

# Spontaneous Flow Transitions in Active Polar Gels

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# Abstract

Active polar gels are a type of viscoelastic soft material formed by polar filaments which are constantly driven out of equilibrium by the consumption of chemical fuel such as ATP. Following the approach of Voituriez *et al*, a generic hydrodynamic theory relying on symmetry arguments only was used to study the effects of quasi one-dimensional confinement on active polar gels. The phenomenological theory based on liquid crystal hydrodynamics is motivated by the dynamics of actin filaments in the cytoskeleton which plays an important role in many cellular processes. Using different boundary conditions, Fredericks-like flow transitions driven by the activity are expected. These transitions occur from homogeneously polarized static states in thin gel layers to flowing states with polarization tilts in larger layers. In addition, a few notes on the limitations of this work and possibilities for additional work are briefly expounded on at the end.

# Acknowledgements

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All concepts taken from external sources are mentioned in the text and fully referenced at the end of the report. Diagrams and Tables adapted from the internet and other sources are also accordingly labelled.

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# Chapter 1

## Introduction

### 1.1 Liquid Crystals

It is widely believed that Matter exists in three distinct and interconvertible phases: The Solid, Liquid and Gaseous phases; with the major distinction between them given by the degree of order (or disorder) in their molecular arrangements. In actual fact however, this is not strictly true for all materials because a wide range of natural and synthetic substances exist that do not display a simple transition from the solid phase to the liquid phase, but rather go through a series of intermediate phases (called *mesophases* or *mesomorphic phases*). These mesophases display properties that are intermediate between the solid and liquid states; and are therefore referred to as **Liquid Crystals**. A liquid Crystal for example may flow like a liquid but does not possess the isotropy an ordinary liquid displays, it may also have interesting optical properties similar to a crystalline material but will not display long-ranged three dimensional order like most crystalline materials. From a microscopic point of view, the major difference between a liquid crystalline phase, the crystalline phase and the liquid phase stems from their molecular arrangement. In a crystalline solid there is long-ranged three dimensional order with a regular arrangement of atoms on a lattice and in a liquid the molecules are oriented in random directions with weak intermolecular forces in all directions. However, in a liquid crystal the intermolecular forces in the crystalline solid are not the same in all directions; in some directions the forces are weaker than in other directions. As such a material is heated, the increased molecular motion overcomes the weaker forces first, but its molecules remain bound by the stronger forces. This produces a molecular arrangement that is random in some directions and regular in others thus leading to liquid-like order in at least one direction and variation in physical

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properties along others (i.e *anisotropy*)

## 1.2 Types of Liquid Crystals

Many Liquid Crystal materials are organic compounds that exhibit liquid crystalline phases either as a function of temperature or concentration of solute molecules in a solvent. The former class of materials are termed *Thermotropic* and the latter, *Lyotropic*. Thermotropic phases usually occur in a certain temperature range, above which the material behaves as an isotropic liquid and below which it forms a regular crystal[1]. Lyotropic phases can be formed in amphiphilic compounds by varying the volume balance between its constituents. There are also certain low-melting inorganic materials such as Zinc Chloride which when mixed with long chain soap-like molecules form mesophases with liquid crystalline behaviour as a function of both temperature and organic-inorganic composition ratio. Such liquid crystals are termed *metallotropic*. Liquid crystals are examples of *mesogenic* materials because they form mesophases under appropriate conditions; this also implies that not all liquid crystal materials will be in liquid crystal phases under all conditions. The major building blocks for liquid crystalline materials have been identified as either small rod-like or disk-like organic molecules, long helical rods in a liquid substrate, polymers and other associated structures such as the amphiphilic molecules above[2].

Various classifications for the different types of liquid crystals have been proposed, the most widely used are as follows:

### 1.2.1 Nematic Liquid Crystals

Nematics are the most commonly encountered liquid crystalline mesophase. In nematics, the long axis of the rod-like constituent molecules tend to align themselves parallel to each other along a common direction called the *anisotropic axis*. This imposes long ranged directional order even though there is no positional order; implying that molecules are free to flow and the centre of mass positions remain randomly distributed as in an isotropic liquid. In many cases, a unit vector called the *director*  $p$  is used to describe the average local direction of molecular alignment; it is often defined without polarity such that its sign has no physical significance i.e the states  $p$  and  $-p$  are indistinguishable. Nematic liquid crystals get their name from the thread-like topological defects (formally called *disclinations*) corresponding to lines of singularity in the director alignment. Examples of extensively studied ne-



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nematic liquid crystals are *p*-azoxyanisole (PAA) and 4-methoxybenzylidene-4'-butylaniline (MBBA). Mixtures of Nematic liquid crystals have interesting optical properties and are often used in liquid crystal displays (LCDs) because they can be easily aligned by external magnetic and electric fields.

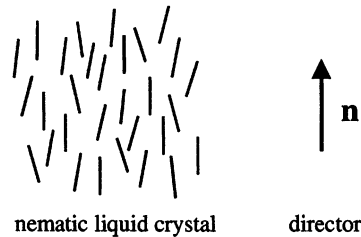


Figure 1.1: Schematic representation of Molecular arrangement in a nematic liquid crystal, the short bold lines represent the molecules

### 1.2.2 Chiral Nematic Liquid Crystals

Chiral nematics exhibit a property called *chirality* or *handedness* meaning they exhibit a twisting of the constituent molecules perpendicular to the director, with the molecular axis parallel to the director giving rise to a helical structure. The structure of chiral nematics is a result of the chiral nature of the constituent molecules. Chiral molecules are different from their mirror images and therefore have either a right-handed or left-handed sense, such molecules are also called *enantiomorphs*. The helical axis of a chiral nematic is often assumed to be in the horizontal direction and the helix itself may be either right-handed or left-handed. At a given temperature, a sample of a cholesteric liquid crystal always produces helices of the same sense but there are cholesterics whose handedness of helix can be changed by varying the temperature[1]. The variation in the director alignment in a chiral nematic sample has a periodicity  $\frac{L}{2}$  where  $L$  is the *helical pitch* defined as the distance measured along the helical axis over which the director rotates through a full  $2\pi$  radians, the periodicity is half of this distance because the states described by  $p$  and  $-p$  are identical.

The chiral pitch is also affected by the concentration of chiral dopants in the liquid crystal host material i.e an achiral liquid crystal host material will form a chiral nematic if doped with chiral molecules.

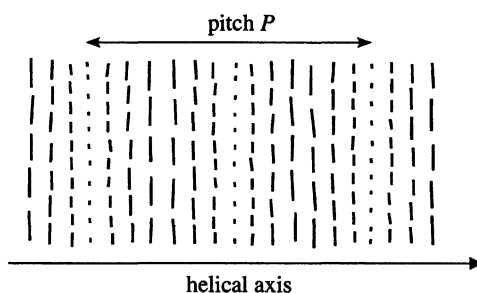


Figure 1.2: Schematic representation of Molecular arrangement in a chiral nematic liquid crystal

### 1.2.3 Smectic Liquid Crystals

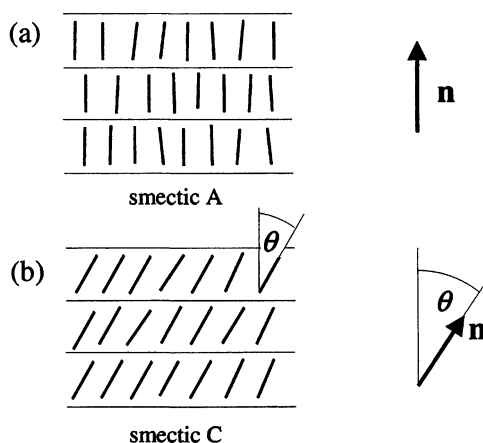


Figure 1.3: Schematic representation of Molecular arrangement in (a) smectic A and (b) smectic C liquid crystal phases

Smectics also derive their name from a greek word meaning “soap”; this is due to the fact that they have mechanical properties similar to those of soaps. They have well defined layered structures (with a fixed interlayer spacing) that can slide over one another similar to soap. Smectics are thus more ordered than nematics and for a given material the smectic phase occurs at temperatures below that for which a nematic phase is observed [1]. Several types of smectics have been identified but the two most common are smectics A and C. In a smectic A phase, the molecules are arranged in layers where

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the director is on an average perpendicular to the layers and parallel to the layer normal.

In a smectic C phase (labelled b), the director is tilted at an angle  $\theta$  relative to the layer normal; in both cases the director has no polarity i.e  $p$  and  $-p$  are indistinguishable.

### 1.3 Biological Liquid Crystals

Many biological systems exhibit liquid crystalline behaviour; in particular, lyotropic phases are found in many living systems. Very common biologically occurring liquid crystalline materials are biological cell membranes where the constituent molecules are perpendicular to the flexible surface of the membrane, such phases often host important proteins such as receptors which float partly inside or outside the membrane itself. Other biological liquid crystal phases are found in DNA, polypeptides and the protein solution spiders use to make silk.

Recently, the physics of liquid crystals has been applied to modelling the behaviour of the cellular *cytoskeleton*, the cytoskeleton is a proteinous network of actin filaments, intermediate filaments and microtubules contained within the cellular cytoplasm. It provides mechanical strength and plays an important role in cellular motility and cell division [3, 4].

### 1.4 The Distortion Free Energy

The previous sections describe the director as a unit vector which describes the average direction of alignment of the molecules in a liquid crystal sample. however, that description is best suited to an ideal, uniaxial nematic liquid crystal [1]. In most practical cases the director alignment is non ideal because of constraints imposed on the sample by say external electric and magnetic fields, or by interaction with limiting surfaces such as the walls of a containing vessel. As such, it is often useful to treat liquid crystals theoretically using a continuum approach; i.e ignoring details of the molecular structure in favour of a coarse grained description of the system. This is especially useful because the distance over which the director alignment varies significantly is often much greater than the molecular dimensions[2]. Two steps involved in this continuum treatment are:

1. The construction of a distortion “free” energy (density) which is a quantity that gives a measure of the *helmholtz free energy* (per unit volume) of the liquid crystal. The distortion is taken with respect to

its preferred conformation with all its molecules roughly parallel to a common axis. This free energy is also commonly called the **Frank free energy** or the **Frank-Oseen elastic energy**. Many standard texts [1, 2] give a full explanation and derivation of this free energy in terms of gradients and curls of the director and some *elastic constants*  $K_i$  called **Frank elastic constants**. The frank elastic constants are dependent on the particular liquid crystal in question and the temprature[1].

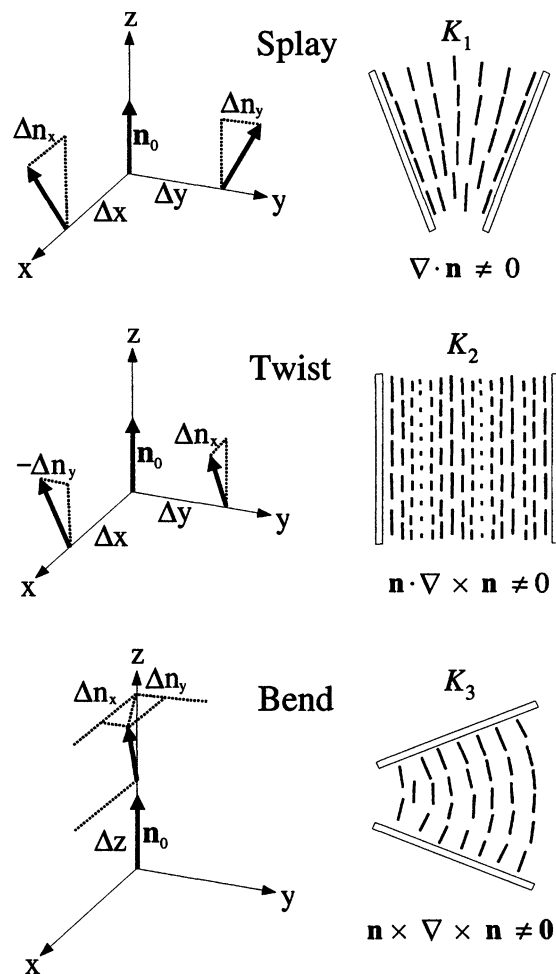


Figure 1.4: Reorientations of the director alignment corresponding to different distortions (left) and the corresponding two-dimensional cross sections; the short bold lines represent the director

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For a non-chiral nematic liquid crystal, the free energy density  $F_d$  is given in terms of the director  $\mathbf{p}$  as:

$$\mathcal{F}_d = \frac{K_1}{2}(\text{div } \mathbf{p})^2 + \frac{K_2}{2}(\mathbf{p} \cdot \text{curl } \mathbf{p})^2 + \frac{K_3}{2}(\mathbf{p} \times \text{curl } \mathbf{p})^2 \quad (1.1)$$

The elastic constants  $K_i$  ( $i = 1 - 3$ ) describe the three most important kinds of distortions found in liquid crystals namely:

- (a)  $K_1$  for distortions where  $\text{div } \mathbf{p} \neq 0$  (*splay*)
- (b)  $K_2$  for distortions where  $\mathbf{p} \cdot \text{curl } \mathbf{p} \neq 0$  (*twist*)
- (c)  $K_3$  for distortions where  $\mathbf{p} \times \text{curl } \mathbf{p} \neq 0$  (*bend*)

A combination of these three constants can be used to represent any arbitrary deformation in a liquid crystal. The elastic constants have a dimension of energy per unit length and are roughly of the same order of magnitude  $10^{-6}$  dynes or  $10^{-11}$ N. The full form of (1.1) is extremely difficult to solve exactly and as such it is often useful to assume that all the frank elastic constants are equal[2]. This is called the **one constant approximation** and it leads to the more compact form:

$$\mathcal{F}_d = \frac{1}{2}K [(\text{div } \mathbf{p})^2 + (\text{curl } \mathbf{p})^2] = \frac{1}{2}K \partial_{\alpha} p_{\beta} \partial_{\alpha} p_{\beta} \quad (1.2)$$

The case of chiral nematics is slightly different, the second term on the right side of 1.1 (called the twist term) has to be modified to take into account the fact that the constituent molecules are achiral. The free energy density is then:

$$\mathcal{F}_d(\text{twist}) = \frac{1}{2}K_2(\mathbf{p} \cdot \text{curl } \mathbf{p} + q_0)^2$$

$q_0$  represents the *helical wavevector* which changes sign depending on whether the helical structure is left-handed or right-handed. The helical pitch is given by  $\frac{2\pi}{q_0}$ . Thus the chiral free energy density is given as:

$$\mathcal{F}_d = \frac{K_1}{2}(\text{div } \mathbf{p})^2 + \frac{K_2}{2}(\mathbf{p} \cdot \text{curl } \mathbf{p} + q_0)^2 + \frac{K_3}{2}(\mathbf{p} \times \text{curl } \mathbf{p})^2 \quad (1.3)$$

It is also possible to have contributions from external electric and magnetic fields due to the anisotropic electric polarizability and diamagnetic

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properties of liquid crystal molecules. Such fields can induce alignment in liquid crystal materials, which consequently decreases their free energy. Sufficiently strong electric and magnetic fields applied to an undistorted liquid crystal can lead to phase transitions called the *frederickz transitions*; this has important technological applications in liquid crystal displays[2].

2. Once the free energy has been constructed, the next step is its minimization to yield differential equations for equilibrium in terms of  $\mathbf{p}$  and its derivatives. The goal of the continuum theory of liquid crystals is to obtain possible equilibrium orientations of the director within a given sample; these correspond to the solutions of the obtained differential equations[1]. As is the usual practice in physics, the solutions with the least energy are interpreted as the physically relevant ones. We will later see that this approach is not adequate for the study of non-equilibrium or **active** systems.

## 1.5 Active Matter

The term active matter according to Menon [3] tentatively refers to *materials (either in the continuum or naturally decomposable into discrete units), which are driven out of equilibrium through the transduction of energy derived from an internal energy depot or ambient medium into work performed on the environment*. This definition implies

1. A large number of diverse systems which may be either macroscopic (e.g flocks of birds) or microscopic (e.g motile bacteria) are described by the term **active matter**.
2. It is often possible to approximate such systems into individual units (called *active particles*) which either interact with each other directly or through disturbances propagated in the medium they are immersed in.
3. Active matter possess an internal source of energy and convert it into useful work on the surroundings with a fraction dissipated as heat. Note that the energy input is internal (located on each unit) and does not act via external fields or at the boundaries. This distinguishes active systems from other driven systems such as sheared fluids and driven vortex lattices.

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The interactions between active particles often result in unusual collective behaviour such as non-equilibrium phase transitions between novel dynamical phases and large fluctuations which violate the central limit theorem. Individual active particles generally exhibit anisotropic behaviour; therefore collections of such units can form **orientationally ordered states**; an example of which is a nematic liquid crystal in thermal equilibrium. In addition, when discussing active particles terms like *active nematic* or *living liquid crystal* are commonly used. The internal energy source is typically the cause of the observed non-equilibrium behaviour in active matter and comes from the hydrolysis of a *nucleoside triphosphate* (**NTP**) such as *adenosine triphosphate* (**ATP**) or *guanosine triphosphate* (**GTP**) into their corresponding *diphosphates* with the release of energy[3].

A class of problems studied in this context include self-organised patterns formed by mixtures of **cytoskeletal filaments** and **molecular motors** in confined geometries. Such patterns include *vortices*, *asters* and *rotating spirals*; these structures require ATP for formation and sustenance and are thus constantly in a non-equilibrium state. **Active gels** provide a general means of describing active matter using a coarse-grained continuum approach on a physical viscoelastic gel constantly driven out of equilibrium by internal energy sources. A *passive* viscoelastic gel is often described by the *maxwell model* which connects the deviatoric stress  $\sigma_{\alpha\beta}$  to the strain rate  $u_{\alpha\beta}$  via:

$$\frac{\partial\sigma_{\alpha\beta}}{\partial t} + \frac{\sigma_{\alpha\beta}}{\tau} = 2Eu_{\alpha\beta} \quad (1.4)$$

Where  $E$  is a short-time shear modulus, the strain rate is defined in terms of the velocity field  $v$  as:

$$u_{\alpha\beta} = \frac{1}{2}(\partial_{\alpha}v_{\beta} + \partial_{\beta}v_{\alpha}) \quad (1.5)$$

# Chapter 2

## Active behaviour of the Cytoskeleton

### 2.1 The Cytoskeleton

The cytoskeleton is a proteinous frame contained within the cytoplasm of cells and has been known to exist in Eukaryotic cells since the first two decades of the 19th century. More recently however, analogous proteinous structures have also been identified in Prokaryotes [5, 6]. The functions of the cytoskeleton to the cell include

1. Establishing shape
2. Providing mechanical strength
3. Assisting in locomotion
4. Chromosome separation in mitosis and meiosis
5. Intracellular transport of organelles

The (eukaryotic) cytoskeleton consists of three kinds of protein filaments: *Actin Filaments*, *Intermediate filaments* and *microtubules*.

#### 2.1.1 Actin Filaments

These are filaments formed by the polymerization of actin monomers into long thin fibres (approximately  $8nm$  in diameter), because they are the thinnest of all cytoskeletal filaments, they are called *microfilaments*. Their major functions include:



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- Provision of mechanical strength to the cell via a band formed just beneath the plasma membrane
  - Generation of locomotion in certain kinds of cells such as Amoeba and white blood cells
  - Generation of cytoplasmic streaming
  - Interaction with other filaments to aid other processes such as contraction in muscular fibres

### 2.1.2 Intermediate Filaments

These cytoplasmic fibres are of intermediate size ( $\sim 10nm$  diameter) compared to microfilaments and microtubules. There are various types such as

**Keratins:** Found in Epithelial cells, which also form hair and nails

**Nuclear Lamins:** These form a stabilizing meshwork for the inner membrane of the nuclear envelope

**Vimentins:** which provide mechanical strength to muscle and other cells and;

**Neurofilaments:** which strengthen the long axons of neurons

All intermediate filaments play similar roles in the cell: the provision of a “scaffolding” for support.

### 2.1.3 Microtubules

Microtubules are straight, hollow cylindrical structures whose wall is made up of a ring of *protofilaments*, they have a diameter  $\sim 25nm$ . They are found in both animal and plant cells and can grow up to 100 times their width. The protofilaments are polymers of two dimers namely  $\alpha$ -*tubulin* and  $\beta$ -*tubulin*. Microtubules are variable in length and grow at each end by the polymerization of tubulin dimers powered by the hydrolysis of GTP and shrink at each end by the release of tubulin dimers i.e by *depolymerization*. These processes always occur more rapidly at one end, called the **plus** end than the other, called the **minus** end.

There are two types of microtubule motors

**Kinesins:** which move towards the plus end of the microtubule and;

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*Dyneins*: which move towards the minus end.

The cellular cytoskeleton has been described in [7, 8, 4] as a viscoelastic material formed by polar filaments maintained in a constant state of non-equilibrium by the consumption of chemical energy. In the Eukaryotic cytoskeleton, the constant polymerization and depolymerization of actin filaments (called *treadmilling*) forms a viscoelastic gel which interacts with ATP-powered myosin motors. We can therefore consider the “*actomyosin*” cytoskeleton as an active polar gel

## 2.2 Constitutive hydrodynamic equations of active polar gels

Different approaches have been taken in the theoretical modelling of active systems which include: detailed microscopic numerical simulations, *mesoscopic* mean-field approaches and phenomenological continuum theories where the active system is modelled in terms of a few coarse-grained fields [9]. These approaches are in fact related, since one would expect that the coarse-graining of the microscopic theory to a mesoscopic or macroscopic scale would yield similar results to those of the mesoscopic or macroscopic approaches [7]. The active gel theory of the cytoskeleton considered here can not rely on the thermodynamic approach of a free-energy minimization, but rather requires a dynamic theory which describes the local force balance in the system. This approach utilizes the phenomenological continuum description [4, 7] to build up a hydrodynamic theory; implying that the macroscopic variables of interest are dictated by conservation laws and symmetry considerations. In a polar liquid for example: the macroscopic variables to consider are the deviatoric stress  $\sigma_{\alpha\beta}$ , the velocity gradient  $u_{\alpha\beta}$  which is given in terms of spatial derivatives of the velocity field  $v$  and the local polarization field  $\mathbf{p}$  which is a vector describing the average local orientation of the molecules [2]. Other additions are the polarization rate, which arises due to the dynamics of the polarization and the orientational field  $\mathbf{h}$  which is related to the second spatial derivative of the polarization vector [7].

The constitutive hydrodynamic equations are obtained by identifying the fluxes and the corresponding conjugate generalized forces. These fluxes are generated by the forces which act on the active gel and induce motion. The flux-force relations define some material properties and characterize how the system reacts to different types of generalized forces [10]. The approaches followed in this Thesis follow the treatments in [8, 10] closely for the description of an active polar gel close to thermodynamic equilibrium. In addition,

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the expansion of fluxes in terms of their conjugate forces is limited to linear order.

### 2.2.1 Polar order, Fluxes and Forces in active gels

The polarization vector  $\mathbf{p}$  has been previously defined as a measure of the average direction of alignment of the molecules in a liquid crystal sample. In active gels, the polar nature of each actin filament allows the assignment of a unit vector in the direction from the *plus* end to the *minus* end. The local polarization field is then defined as the average of these unit vectors in the volume around each point. The thermodynamics of this polarization field can be studied from the standard free energy of a chiral nematic liquid crystal [8] which is given as :

$$F = \int \mathcal{F}_d dr \quad (2.1)$$

Using the free energy density in (1.3), we have:

$$F = \int \left[ \frac{K_1}{2} (\text{div } \mathbf{p})^2 + \frac{K_2}{2} (\mathbf{p} \cdot \text{curl } \mathbf{p} + q_0)^2 + \frac{K_3}{2} (\mathbf{p} \times \text{curl } \mathbf{p})^2 - \frac{1}{2} h_{\parallel} \mathbf{p}^2 \right] dr \quad (2.2)$$

The choice of the free-energy density (1.3) rather than (1.1) is informed by the fact that actin filaments are chiral and we would expect this asymmetry to reflect in the constitutive equations [10, 8]. Furthermore, a term of form  $k \nabla \cdot \mathbf{p}$  allowed by the vector symmetry of the polarization (called the *spontaneous splay* term) has been ignored because of anchoring effects and the assumption that the actin filaments are parallel and have random orientations. The requirement that  $\mathbf{p}^2 = 1$  is enforced by the lagrange multiplier  $h_{\parallel}$  which is the component of the molecular field parallel to the local polarization

$$h_{\alpha} = - \frac{\delta F}{\delta \mathbf{p}_{\alpha}} \quad (2.3)$$

This field also has a perpendicular component  $h_{\perp}$  which creates a torque that tends to align the polarization field. Building up a linear hydrodynamic theory for the cytoskeleton requires the identification of fluxes and their corresponding forces; after which the most general linear relations between them are established[8]. These relations are written such that they obey the symmetries of the problem. It should be noted that such a theory is macroscopic in the sense that it does not depend on microscopically defined parameters describing the action of molecular motors but rather, a few

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phenomenological parameters (called *Onsager* coefficients) which are properties of the cytoskeleton that can be measured experimentally. The fluxes are

- The total stress  $\sigma_{\alpha\beta}^{tot}$  associated with the mechanical properties of the cell
- The rate of change of the polarization  $\dot{\mathbf{P}}$  and
- The ATP consumption rate  $r$

The corresponding conjugate forces are

- The velocity gradient tensor  $\partial_\alpha v_\beta$
- The molecular field  $\mathbf{h}$  defined as the functional derivative of the free energy  $F$  with respect to the polarization  $\mathbf{p}$
- The chemical potential difference  $\Delta\mu$  between ATP and its hydrolysis products i.e the free energy gained per hydrolyzed ATP molecule

The total stress tensor  $\sigma_{\alpha\beta}^{tot}$  conjugate to the velocity gradient  $\partial_\alpha v_\beta$  is in general not symmetric, it can be decomposed into a symmetric part  $\sigma_{\alpha\beta}$  and an antisymmetric part due to the torque exerted on the order parameter  $p_\alpha$  by the field  $h_\alpha$

$$\sigma_{\alpha\beta}^{tot} = \sigma_{\alpha\beta} + \frac{1}{2}(p_\alpha h_\beta - p_\beta h_\alpha) \quad (2.4)$$

Similarly, the velocity gradient tensor  $\partial_\alpha v_\beta$  can be written as the sum of a symmetric *strain rate* tensor  $u$  and an antisymmetric *vorticity* tensor  $\omega$ :

$$\partial_\alpha v_\beta = \frac{1}{2}(\partial_\alpha v_\beta + \partial_\beta v_\alpha) + \frac{1}{2}(\partial_\alpha v_\beta - \partial_\beta v_\alpha) \quad (2.5)$$

$$= u_{\alpha\beta} + \omega_{\alpha\beta} \quad (2.6)$$

Thus our interest may be shifted to the symmetric stress tensor and the strain rate as a flux-force pair. This follows the approach of Kruse, Jülicher *et al* in refs [10] and [8]; the fluxes are decomposed into reactive and dissipative components and written in terms of the corresponding conjugate forces which have well defined signatures under time-reversal. The strain rate  $u_{\alpha\beta}$  is odd under time reversal while the field  $h_\alpha$  and the chemical potential difference  $\Delta\mu$  are positive. Dissipative fluxes have the same signature under time reversal as their conjugate forces, while reactive fluxes have the opposite signature under time reversal.

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## 2.2.2 The Maxwell model

The chemical potential difference  $\Delta\mu$  between ATP and its hydrolysis products are the source of the non-equilibrium behaviour of active gels such as the cytoskeleton [7].

$$\Delta\mu = \mu_{ATP} - \mu_{ADP} - \mu_{P_i} \quad (2.7)$$

The maxwell model is used to describe passive ( $\Delta\mu = 0$ ) viscoelastic systems, it connects the stress tensor to the strain rate via:

$$\left(1 + \tau \frac{D}{Dt}\right) \sigma_{\alpha\beta} = 2\eta u_{\alpha\beta} \quad (2.8)$$

As before,  $\eta$  and  $\tau$  are the shear viscosity and viscoelastic relaxation time, we can identify  $E = \frac{\eta}{\tau}$  with  $E$  representing the short time elastic (shear) modulus of the gel. A major difference between this form and that encountered in (1.4) is the fact that the partial derivative  $\frac{\partial}{\partial t}$  is replaced by a corrotational time derivative  $\frac{D}{Dt}$  which ensures its invariance with respect to translations and rotations; applied to the stress  $\sigma_{\alpha\beta}$ , it gives:

$$\frac{D\sigma_{\alpha\beta}}{Dt} = \frac{\partial\sigma_{\alpha\beta}}{\partial t} + (v_\gamma \partial_\gamma) \sigma_{\alpha\beta} + [\omega_{\alpha\gamma} \sigma_{\gamma\beta} + \omega_{\beta\gamma} \sigma_{\gamma\alpha}] \quad (2.9)$$

It should be noted that this includes geometrical non-linearities, this more general version is commonly called the *convected maxwell model* [10].

## 2.2.3 Dynamic equations

The general hydrodynamic equations for an active viscoelastic polar gel are given[10] by:

$$\begin{aligned} 2\eta u_{\alpha\beta} &= \left(1 + \tau \frac{D}{Dt}\right) \{ \sigma_{\alpha\beta} + \zeta \Delta\mu p_\alpha p_\beta + \zeta' \Delta\mu p_\gamma p_\gamma \delta_{\alpha\beta} + \bar{\zeta} \Delta\mu \delta_{\alpha\beta} - \tau A_{\alpha\beta} \} \\ &\quad - \frac{\nu_1}{2} (p_\alpha h_\beta + p_\beta h_\alpha) - \bar{\nu} p_\gamma h_\gamma \delta_{\alpha\beta} \end{aligned} \quad (2.10)$$

$$\left(1 - \tau^2 \frac{D^2}{Dt^2}\right) \frac{Dp_\alpha}{Dt} = \left(1 - \tau^2 \frac{D^2}{Dt^2}\right) \left(\frac{h_\alpha}{\gamma} + \lambda p_\alpha \Delta\mu\right) - \left(1 - \tau \frac{D}{Dt}\right) (\nu u_{\alpha\beta} p_\beta + \bar{\nu} u_{\beta\beta} p_\alpha) \quad (2.11)$$

$$r = \zeta p_\alpha p_\beta u_{\alpha\beta} + \bar{\zeta} u_{\alpha\alpha} + \zeta' p_\alpha p_\alpha u_{\beta\beta} + \Lambda \Delta\mu + \lambda p_\alpha h_\alpha \quad (2.12)$$

This set of equations is complimented by the force balance condition:

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$$\partial_\alpha (\sigma_{\alpha\beta} - \Pi\delta_{\alpha\beta}) = 0 \quad (2.13)$$

(2.10) is a generalization of the maxwell model to active polar systems; it implies that the activity (characterized by the coefficients;  $\zeta$ ,  $\zeta'$  and  $\bar{\zeta}$ ) generates a finite strain rate. It also implies the generation of a non-trivial stress tensor even in the absence of external flows[10]. Thus we conclude that the hydrolysis of ATP can generate forces and material flow via the action of elements such as molecular motors. The polarization dynamics given by (2.11) also contains an active term described by  $\lambda$ ; the coupling between flow and polarization is described by  $\nu$  and  $\bar{\nu}$ . Note that the rotational viscosity  $\gamma$ , the coupling coefficients between flow and polarization:  $\nu$  and  $\bar{\nu}$  are standard liquid crystal parameters[2]. In (2.12) the ATP consumption rate proportional to  $\Delta\mu$  is characterized by  $\Lambda$  but it is also coupled to the gel flow and the field  $\mathbf{h}$  acting on  $\mathbf{p}$ . The force balance condition (2.13) shows that there are two local forces acting on the gel: the stress  $\sigma_{\alpha\beta}$  and the pressure  $\Pi$  which ensures that the gel is incompressible[11]. In the viscous limit we set  $\tau = 0$ , leading to a simplification of (2.10) and (2.11) thus:

$$\begin{aligned} 2\eta u_{\alpha\beta} &= \sigma_{\alpha\beta} + \zeta\Delta\mu p_\alpha p_\beta + \zeta'\Delta\mu p_\gamma p_\gamma \delta_{\alpha\beta} + \bar{\zeta}\Delta\mu \delta_{\alpha\beta} - \frac{\nu}{2}(p_\alpha h_\beta + p_\beta h_\alpha) \\ &\quad - \bar{\nu} p_\gamma h_\gamma \delta_{\alpha\beta} \end{aligned} \quad (2.14)$$

$$\frac{DP_\alpha}{Dt} = \frac{h_\alpha}{\gamma} + \lambda_1 p_\alpha \Delta\mu - \nu u_{\alpha\beta} p_\beta - \bar{\nu} u_{\beta\beta} p_\alpha \quad (2.15)$$

Note the use of the corotational time derivative of the vector  $\mathbf{p}$  given by:

$$\frac{D}{Dt} p_\alpha = \frac{\partial}{\partial t} p_\alpha + (v_\gamma \partial_\gamma) p_\alpha + \omega_{\alpha\beta} p_\beta \quad (2.16)$$

## 2.2.4 Boundary Conditions and Anchoring

Generally, There is the requirement that the bulk energy and bulk applicable equilibrium equation for any given liquid crystal sample be supplemented by a relevant surface energy and a description of the director alignment at the boundary surfaces of the sample. These descriptions are called *anchoring* and they enter the physics via boundary conditions. Thus, we may correctly expect that different equilibrium solutions for the director on the boundary surfaces satisfy different equations for different anchoring conditions. The main types of anchoring other than the *Natural* boundary condition (where there is no anchoring) are *strong* and *weak* anchoring

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Strong anchoring occurs in situations when surface forces are sufficiently large to enforce a clearly defined direction for the director  $\mathbf{p}$  on the physical surface at the boundary of the sample. Two common examples of strong anchoring between two parallel plates are shown below:

Incorporating strong anchoring into the equilibrium solution is thus reduced to the minimization of the bulk energy subject to the director taking prescribed fixed values at the boundary, i.e  $\mathbf{p} = \mathbf{p}_b$  at the boundary for some fixed  $\mathbf{p}_b$ . Weak anchoring occurs when the angle between the director  $\mathbf{p}$  and the layer normal at a boundary interface varies under the influence of applied fields. This often leads to the introduction of additional surface energies called *weak anchoring energy*[1].

# Chapter 3

## Spontaneous Flow Transitions in 2-Dimensions

### 3.1 Linear Approximation

In the previous chapter, The generalized hydrodynamic equations for a viscoelastic polar gel were introduced with the simplification involved when we only consider the viscous limit. Spontaneous flow transitions are an example of active behaviour in 2–dimensions as described by the dynamic equations (2.10) - (2.12). We now note that the maxwell equation (2.10) may now be re-written with the symmetric and antisymmetric parts resolved in 2–dimensional cartesian co'ordinates and to linear order, we write it and (2.11) as:

$$2\mu u_{\alpha\beta} = \sigma_{\alpha\beta} - \frac{\nu}{2} (p_{\alpha}h_{\beta} + p_{\beta}h_{\alpha}) + \frac{1}{2} (p_{\alpha}h_{\beta} - p_{\beta}h_{\alpha}) + \bar{\zeta}\Delta\mu\delta_{\alpha\beta} \quad (3.1)$$

$$\frac{Dp_{\alpha}}{Dt} = \frac{1}{\gamma}h_{\alpha} + \lambda p_{\alpha}\Delta\mu - \nu u_{\alpha\beta}p_{\beta} \quad (3.2)$$

The use of the corotational time derivative of the vector  $p_{\alpha}$  ensures the rotational and translational invariance of the derivative:

$$\frac{Dp_{\alpha}}{Dt} = \frac{\partial p_{\alpha}}{\partial t} + (v_{\gamma}\partial_{\gamma})p_{\alpha} + \omega_{\alpha\beta}p_{\beta} \quad (3.3)$$

Where  $\omega_{\alpha\beta}$  is the local vorticity, which is defined in terms of the velocity flow field as  $\omega_{\alpha\beta} = \frac{1}{2}(\partial_{\alpha}v_{\beta} - \partial_{\beta}v_{\alpha})$ . We also note that the distortion free energy



in a 2–dimensional case does not include the *twist* term, and may therefore be written as:

$$F = \int \left[ \frac{K_1}{2} (\nabla \cdot \mathbf{p})^2 + \frac{K_3}{2} (\nabla \times \mathbf{p})^2 - \frac{1}{2} h_{\parallel} \mathbf{p}^2 \right] dr \quad (3.4)$$

As before, a term of the form  $k \nabla \cdot \mathbf{p}$  called the spontaneous splay term allowed by polar symmetry has been ignored because of the strong anchoring,  $K_i$  are the *bend* and *splay* Frank elastic constants and the langrange multiplier  $h_{\parallel}$  ensures that the polarization is a unit vector.

### 3.2 Non-equilibrium steady states

For an active system  $\Delta\mu \neq 0$ , we expect non-trivial flow and stress profiles<sup>[10]</sup>. Assuming that the system is incompressible i.e  $\nabla \cdot v = u_{xx} + u_{yy} = 0$  and imposing the conditions that:

1. The system is translationally invariant along the  $y$ –direction; and that it is confined between  $x = 0$  and  $x = L$
2. The anchoring is planar; with the polarization at the confining surfaces parallel to the  $y$ –direction i.e *Homogeneous anchoring* with  $\theta = \frac{\pi}{2}$

The symmetry of the problem implies:

$$v_x = \text{const} = 0; \text{ this leads us to conclude that } u_{xx} = 0 = u_{yy}$$

The transverse component of the stress tensor  $\sigma_{xy} = \text{constant}$  because the force balance condition imposes:  $\partial_x \sigma_{xy} = 0$

The perpendicular component of the molecular field<sup>1</sup>  $h_{\perp} = K \partial_x^2 \theta$ ; which is

- only exact provided the *One constant approximation* holds i.e  $K_1 = K_3 = K$
- valid only for small values of  $\theta - \frac{\pi}{2}$  if  $K_1 = K \neq K_3$

In this 2–Dimensional cartesian geometry; we note that the unit vector polarization field  $p$  is given by  $(\cos \theta, \sin \theta)$ ; and the molecular field components  $h_x$  and  $h_y$  in terms of its components parallel and perpendicular to the polarization are respectively:

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<sup>1</sup>see Appendix II

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$$h_x = h_{\parallel} \cos \theta - h_{\perp} \sin \theta \quad (3.5)$$

$$h_y = h_{\parallel} \sin \theta + h_{\perp} \cos \theta \quad (3.6)$$

which is equivalent to:

$$h_{\parallel} = h_x \cos \theta + h_y \sin \theta \quad (3.7)$$

$$h_{\perp} = -h_x \sin \theta + h_y \cos \theta \quad (3.8)$$

equation (3.1) above is then rewritten as:

$$2\mu u_{xy} = \sigma_{xy} + \zeta \Delta\mu \cos \theta \sin \theta - \frac{\nu}{2} (p_x h_y + p_y h_x) + \frac{1}{2} (p_x h_y - p_y h_x) \quad (3.9)$$

$$2\mu u_{yx} = \sigma_{yx} + \zeta \Delta\mu \cos \theta \sin \theta - \frac{\nu}{2} (p_y h_x + p_x h_y) + \frac{1}{2} (p_y h_x - p_x h_y) \quad (3.10)$$

Adding and subtracting equations (3.9) and (3.10) and then dividing by two; we obtain:

$$2\mu u_{xy} = \frac{1}{2} (\sigma_{xy} + \sigma_{yx}) + \frac{\zeta}{2} \Delta\mu \sin 2\theta - \frac{\nu}{2} (p_x h_y + p_y h_x) \quad (3.11)$$

$$0 = \frac{1}{2} (\sigma_{xy} - \sigma_{yx}) + \frac{1}{2} (p_x h_y - p_y h_x) \quad (3.12)$$

which simplify to

$$2\mu u_{xy} = \frac{1}{2} (\sigma_{xy} + \sigma_{yx}) + \frac{\zeta}{2} \Delta\mu \sin 2\theta - \frac{\nu}{2} (h_{\parallel} \sin 2\theta + h_{\perp} \cos 2\theta) \quad (3.13)$$

$$0 = \frac{1}{2} (\sigma_{xy} - \sigma_{yx}) + \frac{h_{\perp}}{2} \quad (3.14)$$

The polarization equation (3.2) at steady-state is

$$\omega_{xy} \sin \theta = \frac{1}{\gamma} h_x + \lambda \cos \theta \Delta\mu - \nu u_{xy} \sin \theta \quad (3.15)$$

$$\omega_{yx} \cos \theta = \frac{1}{\gamma} h_y + \lambda \sin \theta \Delta\mu - \nu u_{yx} \cos \theta \quad (3.16)$$

---

Since the term proportional to the vorticity in (3.2) remains in steady-state. Noting that the strain rate is symmetric i.e  $u_{xy} = u_{yx}$  and the vorticity is anti-symmetric i.e  $\omega_{yx} = -\omega_{xy}$ ; Multiplying (3.15) by  $\cos \theta$  and (3.16) by  $\sin \theta$  then adding, we get:

$$0 = \frac{h_x \cos \theta + h_y \sin \theta}{\gamma} + \lambda \Delta \mu - \nu u_{xy} (\sin \theta \cos \theta + \sin \theta \cos \theta) \quad (3.17)$$

Multiplying (3.15) by  $\sin \theta$  and (3.16) by  $\cos \theta$  and subtracting  $\sin \theta \times$  (3.15) from  $\cos \theta \times$  (3.16); we obtain:

$$-\omega_{xy} (\cos^2 \theta + \sin^2 \theta) = \frac{h_y \cos \theta - h_x \sin \theta}{\gamma} - \nu u_{xy} (\cos^2 \theta - \sin^2 \theta) \quad (3.18)$$

Hence the polarization equation (3.2) reduces to:

$$\nu u_{xy} \sin 2\theta = \frac{h_{\parallel}}{\gamma} + \lambda \Delta \mu; \quad (3.19)$$

$$u_{xy} (\nu \cos 2\theta - 1) = \frac{h_{\perp}}{\gamma} \quad (3.20)$$

this is because in (3.18), the requirement that  $v_x = 0$  implies that  $\omega_{xy} = u_{xy}$

## 3.3 Boundary Conditions

### 3.3.1 Hydrodynamic free boundary conditions

Here we consider a free standing film, with the gel free to slide on the confining surfaces. The stress  $\sigma_{xy}(x)$  vanishes since  $\sigma_{xy}(x=0) = \sigma_{xy}(x=L) = 0$ ; thus the equations (3.13), (3.14), (3.19) and (3.20) together with the molecular field  $h_{\perp} = K \partial_x^2 \theta$  can be written into a differential equation. From (3.20):

$$u = u_{xy} = \frac{h_{\perp}}{\gamma (\nu \cos 2\theta - 1)} \quad (3.21)$$

Henceforth,  $u_{xy}$  will be written as  $u$  for brevity; equations (3.13), (3.14), (3.19) and (3.20) are then rearranged thus:

---


$$4\eta u = \sigma_{yx} + \zeta \Delta\mu \sin 2\theta - \nu (h_{\parallel} \sin 2\theta + h_{\perp} \cos 2\theta) \quad (3.22)$$

$$h_{\perp} = \sigma_{yx} \quad (3.23)$$

$$\frac{h_{\parallel}}{\gamma} = u\nu \sin 2\theta - \lambda \Delta\mu \quad (3.24)$$

$$\frac{h_{\perp}}{\gamma} = u(\nu \cos 2\theta - 1) \quad (3.25)$$

Multiplying (3.24) by  $\sin 2\theta$ , (3.25) by  $\cos 2\theta$  and adding:

$$h_{\parallel} \sin 2\theta + h_{\perp} \cos 2\theta = \gamma (u\nu - \lambda \Delta\mu \sin 2\theta - u \cos 2\theta) \quad (3.26)$$

Substituting (3.26), (3.21) and (3.23) in (3.22):

$$h_{\perp} \frac{(4\eta + \nu^2 \gamma - 2\nu \gamma \cos 2\theta + \gamma)}{\gamma(\nu \cos 2\theta - 1)} = (\zeta + \nu \gamma \lambda) \Delta\mu \sin 2\theta \quad (3.27)$$

with  $\bar{\zeta} = \zeta + \nu \gamma \lambda$ ; we can then write:

$$h_{\perp} = \frac{\bar{\zeta} \Delta\mu \sin 2\theta (\nu \cos 2\theta - 1)}{\left(4\frac{\eta}{\gamma} + \nu^2 - 2\nu \cos 2\theta + 1\right)} \quad (3.28)$$

OR equivalently

$$\partial_x^2 \theta = \frac{\bar{\zeta} \Delta\mu \sin 2\theta (\nu \cos 2\theta - 1)}{K \left(4\frac{\eta}{\gamma} + \nu^2 - 2\nu \cos 2\theta + 1\right)} = \Phi_f(\theta) \quad (3.29)$$

Equation (3.29) is a differential equation for the polarization orientation  $\theta$ ; we assume that  $\bar{\zeta} \Delta\mu < 0$  which has been shown[12] to be the case generating self-motion in a point-like defect. There is an effective potential  $V_f$  associated with the force  $\Phi_f(\theta)$ :

$$V_f = - \int \Phi_f(\theta) d\theta \quad (3.30)$$

which can be expanded around the value imposed by the anchoring on the confining surfaces,  $\theta = \frac{\pi}{2} + \epsilon$

---


$$\begin{aligned}
V_f(\theta) &= V_f\left(\frac{\pi}{2}\right) + V_f'\left(\frac{\pi}{2}\right)\epsilon + V_f''\left(\frac{\pi}{2}\right)\frac{\epsilon^2}{2!} + O(\epsilon^3) + \dots \\
V_f(\theta) &= V_f\left(\frac{\pi}{2}\right) - \Phi_f\left(\frac{\pi}{2}\right)\epsilon - \Phi_f'\left(\frac{\pi}{2}\right)\frac{\epsilon^2}{2!} + O(\epsilon^3) + \dots
\end{aligned} \tag{3.31}$$

Since we know that (3.30) implies that  $V_f'(\theta) = -\Phi_f(\theta)$  and  $V_f''(\theta) = -\Phi_f'(\theta)$ . It is also clear from (3.29) that the  $\sin 2\theta$  term will cause the term linear in  $\epsilon$  to vanish at  $\theta = \frac{\pi}{2}$  which leaves us with the term in  $\epsilon^2$ . Differentiating (3.29) and evaluating at  $\theta = \frac{\pi}{2}$  yields:

$$\Phi_f'\left(\frac{\pi}{2}\right) = \frac{2\bar{\zeta}\Delta\mu(\nu - 1)}{K\left(4\frac{\eta}{\gamma} + (\nu + 1)^2\right)} \tag{3.32}$$

substituting in the Taylor expansion (3.31) above:

$$\begin{aligned}
V_f(\theta) &= V_f\left(\frac{\pi}{2}\right) - \frac{\bar{\zeta}\Delta\mu(\nu - 1)}{K\left(4\frac{\eta}{\gamma} + (\nu + 1)^2\right)}\epsilon^2 + O(\epsilon^3) + \dots \\
V_f(\theta) &= V_f\left(\frac{\pi}{2}\right) + \frac{\epsilon^2}{\ell^2} + O(\epsilon^3) + \dots
\end{aligned} \tag{3.33}$$

Where

$$\ell^2 = -\frac{K\left[4\frac{\eta}{\gamma} + (\nu + 1)^2\right]}{\bar{\zeta}\Delta\mu(\nu + 1)} \tag{3.34}$$

The effective potential energy  $V$  defined in (3.30) has minima for  $\theta = 0, \frac{\pi}{2}$  and a maximum for an angle  $\theta_0$  such that  $\cos 2\theta_0 = \frac{1}{\nu}$ . It follows from the physics of nematic liquid crystals[2, 11] that if the length  $\ell$  defined above is real i.e  $\bar{\zeta} < 0$  (corresponding to a contractile active stress); the system exhibits a spontaneous flow transition above a certain critical size for a fixed activity, this critical size  $L_c$  is given by:

$$L_c = \frac{\ell\pi}{\sqrt{2}} \tag{3.35}$$

Using (3.34); the critical size  $L_c$  at constant activity or the critical activity  $\Delta\mu_c$  for constant thickness may be expressed as:

---


$$L_c^2 = -\frac{\pi^2 K \left[ 4\frac{\eta}{\gamma} + (\nu + 1)^2 \right]}{2\bar{\zeta}\Delta\mu(\nu + 1)} \quad (3.36)$$

Written in terms of the ATP chemical potential difference  $\Delta\mu$  :

$$\Delta\mu_c = -\frac{\pi^2 K \left[ 4\frac{\eta}{\gamma} + (\nu + 1)^2 \right]}{2\bar{\zeta}L^2(\nu + 1)} \quad (3.37)$$

We now note that when  $L < L_c$  (or  $\Delta\mu < \Delta\mu_c$ ) the gel is dominated by anchoring effects and the polarization orientation is constant in most of the film with  $\theta(x) = \frac{\pi}{2}$ . However, for the case where  $L > L_c$  (or  $\Delta\mu > \Delta\mu_c$ ) the system shows a tilting of the polarization in the bulk down to a minimum angle  $\theta_{min} = \theta(\frac{L}{2}) < \frac{\pi}{2}$ . Near the critical size  $L \sim L_c$ , the tilt amplitude is  $\epsilon(x) = \epsilon_m \sin(\frac{x\pi}{L})$ . The quantity  $\epsilon_m \propto \sqrt{L - L_c}$  or  $\epsilon_m \propto \sqrt{\Delta\mu - \Delta\mu_c}$ . Using the velocity gradient (3.21) it is possible to obtain the velocity flow field at linear order in  $\epsilon_m$ . The velocity gradient is:

$$u = \frac{\bar{\zeta}\Delta\mu \sin 2\theta}{4\eta + \gamma(\nu^2 - 2\nu \cos 2\theta + 1)} \quad (3.38)$$

The velocity at the midplane - the integration constant, is chosen such that the net flow vanishes, i.e there is no net gel flux. To linear order in the tilt amplitude, we have:

$$v_y = \frac{4L\bar{\zeta}\Delta\mu\epsilon_m \cos \frac{x\pi}{L}}{\pi(4\eta + \gamma(\nu + 1)^2)} \quad (3.39)$$

### 3.3.2 Hydrodynamic no-slip boundary conditions

In a case where the gel is confined between solid surfaces and does not slide on the walls,  $v_y(x = 0) = v_y(x = L) = 0$ , the differential equation for the polarization orientation is:

$$\partial_x^2 \theta = \frac{(\bar{\zeta}\Delta\mu \sin 2\theta + 2\sigma_{xy})(\nu \cos 2\theta - 1)}{K \left( 4\frac{\eta}{\gamma} + \nu^2 - 2\nu \cos 2\theta + 1 \right)} = \Phi_{ns}(\theta) \quad (3.40)$$

---

To linear order in the polarization tilt, the polarization equation may be written as:

$$\partial_x^2 \epsilon = \frac{2(\nu + 1)}{K \left( 4\frac{\eta}{\gamma} + (\nu + 1)^2 \right)} (\bar{\zeta} \Delta \mu \epsilon - \sigma_{xy}) \quad (3.41)$$

with the polarization angle  $\epsilon$  given by:

$$\epsilon = \frac{\sigma_{xy}}{\bar{\zeta} \Delta \mu} \left( 1 - \cos \left( \frac{\pi x}{L_c} \right) - \tan \left( \frac{\pi L}{2L_c} \right) \sin \left( \frac{\pi x}{L_c} \right) \right) \quad (3.42)$$

According to Voituriez *et al*[11], when the activity  $\Delta \mu$  is small, the tilt angle  $\epsilon$  is small as well. In this low activity regime the stress  $\sigma_{xy} = 0$  and a spontaneous flow transition occurs. For cases when the stress  $\sigma_{xy} \neq 0$ , the velocity gradient:

$$u = \frac{\bar{\zeta} \Delta \mu \sin 2\theta + 2\sigma_{xy}}{4\eta + \gamma(\nu^2 - 2\nu \cos 2\theta + 1)} \quad (3.43)$$

does not change sign for any constant  $\sigma_{xy} \neq 0$ , this does not agree with the no slip condition and we conclude that  $\sigma_{xy} = 0$  must be fulfilled at all times. As a consequence, the polarization remains uniform. When the activity  $\Delta \mu$  is larger, there is also a spontaneous flow transition. Near threshold, the maximum tilt angle is small[11] and it is possible to take a linear approximation to (3.40) with the polarization tilt  $\epsilon$  given by (3.42). Using the boundary conditions for the no-slip condition and integrating (3.43), we get:

$$v_y = \frac{4\sigma_{xy}L_c}{\pi(4\eta + \gamma(\nu + 1)^2)} \left( \sin \left( \frac{\pi x}{L_c} \right) - \tan \left( \frac{\pi L}{2L_c} \right) \left( \cos \left( \frac{\pi x}{L_c} \right) - 1 \right) \right) \quad (3.44)$$

Because it is required that the velocity  $v_y$  vanishes at  $x = L$ , the spontaneous flow transition occurs when  $L = 2L_c$  since that is when the boundary condition is satisfied, this is equivalent to  $\Delta \mu = 4\Delta \mu_c$ . As before, close to the transition; the maximum tilt angle and the transverse stress, are proportional to  $\sqrt{L - L_c}$ ; that is  $\epsilon_m \propto \sigma_{xy} \propto \sqrt{L - L_c}$

---

### 3.3.3 Hydrodynamic mixed boundary conditions

This is achieved experimentally by placing a gel film on a solid plane with a free surface[11], this imposes the condition that the velocity at the plane  $v_y$  vanishes ( $v_y(x=0) = 0$ ) with the transverse stress at the free surface ( $\sigma_{xy}(x=L) = 0$ ). As the stress vanishes everywhere, the polarization field is the same as a free standing film with hydrodynamic free boundary conditions (refer to 3.29), with the transition threshold described by (3.37) or (3.36). Above threshold, there is a finite gel flux  $Q$ , given by:

$$Q = \int_0^L v_y dx = -\frac{4L\bar{\zeta}\Delta\mu \epsilon_m}{\pi(4\eta + \gamma(\nu + 1)^2)} \quad (3.45)$$

In this case

$$\epsilon_m = -\sqrt{\frac{2\pi(L - L_c)}{L_c}}$$

### 3.3.4 Active boundary conditions

When the gel is confined between two planar surfaces coated with molecular motors, the boundary condition is referred to as *active*. In this case, there is an imposition of a finite gel velocity on the surfaces. There are two cases:

1. Identical confining surfaces: The velocities at the two surfaces  $x = 0$  and  $x = L$  are equal; this is equivalent to no-slip boundary conditions with a constant drift velocity set by the motors. (3.43) is thus integrated with the new molecular motor-imposed drift velocity.
2. Non-identical confining surfaces: In this case, the velocities imposed by the motors are different. There is always a finite shear stress  $\sigma_{xy}$  and polarization tilt. There is however, no spontaneous flow transition as in the no-slip case with non vanishing transverse stress.



# Chapter 4

## Endnotes

### 4.1 Scope of work and Recommendations for further study

This project covers the use of a generic hydrodynamic theory to describe spontaneous flow transitions induced by boundary conditions on cytoskeletal filaments. There are however certain simplifications that were made to make the model more mathematically tractable. It is expected that taking them into account will yield a better qualitative explanation of the behaviour of the cytoskeleton. They include:

1. The hydrodynamic theory is mainly limited to large length scales and long time scales, in an active gel this would mean a length scale larger than the mesh size.
2. The theory is linear, it ignores geometric non-linearities as contained in  $A_{\alpha\beta}$  and does not take into account the fact that the rheological properties of the cytoskeleton are best described by a wide distribution of relaxation times; rather than a single viscoelastic relaxation time. There are also permeation effects, non-linear couplings and noise; which could play non-trivial roles.
3. Possible experimental realizations of spontaneous flows described in Chapter 3 will have to rely on a Quasi 2-dimensional confined geometry; which is inadequate to fully describe chiral systems such as cytoskeletal filaments.

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## 4.2 Conclusion

Active systems display a range of interesting and novel physical effects including topological defects, propagating waves and spontaneous flows. In this report, we discuss the existence of *Frederiks*-like spontaneous flow transitions in the **absence** of an external field. This is caused by a polarization tilt arising as a result of the activity of a viscoelastic gel above a certain critical thickness or activity. In active polar materials below this threshold, the gel remains in a static, homogeneously polarized state with anchoring conditions prevailing. The flow transitions and critical thickness (or activity) are dependent on the imposed anchoring conditions and hydrodynamic boundary conditions respectively.

The phenomenological coefficients can be measured from experiments or using simple limits from microscopic models. Measuring the critical transition parameters will give direct access to the active stress  $\bar{\zeta}\Delta\mu$  OR more generally other active parameters of the gel such as  $\lambda$  and  $\zeta$  as well as the more standard liquid crystalline parameters:  $\gamma$  and  $\nu$ . Detailed experimental studies will be made possible by a careful choice of anchoring and boundary conditions in a suitable geometry[11]. The use of spontaneous flows to quantitatively describe active systems such as the cellular cytoskeleton will require the inclusion of other components and the extension of the theory beyond the linear approximation. This together with other works in this area, should aid in improving our understanding of the physics of active systems.

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# APPENDICES

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## APPENDIX I

### Typical values of Frank elastic constants

$T(^{\circ}\text{C})$	Elastic constants ( $10^{-7}$ dyn)		
	$K_1$	$K_2$	$K_3$
120	5.0	3.8	10.1
125	4.5	2.9	9.5
129	3.85	2.4	7.7
120	7.01	4.26	—
124.9	6.06	3.7	—
130	4.84	2.89	—
129	—	$3.1 \pm 0.6$	—

Figure 4.1: Typical values of  $K_i$  ( $i = 1, 2, 3$ ) for  $p$ -azoxyanisole (PAA)

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$T$ (°C)	Elastic constants ( $10^{-7}$ dyn)		
	$K_1$	$K_2$	$K_3$
22	5.8		7
~24		$K_{2,\max} = 3.8$	
22	$6.2 \pm 0.6$		$8.6 \pm 0.4$
22			$7.3 \pm 1.5$
22		$3.4 \pm 0.3$	$8 \pm 0.8$
22		$3.34 \pm 0.04$	
22	$5.3 \pm 0.5$	$2.2 \pm 0.7$	$7.45 \pm 1.1$
25	3.5		
22		3.35	
23			8.1
23			
24			$7.2 \pm 1$
26	$3.2 \pm 1$		$6.1 \pm 1$
22			
$23.5 \pm 0.5$	3.88		4.66

Figure 4.2: Typical values of  $K_i$  ( $i = 1, 2, 3$ ) for 4-methoxybenzylidene-4'-butylaniline (MBBA)

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## APPENDIX II

### Molecular Field

Consider a free energy of the form below with the one constant approximation:

$$F[p(r)] = \int \frac{K}{2} [(\operatorname{div} \mathbf{p})^2 + (\mathbf{p} \cdot \operatorname{curl} \mathbf{p} + q_0)^2 + (\mathbf{p} \times \operatorname{curl} \mathbf{p})^2] dr$$

Using the levi-civita symbol  $\epsilon_{ijk}$  and Einstein's summation convention, we may simplify the free energy to:

$$F[p] = \frac{K}{2} \int [(\partial_i p_i)(\partial_j p_j) + (\partial_i p_j)(\partial_i p_j) - (\partial_i p_j)(\partial_j p_i)]$$

From which follows:

$$\frac{\delta F}{\delta p_l(r)} = -\partial_k \left[ \frac{\partial F}{\partial (\partial_k p_l(r))} \right] = -K(\partial_l \partial_i p_i + \partial_i \partial_i p_l - \partial_l \partial_i p_i) = -K \nabla^2 p_l(r)$$

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Figures 1.1 - 1.4 I. W. Stewart, *The Static and Dynamic Continuum Theory of Liquid Crystals: A Mathematical Introduction*. Taylor and Francis, January 2004.

Figures 4.1 - 4.2 P. G. De Gennes and J. Prost, *The Physics of Liquid Crystals*. New York: Clarendon Press, second edition ed., 1993.