\langle \mathcal{Z} \rangle = \int \mathcal{D}\tilde{r}(\omega) \mathcal{D}\hat{\tilde{r}}(\omega) \exp\left(-\frac{\lambda}{2} \int \hat{\tilde{r}}^2 + i \int \hat{\tilde{r}} \left[-\gamma\omega\tilde{r} + \kappa\tilde{r} \right] \right) , \qquad (4.18)$$

where the source term is suppressed and the thermal average over the stochastic force has been taken. First let us suppose that we can write

$$\rho(r, v, t) = \delta(r - \int d\omega \, e^{i\omega t}\tilde{r}(\omega))\delta(v - \int d\omega \, e^{i\omega t}\tilde{v}(\omega)) ,$$

where

$$\tilde{v}(\omega) = i\omega\tilde{r}(\omega)\,.$$

This allows us to write the generalised density-density correlation function as

$$\langle\rho(r,v,t)\rho(r',v',t')\rangle = \left\langle\prod_{i=1}^{n}\delta(r_i - \int d\omega\, e^{i\omega t}\tilde{r}(\omega))\delta(v_i - \int d\omega\, e^{i\omega t}\tilde{v}(\omega))\right\rangle$$

where we may now apply the Fourier transformation to the Dirac delta functions to get

$$\langle\rho(r,v,t)\rho(r',v',t')\rangle = \left\langle\int dk_1 dk_2 dk_3 dk_4 \exp\left(ik_1 r - ik_1\int_\omega e^{i\omega t}\tilde{r} + ik_2 v - ik_2\int_\omega e^{i\omega t}\tilde{v}\right.\right.$$
$$\left.\left. + ik_3 r' - ik_3\int_\omega e^{iwt'}\tilde{r} + ik_4 v' - ik_4\int_\omega e^{i\omega t'}\tilde{v}\right)\right\rangle\,.$$

The thermal average may now be rewritten by using equation 4.18, which leads to

$$\langle\rho(r,v,t)\rho(r',v',t')\rangle = \int dk_1 dk_2 dk_3 dk_4 \int \mathcal{D}\tilde{r}(\omega)\mathcal{D}\hat{\tilde{r}}(\omega)$$
$$\times \exp\left(-\frac{\lambda}{2}\int\hat{\tilde{r}}^2 + i\int\hat{\tilde{r}}\left[-\gamma\omega\tilde{r} + \kappa\tilde{r}\right]\right)$$
$$\times \exp\left(ik_1 r - ik_1\int_\omega e^{i\omega t}\tilde{r} + ik_2 v - ik_2\int_\omega e^{i\omega t}\tilde{v} + ik_3 r'\right.$$
$$\left. - ik_3\int_\omega e^{iwt'}\tilde{r} + ik_4 v' - ik_4\int_\omega e^{i\omega t'}\tilde{v}\right)\,,$$

where we can now integrate over the fields $\tilde{r}(\omega)$ and $\hat{\tilde{r}}(\omega)$. Integrating over $\hat{\tilde{r}}(\omega)$ results in

$$\langle\rho(r,v,t)\rho(r',v',t')\rangle = \int dk_1 dk_2 dk_3 dk_4 \int \mathcal{D}\tilde{r}(\omega)$$
$$\times \exp\left(-\frac{1}{2\lambda}\int\tilde{r}^2\left[\gamma^2\omega^2 + \kappa^2\right]\right)$$
$$\times \exp\left(ik_1 r - ik_1\int_\omega e^{i\omega t}\tilde{r} + ik_2 v - ik_2\int_\omega e^{i\omega t}\tilde{v} + ik_3 r'\right.$$
$$\left. - ik_3\int_\omega e^{iwt'}\tilde{r} + ik_4 v' - ik_4\int_\omega e^{i\omega t'}\tilde{v}\right)\,,$$

and integrating over $\tilde{r}(\omega)$ leads to

$$\int dk_1 dk_2 dk_3 dk_4 \exp\left(ik_1 r + ik_2 v + ik_3 r' + ik_4 v'\right)$$
$$\times \exp\left(-\frac{\lambda}{2}\int_\omega\left[\gamma^2\omega^2 + \kappa^2\right]^{-1}\times\left[k_1^2 + \omega^2 k_2^2 + k_3^2 + \omega^2 k_4^2\right.\right.$$
$$+ k_1 k_3 e^{-i\omega(t'-t)} + ik_1 k_4\omega e^{-\omega(t'-t)} - ik_2 k_3\omega e^{-i\omega(t'-t)} + k_2 k_4\omega^2 e^{-i\omega(t'-t)}$$
$$\left.\left. + k_1 k_3 e^{i\omega(t'-t)} + ik_2 k_3\omega e^{i\omega(t'-t)} - ik_1 k_4\omega e^{i\omega(t'-t)} + \omega^2 k_2 k_4 e^{i\omega(t'-t)}\right]\right)\,, \tag{4.19}$$

where the time ordering $t' > t$ has been explicitly applied.

We now have to deal with the integral over ω in this lengthy expression. Most of the integrals are Fourier transformations (up to a normalisation constant) and we find that

$$\int d\omega \, \frac{1}{\gamma^2\omega^2 + \kappa^2} e^{i\omega(t'-t)} = \frac{1}{\gamma\kappa} \exp\left(-\frac{\kappa(t'-t)}{\gamma}\right)$$

$$\int d\omega \, \frac{\omega}{\gamma^2\omega^2 + \kappa^2} e^{i\omega(t'-t)} = \frac{1}{i\gamma^2} \exp\left(-\frac{\kappa(t'-t)}{\gamma}\right)$$

$$\int d\omega \, \frac{\omega^2}{\gamma^2\omega^2 + \kappa^2} e^{i\omega(t'-t)} = -\frac{\kappa}{\gamma^3} \exp\left(-\frac{\kappa(t'-t)}{\gamma}\right)$$

and

$$\int d\omega \, \frac{1}{\gamma^2\omega^2 + \kappa^2} = \frac{1}{\kappa\gamma} \, .$$

Dealing with integrals of the form

$$\int d\omega \, \frac{\omega^2}{\gamma^2\omega^2 + \kappa^2}$$

is a bit more difficult. Let us extend the domain to the complex plane and consider the integral

$$\int_C dz \, \frac{z^2}{\gamma^2 z^2 + \kappa^2}$$

where the curve C is a semi-circle in the upper complex plane that encloses the pole $z = \frac{i\kappa}{\gamma}$. The residue at this point is given by

$$\text{Res}_{z=\frac{i\kappa}{\gamma}} \frac{z^2}{\gamma^2 z^2 + \kappa^2} = \frac{i\kappa}{2\gamma^3} \, .$$

The residue at the other pole $z = -\frac{i\kappa}{\gamma}$ is zero because it is not enclosed by the semi-circle. From the residue theorem the result of the contour integral follows:

$$\int_C dz \, \frac{z^2}{\gamma^2 z^2 + \kappa^2} = 2\pi i \, \text{Res}_{z=\frac{i\kappa}{\gamma}} \frac{z^2}{\gamma^2 z^2 + \kappa^2}$$

$$= -\frac{\kappa\pi}{\gamma^3}$$

We may decompose the contour C into a straight line and an arc, i.e.

$$\int_{-a}^{a} dz \, \frac{z^2}{\gamma^2 z^2 + \kappa^2} + \int_{\text{arc}} dz \, \frac{z^2}{\gamma^2 z^2 + \kappa^2} = -\frac{\kappa \pi}{\gamma^3}$$

and show that the integral along the arc is zero as $a \to \infty$. Unfortunately no way has been found to do so. One may introduce a *regulator* $\varepsilon > 0$ such that

$$\int_{-\infty}^{\infty} d\omega \, \frac{\omega^2}{\left(\kappa^2 + \gamma^2 \omega^2\right)\left(1 + \varepsilon^2 \omega^2\right)}$$

reduces to the original integral in the limit where $\varepsilon \to 0$. This integral is convergent and we find that

$$\int_{-\infty}^{\infty} d\omega \, \frac{\omega^2}{\left(\kappa^2 + \gamma^2 \omega^2\right)\left(1 + \varepsilon^2 \omega^2\right)} = \frac{\pi}{\gamma^2 \varepsilon} - \frac{\kappa \pi}{\gamma^3} + \mathcal{O}(\varepsilon),$$

where the divergent behaviour is now parametrised by ε. Dealing with this divergent term requires the use of *renormalisation*[2] and is outside the scope of our research.

Returning the our correlation function, we can restrict the function to small time differences, i.e. $t' - t \ll 1$ and furthermore where $\frac{\kappa(t'-t)}{\gamma} \ll 1$. This allows us to make the following expansion:

$$\exp\left(-\frac{\kappa(t'-t)}{\gamma}\right) \approx 1 - \frac{\kappa}{\gamma}(t'-t).$$

Substituting the results for the integrals over ω into equation 4.19, we find that the generalised density-density correlation function is given by

$$\langle \rho(r, v, t) \rho(r', v', t') \rangle = \int dk_1 dk_2 dk_3 dk_4$$

$$\times \exp\left\{ ik_1 r + ik_2 v + ik_3 r' + ik_4 v' \right.$$

$$- \frac{\lambda}{2}\left[\frac{k_1^2}{\kappa \gamma} + k_2^2\left(\frac{1}{\gamma^2 \epsilon} - \frac{\kappa}{\gamma^3} + \mathcal{O}(\epsilon)\right) + \frac{k_3^2}{\kappa \gamma} + k_4^2\left(\frac{1}{\gamma^2 \epsilon} - \frac{\kappa}{\gamma^3} + \mathcal{O}(\epsilon)\right) \right.$$

$$\left.\left. + 2\frac{\kappa}{\gamma}(t'-t)\left(\frac{k_2 k_3}{\gamma^2} - \frac{k_1 k_4}{\gamma^2}\right) + 2\frac{k_1 k_2}{\gamma \kappa} - 2\frac{\kappa k_2 k_4}{\gamma^3} \right]\right\}.$$

We may now notice that the divergent terms parametrised by ϵ are coupled to k_2 and k_4, which were introduced by the Fourier transformation of the Dirac delta function associated with the velocity components. At this point it is not clear how the

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[2]It is not clear how renormalisation that arises in quantum field theories would be applicable here. If we were to absorb the divergences into the coupling constants, then we have to rework the entire model.

velocity terms are responsible for the divergent behaviour. We may also note that the divergent quantities only couple to terms that are not explicitly time dependent. In theory we should now integrate over k_1, k_2, k_3 and k_4, but this leads to an expression that is not algebraically tractable to work with and we are still left with the problem of dealing with the divergent behaviour. We will defer this to further study.

4.5   Remarks and Outlook

In this section we constructed some simple mesoscopic theories for the dynamics of a polymer network as yet much of these remain at the level of the formalism. Unfortunately the constraint problem of forming a network leads to all sorts of mathematical difficulties as was seen in this section.

For the renormalisation calculation we were able to calculate the renormalised drag γ_n and spring constant k_n for N integrating steps in terms of a coupled set of recurrence relations. While we were not able to find closed form solutions, the numerical analysis agreed with our brief theoretical treatment of the problem. The complicated transient behaviour that was observed via numerical analysis might indicate that there is most likely no closed form solution in terms of elementary functions.

The Edwards type theory did not deliver any results that are related to macroscopic quantities such as the shear modulus, but only a relation between the various density functions. We also found that a generalised density-density correlation function exhibits divergent behaviour due to the inclusion of the velocity dependence. Further study is required to see if this can be handled using a renormalisation process such as found in quantum field theories. For reversible crosslinks it might not be needed to include a velocity dependent density function, but it is not clear what mathematical structures will arise in this case.

If one compares the work in this section to that of the first two sections, then we see that the mathematical complexity definitely arises from the constraint problem of forming a permanent network. The dynamics of individual strands are more or less simple compared to this. A breakthrough in the dynamics of polymer networks can only be made if we find a clever way to enforce the constraint problem without introducing complexity that makes the model mathematically intractable.

Chapter 5

Conclusion

In this thesis we constructed and investigated analytical mesoscopic models to study the dynamical behaviour of some aspects of ordinary and active networks.

In our first model, which was that of a single active crosslinked flexible filament, we formulated the model using a Langevin equations approach and then analysed the model using functional integral techniques. A key point of our analysis was to make the ansatz that in the long time limit we can separate the dynamical behaviour of the system into steady steady and fluctuating behaviour. We calculated the steady state behaviour perturbatively up to first order in the motor force f_s. In the dynamical study of the model, we were able to calculate the dependence of autocorrelation of the fluctuations of the position of the active crosslink on the motor force. This dynamical calculation led to complicated mathematical expressions even when we simplified to the case where we only considered the lowest vibrational mode of the filament. We find that autocorrelation does not depend on the motor force to first order in the symmetrical case where the position of the motor is situated in the middle of the contour length of filament. This correlation function is only dependent on f_s^2, where we still have to calculate the second order corrections to the steady state solutions.

We also showed that the fluctuations of the spring force that anchors the motor is proportional to the autocorrelation function of the motor fluctuations, i.e.

$$k^2 \langle (r(\sigma, \omega) - X) \sim \langle \tilde{\Delta}^2(\omega) \rangle. \tag{5.1}$$

While this quantity is not directly related to the elasticity of the filament, we also find an f_s^2 dependence like Liverpool et al. found for the shear modulus of a similar

system.

We then briefly considered a modification to this model where we added a curvature dependent term to create a model for a directed polymer. We then argued that this should not drastically change the results that we have obtained for the ordinary flexible case.

Lastly we explored some dynamical network models in the literature and then presented some ideas of our own. First we presented an idea inspired by Jones and Ball to model the dynamical behaviour of a Cayley-tree type network consisting of Brownian particles. We were able to derive recurrence relations for the renormalised drag and spring constants of the system, but have yet to to find closed form solutions to these recurrence relations. Our numerical analysis of the problem was in agreement with the limited theoretical treatment,

We then considered an Edwards style dynamical theory for crosslinking of filaments. A generalised density function that is velocity and time dependent is proposed to solve the time ordering problem that arises from employing Wick's theorem to solve the constraint problem. While we are able to calculate the saddle points of this field theory, we are not able to calculate quantities that are related to macroscopic observables. The mathematical structure of a generalised density-density correlation is also problematic because the inclusion of the velocity dependence leads to divergent behaviour.

Looking forward there are various aspects that we may still consider. Firstly it would be useful if we could rewrite our first model of a flexible filament in terms of less fundamental parameters such that more mathematically tractable analytical work can be performed. This is of course a difficult procedure because we would like to be able to express all macroscopic quantities in terms of microscopic quantities.

The case of a semiflexible polymer with an active crosslinker is the obvious next model to study. We have discussed how the inflexibility constraint also leads to additional mathematical problems, but if we want to study a system closer to a real biological system, then we have to handle these difficulties.

The network models still require substantial work to see if they can be aligned with results found in the literature. We are hopeful that the Edwards style theory might be able to provide sensible results, based on the successes the technique has provided in the equilibrium case.

While we were not able to provide results that are easily matched or differ from those found in the literature, we do believe that a great deal of insight has

been gained in the understanding of active systems and the problems related to crosslinking. It is our hope that further study will lead to formulating models and analysis that could provide the mesoscopic framework that explains macroscopic quantities found in models in the literature.

Appendix A

Functional Derivative

In this section we will briefly explain how functional derivatives work and also apply the technique to deriving equations of motion from a Hamiltonian. A functional is a map that takes a vector space and maps it to the field that underlies said vector space. For our purposes we will work with the space of normalisable functions that gets mapped to the complex numbers. Formally we can write for the functional $F[\phi(x)]$ that

$$F : \Phi \to \mathbb{C} \, ,$$

where

$$\Phi = \{ \phi(x) : x \in \mathbb{C} \} \, .$$

We now turn to defining the functional derivative $\frac{\delta F[\phi(x)]}{\delta \phi(y)}$ as a measure of how the functional $F[\phi]$ changes when when the function $\phi(y)$ is changed at point y. The functional derivative is an ordinary function where the following relation holds:

$$\delta F[\phi(x)] = \int dy \frac{\delta F[\phi(x)]}{\delta \phi(y)} \delta \phi(y) \, .$$

Or more simply the change in the functional F when variating $\phi(y)$ is just the sum of all the local changes over all possible allowed values for y. This formal definition is not so useful for directly calculating quantities and by substituting the variation at point y, $\phi(x) = \epsilon \delta(x - y)$ (where ϵ is an infinitesimal quantity) into the above expression results in the following divided differences equation:

$$\frac{\delta F[\phi(x)]}{\delta \phi(y)} = \lim_{\epsilon \to 0} \frac{F[\phi(x) + \epsilon \delta(x - y)] - F[\phi(x)]}{\epsilon} \, . \tag{A.1}$$

To make this a unique map, we have to use the convention that if there are other limiting procedures required then that we first takes the limit where ϵ goes to zero before considering other limits. Let us now consider our Hamiltonian

$$\mathcal{H} = \frac{3k_B T}{2l} \int_0^L ds \left(\frac{\partial r(s,t)}{\partial s} \right)^2 + \frac{k}{2} \left(r(\sigma(t),t) - X \right)^2$$

and consider the quantities $\frac{\delta \mathcal{H}}{\delta r(s,t)}$ and $\frac{\delta \mathcal{H}}{\delta \sigma(t)}$. These quantities are analogue to taking the ordinary derivatives of a scalar potential in a force balance equation. Let us consider

$$F_1[r(s,t)] \equiv \int_0^L ds \left(\frac{\partial r(s,t)}{\partial s} \right)^n$$

and substitute this into equation A.1. This leads to

$$\frac{\delta F_1[r(s,t)]}{\delta r(s',t)} = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left(\int ds \left(\frac{\partial}{\partial s} \left[r(s,t) + \epsilon \delta(s-s') \right] \right)^n - \int ds \left(\frac{\partial}{\partial s} r(s,t) \right)^n \right)$$

$$= \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int ds \left(\left(\frac{\partial r(s,t)}{\partial s} \right)^n + n\epsilon \left(\frac{\partial r(s,t)}{\partial s} \right)^{n-1} \right.$$

$$\times \frac{\partial}{\partial s} \delta(s-s') + \mathcal{O}(\epsilon^2) - \left(\frac{\partial r(s,t)}{\partial s} \right)^n \right)$$

$$= n \int ds \left(\frac{\partial r(s,t)}{\partial s} \right)^{n-1} \frac{\partial}{\partial s} \delta(s-s')$$

and using integration by parts

$$= -n \frac{\partial}{\partial s} \left(\frac{\partial r(s,t)}{\partial s} \right)^{n-1} \bigg|_{s=s'} .$$

For the case of our Hamiltonian where $n = 2$ this reduces to

$$\frac{\delta}{\delta r} \int_0^L ds \left(\frac{\partial r(s,t)}{\partial s} \right)^2 = -2 \frac{\partial^2 r(s,t)}{\partial s^2} .$$

Note that it does not matter what we name r and what r' as this is purely a labelling scheme. The functional F_1 does not depend on $\sigma(t)$ and thus

$$\frac{\delta F_1[r(s,t)]}{\delta \sigma(t')} = 0 .$$

Let us now turn to the functional (which is actually an ordinary function)

$$F_2[r(s, t), \sigma(t)] \equiv (r(\sigma(t), t) - X)^2 . \tag{A.2}$$

It can be shown that the chain rule

$$\frac{\delta F}{\delta \phi(y)} F[g(\phi)] = \frac{\delta F}{\delta g(\phi(y))} \frac{dg(\phi(y))}{d\phi(y)}$$

holds where g is an ordinary function. It is straight forward to see that power rule also holds by directly substituting $F \equiv \int dx \, (\phi(x))^n$ into equation A.1 and taking the limit $\epsilon \to 0$ before calculating the integral or equivalently just work up to first order in ϵ. This will result in

$$\frac{\delta}{\delta \phi(y)} \int ds \, (\phi(x))^n = n \, (\phi(y))^{n-1} .$$

We now calculate the functional derivative of F_2 with respect to $r(s', t)$:

$$\frac{\delta F_2}{\delta r(s', t)} \overset{\text{chain rule}}{=} 2 \, (r(s, t) - X) \frac{\delta}{\delta r(s', t)} (r(\sigma(t), t) - X) ,$$

where $r(\sigma(t), t)$ is an ordinary function. The functional derivative of an ordinary function is trivial is one refers to equation A.1 and we find that

$$\frac{\delta r(\sigma(t), t)}{\delta r(s', t)} = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \Big(r(\sigma(t), t) + \epsilon \delta(\sigma(t) - s') - r(\sigma(t), t) \Big)$$

$$= \delta(\sigma(t) - s') .$$

From this we can conclude that

$$\frac{\delta F_2}{\delta r(s', t)} \overset{\text{chain rule}}{=} 2 \, (r(s, t) - X) \, \delta(\sigma(t) - s') .$$

Lastly we have to consider the functional derivative of F_2 with respect to $\sigma(t)$. By making use of equation A.2 we find that

$$\frac{\delta F_2}{\delta \sigma(t')} = 2 \, (r(\sigma(t), t) - X) \frac{\delta r(\sigma(t), t)}{\delta \sigma(t')}$$

$$= 2 \, (r(\sigma(t), t) - X) \frac{\partial r(s, t)}{\partial s} \bigg|_{s = \sigma(t)} .$$

where again the t and t' are purely for labelling.

Appendix B

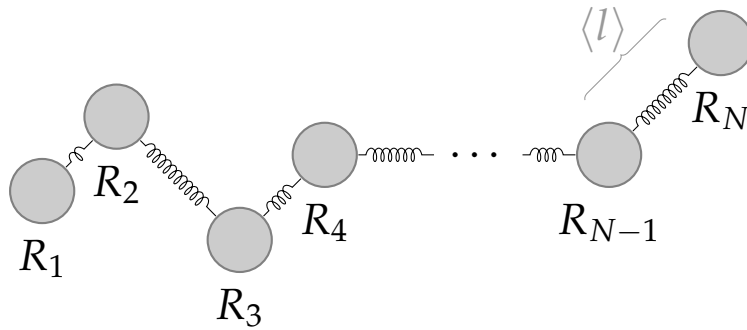# Derivation of Polymer Dynamics

Figure B.1: *N* identical monomers are linked with a harmonic potential with spring constant $k = \frac{3k_B T}{l^2}$ where *l* is the average inter-monomer distance also known as the Kuhn length. Each node experiences a drag force with drag coefficient γ and a stochastic force f_n.

We would like to briefly explain and derive a Langevin equation for the dynamics of a flexible polymer where we do not take the hydrodynamic interaction or the excluded volume effect into consideration. This is known as the Rouse model[7]. First let us suppose that a homogeneous polymer consists of *N* identical monomers connected by harmonic potentials with spring constant $k = \frac{3k_B T}{l^2}$ in a linear fashion as depicted in figure B.1. The average inter-monomer distance is given by *l* and thus the total length of the polymer by $L = lN$. Each monomer experiences a velocity dependent drag force with drag coefficient γ and a time dependent stochastic force $f_n(t)$. We label the monomers by $R_1, \ldots, R_N$ where for the case $n = 2, \ldots, N - 1$ we

can write down the following overdamped Langevin equations:

$$\gamma \frac{\partial R_n(t)}{\partial t} = k\left(R_{n+1}(t) - R_n(t)\right) + k\left(R_{n-1}(t) - R_n(t)\right) + f_n(t)$$

$$= k\left(R_{n+1}(t) - 2R_n(t) + R_{n-1}(t)\right) + f_n(t)\,. \tag{B.1}$$

For the case $n = 1$ we have

$$\gamma \frac{\partial R_1(t)}{\partial t} = k(R_2(t) - R_1(t)) + f_1(t) \tag{B.2}$$

and for $n = N$ it must hold that

$$\gamma \frac{\partial R_N(t)}{\partial t} = k(R_{N-1}(t) - R_N(t)) + f_N(t)\,. \tag{B.3}$$

We can now rewrite equation B.1 by taking the continuum limit where $N \gg 1$ and $l \ll 1$ and changing from the discrete variable n to the continuous variable s. The continuum representation is given by

$$\gamma \frac{\partial R(s,t)}{\partial t} = k \frac{\partial^2 R(s,t)}{\partial s^2} + f(s,t)\,.$$

For a free chain there can be no elastic forces at the end points of the polymer and thus from the continuum limit of equations B.2 and B.3 we find that

$$\left. \frac{\partial R(s,t)}{\partial s} \right|_{s=0} = 0$$

and

$$\left. \frac{\partial R(s,t)}{\partial s} \right|_{s=L} = 0$$

respectively.

Appendix C

Martin-Siggia-Rose Formalism

In this chapter we will briefly explain how the Martin-Siggia-Rose[18] formalism works. We will not present the original operator based formalism, but the equivalent functional integral formulation presented by Jouvet, Phythian[19] and Jensen[20] for additive noise. This is equivalent to how one my find a functional integral representation of an operator and state vector based quantum mechanical problem. This section will also draw upon ideas and results presented by Arenas and Barci[40] who discusses the extended multiplicative noise case. For the purpose of this section we only consider additive noise.

Consider a random variable $x(t)$ that obeys the following Langevin or equation of motion:

$$\frac{dx(t)}{dt} = F(x(t)) + f(t)\,, \tag{C.1}$$

where F is a function of $x(t)$ and $f(t)$ a random variable that represents the noise on the system. We take this stochastic force to be Gaussian, i.e.

$$\langle f(t) \rangle = 0$$

$$\langle f(t)f(t') \rangle = \lambda \delta(t - t')\,,$$

where λ parametrises the strength of the noise. We want to be able to find autocorrelation functions of the random variable $x(t)$ i.e. $\langle x(t_1) \dots x(t_n) \rangle$ which is equivalent to solving the Langevin equation, calculating the n-product of $x(t)$ for different realisations of $f(t)$ and then in turn averaging over the stochastic force $f(t)$. This can

be formally written as

$$\langle x(t_1)\ldots x(t_n)\rangle = \langle \bar{x}_{[f]}(t_1)\ldots \bar{x}_{[f]}(t_n)\rangle_f$$

where $\bar{x}_{[f]}$ is a solution to equation C.1 for a specific realisation of $f(t)$. It is assumed that the initial conditions $x(t_n) = x_n$ are given. If we only know the probability distribution of the initial conditions, then this required averages should also be taken at this point.

One can also derive a correlation function from a generating functional

$$\mathcal{Z}\left[J(t)\right] = \left\langle e^{\int_t J(t)\bar{x}(t)_{[f]}}\right\rangle_f \tag{C.2}$$

by taking the n'th order functional derivative

$$\frac{\delta^n \mathcal{Z}[J(t)]}{\delta J(t_n)\ldots \delta J(t_1)}\bigg|_{J=0} = \left\langle \bar{x}_{[f]}(t_1)\ldots \bar{x}_{[f]}(t_n)e^{\int_t J(t)\bar{x}(t)_{[f]}}\right\rangle_f\bigg|_{J=0}$$

$$= \left\langle \bar{x}_{[f]}(t_1)\ldots \bar{x}_{[f]}(t_n)\right\rangle_f ,$$

where $J[0] = 1$ by definition and the measure of $\mathcal{Z}$ is unity. One refers to $J(t)$ as the source term. Of course we are still left with the problem of solving the Langevin equation and the purpose of this formalism is to avoid having to explicitly do so. To find a functional representation of our system we will introduce a functional integral over $x(t)$ and a Dirac Delta functional. Doing so we find that equation C.2 can be transformed as follows,

$$\left\langle e^{\int_t J(t)\bar{x}(t)_{[f]}}\right\rangle_f = \left\langle \int \mathcal{D}x(t)\delta\left[x - \bar{x}_{[f]}(t)\right] e^{\int_t J(t)x(t)}\right\rangle_f .$$

The stochastic dependence is only via the particular solutions $\bar{x}_{[f]}$ and thus we only have to take the stochastic average of these terms. Doing so we find for the generating functional

$$\mathcal{Z}[J(t)] = \int \mathcal{D}x(t) \left\langle \delta\left[x - \bar{x}_{[f]}(t)\right]\right\rangle_f e^{\int_t J(t)x(t)} .$$

The key point of this formalism is to now transform the delta functional from a functional of the solutions of the system to a functional of the equation of motion (C.1). We will assume there there is one unique solution and will point out where a problem may arise with this argument.

Let us first consider the change of variables for a delta functional. It will be sufficient to study the ordinary delta function seeing as we can always slice the delta functional into a set of ordinary delta functions. Consider the integral

$$\int_{\mathbb{R}} dx\, f(x)\delta(g(x))$$

where $f(x)$ is any test function and $g(x)$ has real roots x_i, whereas the derivative $g'(x)$ has no real roots. Thus $\delta(g(x))$ is non-zero only for $x = x_i$, which leads to

$$\int_{\mathbb{R}} dx\, f(x)\delta(g(x)) = \sum_i \int_{x_i-\epsilon}^{x_i+\epsilon} dx\, f(x)\delta(g(x))\,,$$

where $\epsilon > 0$ is some positive infinitesimal number. We may now introduce the change of variables $u = g(x)$ and $du = |g'(x)|\, dx$ which leads to

$$\sum_i \int_{g(x_i-\epsilon)}^{g(x_i+\epsilon)} \frac{1}{|g'(x)|} du\, \delta(u) f(g^{-1}(u)) = \sum_i \frac{f(x_i)}{|g'(x_i)|}\,.$$

This should all for any test function $f(x)$ and thus

$$\delta(g(x)) = \sum_i \frac{\delta(x - x_i)}{|g'(x_i)|}.$$

Where in turn we may now generalise the result to functionals, which leads to

$$\sum_i \delta\left[y(t) - y_i'(t)\right] = \delta\left[G(y(t))\right] \left|\det \frac{\delta G}{\delta y(t)}\right|\,,$$

where $y_i'(t)$ are the simple roots of $G(y(t))$.

For the rest of this formalism to hold, we have to assume to that there is only one unique solution and that the Jacobian $\frac{\delta G}{\delta y(t)}$ is always positive, i.e.

$$\det \frac{\delta G}{\delta y(t)} = \left|\det \frac{\delta G}{\delta y(t)}\right| \quad \forall y(t)\,.$$

Of course one might end up with a pathological system where these conditions might not hold.

For the type of systems we want to consider, we will show that the Jacobian can be chosen to always be positive. We refer the reader to an article by Tarski[41] for more rigorous details on the functional delta and functional Fourier transformation. The derivations presented up to now are sufficient for our purposes. We now turn

to the transformation of the delta functional in our generating functional

$$\delta\left[x(t) - \bar{x}_{[f]}(t)\right] = \delta[\hat{L}(x)]\det\frac{\delta\hat{L}}{\delta x(t)}$$

where $\bar{x}_{[f]}(t)$ is the only functional form that is a solution to $\hat{L}(x)$ with

$$\hat{L}(x) \equiv \frac{dx(t)}{dt} - F(x(t)) - f(t)\,.$$

The quantity $\det\frac{\delta\hat{L}}{\delta x(t)}$ is a differential operator given by

$$\frac{\delta\hat{L}[(x(t)]}{\delta x(t')} = \left[\frac{d}{dt} - \frac{df(x(t))}{dx}\right]\delta(t - t')\,,$$

where we see that it is independent of the stochastic force f. Our generating functional at this point is now given by

$$\mathcal{Z}[J(t)] = \int \mathcal{D}x(t)\det\left(\frac{\delta L}{\delta x(t)}\right)\langle\delta\left[L(x(t))\right]\rangle_f\, e^{\int_t J(t)x(t)}$$

where it is still required that we explicitly deal with the Jacobian. This can be done introducing Grassmann integrals[40], but we will follow the technique presented by Jouvet and Phythian[19]. We begin this discussion by thinking of our formalism as limit process. The time interval from 0 to T can be divided into N subintervals of equal length $l = T/N$ and we can replace our Langevin equation C.1 with a finite difference equation for example

$$\frac{x_{n+1} - x_n}{l} = F(x_n) + f_n$$

where the functional Jacobian that relates $\{f_n\}$ to $\{x_n\}$ is now the limit of the ordinary Jacobian

$$\det\left(\frac{\partial f_n}{\partial x_m}\right) = \frac{1}{l^N}$$

as $N \to \infty$. The functional integral is also now defined in its usual sense of N integrals over $x_1 \ldots x_N$ as $N \to \infty$. Of course we can choose any other discretisation process and get a different ordinary Jacobian. It is assumed that in the continuum limit that all discretisation processes lead to the same end result and thus we can choose the functional Jacobian as unity.

The generating functional

$$\mathcal{Z}[J(t)] = \int \mathcal{D}x(t) \left\langle \delta\left[L(x(t))\right] \right\rangle e^{\int_t J(t)x(t)}$$

can now be rewritten using the functional Fourier transformation which results in

$$\mathcal{Z}[J(t)] = \int \mathcal{D}x(t)\mathcal{D}\hat{x}(t) \left\langle e^{i\int_t \hat{x}(t)L(x(t))} \right\rangle e^{\int_t J(t)x(t)} ,$$

where $\hat{x}(t)$ is now an auxiliary field that couples to the system. Finally one can introduce the probability distribution for the Gaussian noise

$$P\left[f(t)\right] = \int \mathcal{D}f e^{-\frac{1}{2\lambda}\int_t f^2(t)}$$

to obtain the final expression

$$\mathcal{Z}[J(t)] = \int \mathcal{D}x(t)\mathcal{D}\hat{x}(t)\mathcal{D}f e^{-\frac{1}{2\lambda}\int_t f^2(t) + i\int_t \hat{x}(t)L(x(t)) + \int_t J(t)x(t)} .$$

One is now able to explicitly average over the stochastic force by integrating over f. Doing so one will be left with

$$\mathcal{Z}[J(t)] = \int \mathcal{D}x(t)\mathcal{D}\hat{x}(t) e^{-\frac{\lambda}{2}\int_t \hat{x}^2 + i\int_t \hat{x}[\dot{x} - F(x(t))]} ,$$

where one may now interpret $\hat{x}(t)$ as a Gaussian fluctuating field that couples to the system.

In practise one will not be able to calculate all the functional integrals, but one can employ the various approximation schemes associated with functional integrals in quantum theory. In our case we will only deal with 2-point correlation functions and given our functional form of the noise and Langevin equation, we do not have to explicitly integrate over our dynamical quantity for which we are seeking the correlation function. We always aim to find Gaussian approximations for our systems and thus integrating out all the other fields is sufficient as the functional derivatives with respect to the source term will just return the inverse of the pre-factor associated with the square of the dynamical quantity at hand. We have only presented this formalism for a single variable system, but it generalises to more degrees of freedom quite naturally using matrix equations of the same functional form.

Appendix D

Details of Flexible Chain Calculation

D.1   Linearisation

Consider the expression:

$$\gamma_r \frac{\partial r(s,t)}{\partial t} - \frac{3k_B T}{l} \frac{\partial^2 r(s,t)}{\partial s^2} + k\left(r(s,t) - X\right)\delta(s - \sigma(t)),$$

where we may now use equations 2.7 and 2.8 to rewrite it as

$$\gamma_r \frac{\partial \rho(t)}{\partial t} - \frac{3k_B T}{l} \frac{\partial^2 r_\infty(s)}{\partial s^2} - \frac{3k_B T}{l} \frac{\partial^2 \rho(s,t)}{\partial s^2} + k\left(r_\infty(s) + \rho(s,t) - X\right)\delta(s - \sigma_\infty - \Delta(t)).$$

Expanding the Dirac Delta function up to first order in $\Delta(t)$ results in

$$\begin{aligned}
&\gamma_r \frac{\partial \rho(t)}{\partial t} - \frac{3k_B T}{l} \frac{\partial^2 r_\infty(s)}{\partial s^2} - \frac{3k_B T}{l} \frac{\partial^2 \rho(s,t)}{\partial s^2} \\
&+ k\left(r_\infty(s) + \rho(s,t) - X\right)\left[\delta(s - \sigma_\infty) - \Delta(t)\delta'(s - \sigma_\infty)\right] \\
&= \gamma_r \frac{\partial \rho(t)}{\partial t} - \frac{3k_B T}{l} \frac{\partial^2 r_\infty(s)}{\partial s^2} - \frac{3k_B T}{l} \frac{\partial^2 \rho(s,t)}{\partial s^2} \\
&+ k\left(r_\infty(s) + \rho(s,t) - X\right)\left[\delta(s - \sigma_\infty) - \Delta(t)\delta'(s - \sigma_\infty)\right],
\end{aligned}$$

where all higher order fluctuation terms can be neglected to result in

$$\begin{aligned}
&\gamma_r \frac{\partial \rho(t)}{\partial t} - \frac{3k_B T}{l} \frac{\partial^2 r_\infty(s)}{\partial s^2} - \frac{3k_B T}{l} \frac{\partial^2 \rho(s,t)}{\partial s^2} + k\left(r_\infty(s) + \rho(s,t) - X\right)\delta(s - \sigma_\infty) \\
&- k\left(r_\infty(s) + \rho(s,t) - X\right)\Delta(t)\delta'(s - \sigma_\infty).
\end{aligned}$$

D.2   Fourier Transformation

We would like to briefly discuss how various terms of our model will transform under the Fourier transformation. Let us first consider integrals of the form

$$\int dt\, f(t)g(t)\,,$$

where $f(t)$ and $g(t)$ are square-integrable functions. Introducing a Dirac Delta function we may rewrite this as

$$\int dt dt'\, f(t)\delta(t -' t)g(t')$$

and then raise the argument of the delta function into an exponent using a Fourier transformation. Doing so results in

$$\int dt dt' d\omega\, f(t) \exp\left(\omega(t - t')\right) g(t') =$$
$$\int dt dt' d\omega\, f(t) \exp\left(\omega t\right) \exp\left(-\omega t'\right) g(t')\,,$$

where we may perform the integrals over t and t', which leads to

$$\int d\omega\, f(\omega)g(-\omega)\,.$$

Note that we integrate over the entire real line and thus the result after integration does not dependent on the sign of ω in the functions $f(\omega)$ and $g(\omega)$ i.e.

$$\int d\omega\, f(\omega)g(-\omega) = \int d\omega\, f(-\omega)g(\omega)\,.$$

Terms of the form

$$\int dt\, f(t)\,,$$

may be rewritten in the a frequency basis. First let us introduce the inverse Fourier transformation such that

$$\int dt\, f(t) = \int dt d\omega\, \tilde{f}(\omega) \exp\left(i\omega t\right)\,.$$

Performing the integral over t results in

$$= \int dw\, \tilde{f}(\omega)\delta(\omega)$$

and integrating over ω we are left with

$$\int dt\, f(t) = \tilde{f}(0)\,.$$

D.3 Integration over spatial variable

In this section we will provide details on integrating over the spatial variable s. Consider for example the term

$$\sum_{m,m'}^{\infty} \tilde{b}_m(\omega)\tilde{b}_{m'}(-\omega)\sin\frac{\pi m s}{L}\sin\frac{\pi m' s}{L}\,.$$

Integrating over s and making use of orthogonality relations of the sines, we find that

$$\sum_{m,m'}^{\infty} \tilde{b}_m(\omega)\tilde{b}_{m'}(-\omega)\frac{L}{4}\delta_{mm'} = \sum_{m}^{\infty} \tilde{b}_m(\omega)\tilde{b}_m(-\omega)\frac{L}{4}\,.$$

The only other type of term we have to deal with explicitly is

$$\int_{s,\omega} \sum_{m}^{\infty} \tilde{b}_m(-\omega)\sin\frac{\pi m s}{L}k\tilde{\Delta}(r_\infty - X)\delta'(s - \sigma_\infty)\,,$$

where we may integrate by parts to find that

$$= \cancel{\int_{\omega} \sum_{m}^{\infty} \tilde{b}_m(-\omega)\sin\frac{\pi m s}{L}k\tilde{\Delta}(r_\infty - X)\delta(s - \sigma_\infty)\Big|_{-\infty}^{\infty}}$$
$$- \int_{s,\omega} \delta(s - \sigma_\infty)\frac{\partial}{\partial s}\left(\sum_{m}^{\infty} \tilde{b}_m(-\omega)\sin\frac{\pi m s}{L}k\tilde{\Delta}(r_\infty(s) - X)\right)$$

$$= -\int_{s,\omega} \delta(s - \sigma_\infty)\frac{\pi m}{L}\sum_{m}^{\infty} \tilde{b}_m(\omega)\cos\frac{\pi m s}{L}k\tilde{\Delta}\left(r_\infty(s) - X\right)$$
$$- \int_{s,\omega} \delta(s - \sigma_\infty)\sum_{m}^{\infty}\sin\frac{\pi m s}{L}k\tilde{\Delta}\frac{\partial r_\infty(s)}{\partial s}$$

$$= -\int_{\omega} \frac{\pi m}{L}\sum_{m}^{\infty} \tilde{b}_m(\omega)\cos\frac{\pi m \sigma_\infty}{L}k\tilde{\Delta}\left(r_\infty(\sigma_\infty) - X\right) - \int_{\omega} \sum_{m}^{\infty}\sin\frac{\pi m \sigma_\infty}{L}k\tilde{\Delta}\frac{\partial r_\infty}{\partial s}\Big|_{s=\sigma_\infty}\,.$$

We cross out the term in the above equation because we assume that $r_\infty(s)$ is square-integrable.

D.4   Hubbard-Stratonovich

Consider the expression

$$
k^2 \left(\sum_m \sin^2 \frac{\pi m \sigma_\infty}{L} \right) \left(\sum_m \sin \frac{\pi m \sigma_\infty}{L} \tilde{a}_m \right)^2
$$
$$
- 2k \frac{3k_B T}{l} \frac{\pi^2}{2L} \sum_m m^2 \tilde{a}_m \sin \frac{\pi m \sigma_\infty}{L} \sum_{m'} \tilde{a}_{m'} \sin \frac{\pi m' \sigma_\infty}{L}
$$

and note that we may complete the square to get

$$
\left[k \left(\sum_m \sin^2 \frac{\pi m \sigma_\infty}{L} \right)^{1/2} \left(\sum_m \sin \frac{\pi m \sigma_\infty}{L} \tilde{a}_m \right) \right.
$$
$$
\left. - \left(\sum_m \sin^2 \frac{\pi m \sigma_\infty}{L} \right)^{-1/2} \sum_m m^2 \sin \frac{\pi m \sigma_\infty}{L} \tilde{a}_m \frac{3k_B T}{l} \frac{\pi^2}{2L} \right]^2
$$
$$
- \left[\left(\sum_m \sin^2 \frac{\pi m \sigma_\infty}{L} \right)^{-1/2} \sum_m m^2 \sin \frac{\pi m \sigma_\infty}{L} \frac{3k_B T}{l} \frac{\pi^2}{2L} \tilde{a}_m \right]^2 .
$$

We can now write our generating functional as

$$
\langle \mathcal{Z} \rangle = \int \prod_m \mathcal{D}\tilde{a}_m \mathcal{D}\tilde{\Delta} \exp \left\{ -\frac{1}{\lambda_r} \int_\omega \sum_m \tilde{a}_m^2 \left(\omega^2 \gamma_r^2 \frac{L}{4} + \left(\frac{3k_B T}{l} \right)^2 \frac{\pi^4 m^4}{4L^2} \right) \right.
$$
$$
+ 2 \int_\omega \sum_m \tilde{a}_m \tilde{\Delta} \left[\phi_m \left(\frac{1}{\lambda_r L} k \frac{3k_B T}{l} \frac{\pi^2 m^2}{2L} - \frac{1}{\lambda_r L} k^2 \sin \frac{\pi m \sigma_\infty}{L} \sum_{m'} \sin \frac{\pi m' \sigma_\infty}{L} \right) \right.
$$
$$
\left. - \frac{k^2}{2\lambda_\sigma} \left(\left(\frac{\partial r_\infty(\sigma_\infty)}{\partial s} \right)^2 + (r_\infty(\sigma_\infty) - X) \frac{\partial^2 r_\infty(\sigma_\infty)}{\partial s^2} \right) \phi_m \right] - \int_\omega \tilde{\Delta}^2 \sum_m \left[\frac{k^2}{\lambda_r L} \phi_m^2 \right.
$$
$$
\left. + \frac{1}{2\lambda_\sigma} \omega^2 \gamma_\sigma^2 + k^2 \left(\left(\frac{\partial r_\infty(\sigma_\infty)}{\partial s} \right)^2 + (r_\infty(\sigma_\infty) - X) \frac{\partial^2 r_\infty(\sigma_\infty)}{\partial s^2} \right)^2 \right]
$$

$$
- \frac{1}{\lambda_r L} \int_\omega \left[k \left(\sum_m \sin^2 \frac{\pi m \sigma_\infty}{L} \right)^{1/2} \left(\sum_m \sin \frac{\pi m \sigma_\infty}{L} \tilde{a}_m \right) \right.
$$
$$
\left. - \left(\sum_m \sin^2 \frac{\pi m \sigma_\infty}{L} \right)^{-1/2} \sum_m m^2 \sin \frac{\pi m \sigma_\infty}{L} \tilde{a}_m \frac{3k_B T}{l} \frac{\pi^2}{2L} \right]^2
$$
$$
- \frac{1}{\lambda_r L} \int_\omega \left[\left(\sum_m \sin^2 \frac{\pi m \sigma_\infty}{L} \right)^{-1/2} \sum_m m^2 \sin \frac{\pi m \sigma_\infty}{L} \frac{3k_B T}{l} \frac{\pi^2}{2L} \tilde{a}_m \right]^2
$$
$$
\left. - \frac{1}{\lambda_\sigma} \int_\omega k^2 \left(\sum_m \phi_m \tilde{a}_m \right)^2 \right\},
$$

where we may now introduce three Gaussian fluctuating fields ξ, ψ and χ to rewrite the above in to the following functional form:

$$
\langle \mathcal{Z} \rangle = \int \prod_m \mathcal{D}\tilde{a}_m \mathcal{D}\tilde{\Delta} \mathcal{D}\xi \mathcal{D}\psi \mathcal{D}\chi \exp \left\{ -\frac{1}{\lambda_r} \int_\omega \sum_m \tilde{a}_m^2 A_m(\omega) + \int_\omega \sum_m \tilde{a}_m^2 \tilde{\Delta}^2 \tilde{\Delta} B_m(\omega) \right.
$$
$$
- \int_\omega \sum_m \tilde{\Delta}^2 C_m + i \int_\omega \sum_m \tilde{a}_m D_m \xi + \int_\omega \sum_m \tilde{a}_m E_m \psi + i \int_\omega \sum_m \tilde{a}_m F_m \chi
$$
$$
\left. - \frac{\lambda_r L}{4} \int_\omega \xi^2 - \frac{\lambda_r L}{4} \int_\omega \psi^2 - \frac{\lambda_\sigma}{2} \int_\omega \chi^2 \right\},
$$

where

$$
A_m(\omega) = \omega^2 \gamma_r^2 \frac{L}{4} + \left(\frac{3k_B T}{l} \right)^2 \frac{\pi^4 m^4}{4L^2}
$$

$$
B_m(\omega) = \phi_m \left(\frac{1}{\lambda_r L} k \frac{3k_B T}{l} \frac{\pi^2 m^2}{2L} - \frac{1}{\lambda_r L} k^2 \sin \frac{\pi m \sigma_\infty}{L} \sum_{m'} \sin \frac{\pi m' \sigma_\infty}{L} \right)
$$
$$
- \frac{k^2}{2\lambda_\sigma} \left(\left(\frac{\partial r_\infty(\sigma_\infty)}{\partial s} \right)^2 + (r_\infty(\sigma_\infty) - X) \frac{\partial^2 r_\infty(\sigma_\infty)}{\partial s^2} \right) \phi_m
$$

$$
C_m(\omega) = \frac{k^2}{\lambda_r L} \phi_m^2 + \frac{1}{2\lambda_\sigma} \omega^2 \gamma_\sigma^2 + k^2 \left(\left(\frac{\partial r_\infty(\sigma_\infty)}{\partial s} \right)^2 + (r_\infty(\sigma_\infty) - X) \frac{\partial^2 r_\infty(\sigma_\infty)}{\partial s^2} \right)^2
$$

$$
D_m(\omega) = k \left(\sum_m \sin^2 \frac{\pi m \sigma_\infty}{L} \right)^{1/2} \left(\sum_m \sin \frac{\pi m \sigma_\infty}{L} \tilde{a}_m \right)
$$
$$
- \left(\sum_m \sin^2 \frac{\pi m \sigma_\infty}{L} \right)^{-1/2} \sum_m m^2 \sin \frac{\pi m \sigma_\infty}{L} \tilde{a}_m \frac{3k_B T}{l} \frac{\pi^2}{2L}
$$

$$
E_m(\omega) = \left(\sum_m \sin^2 \frac{\pi m \sigma_\infty}{L} \right)^{-1/2} \sum_m m^2 \sin \frac{\pi m \sigma_\infty}{L} \frac{3k_B T}{l} \frac{\pi^2}{2L} \tilde{a}_m
$$

$$
F_m(\omega) = k \phi_m \tilde{a}_m .
$$

It is now possible to integrate over the vibrational modes of the filament $\tilde{a}_m(\omega)$, with the resulting expression given by

$$
\langle \mathcal{Z} \rangle = \int \mathcal{D}\tilde{a}_m \mathcal{D}\tilde{\Delta} \mathcal{D}\xi \mathcal{D}\psi \mathcal{D}\chi \exp \left\{ \int_\omega \sum_m \frac{\lambda_r L}{4} A_m^{-1} \left[\tilde{\Delta}^2 B_m^2 + 2i\tilde{\Delta} B_m D_m \xi + 2\tilde{\Delta} B_m E_m \psi \right. \right.
$$
$$
\left. + 2i\tilde{\Delta} B_m F_m \chi + 2i D_m E_m \xi \phi - 2 D_m F_m \xi \chi + 2i E_m F_m \psi \chi \right]
$$
$$
- \int_\omega \sum_m \tilde{\Delta}^2 C_m - \int_\omega \xi^2 \left(\frac{\lambda_r L}{4} + \sum_m \frac{\lambda_r L}{4} A_m^{-1} D_m^2 \right)
$$
$$
\left. - \int_\omega \psi^2 \left(\frac{\lambda_r L}{4} - \sum \frac{\lambda_r L}{4} A_m^{-1} E_m^2 \right) - \int_\omega \chi^2 \left(\frac{\lambda_\sigma}{2} + \sum_m \frac{\lambda_r L}{4} A_m^{-1} F_m^2 \right) \right\},
$$

where we now have to integrate over the fields ξ, ψ and χ if were to find correlation functions of $\tilde{\Delta}(\omega)$. Unfortunately these fields are coupled in a non-trivial way and while this procedure is analytically possible, the resulting mathematical expression is too complicated to be of any practical use.

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