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Spiral Patterns in Liquid Crystals

By Gavin Hartnett

with

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Abstract

The macroscopic configurations of various two-dimensional liquid crystal systems are explored. Aster, vortex and spiral patterns are analyzed for both inactive nematic and polar liquid crystals, as well as for active nematic and polar liquid crystals. The relevance of these systems to the cellular cytoskeleton is discussed. Differing theoretical models of the cytoskeleton are compared and extended to include a more general description of cytoskeletal dynamics.

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Chapter 1

Introduction

Condensed matter is a very broad subfield of physics that encompasses many different types of physical systems. Generally speaking, condensed matter is the study of how the microscopic details of a system lead to its overall behavior. Whereas high-energy physicists attempt to understand elementary particles and laws governing nature on the smallest distance scales, condensed matter physicists study how large numbers of elementary particles interact to form material substances. Condensed matter physicists are interested in a wide range of substances, including crystals, solids, liquids, superfluids, superconductors, semiconductors, magnets and liquid crystals, to name just a few. Condensed matter physicists are also interested in transitions between different phases of matter, as well as transport phenomena such as conduction, diffusion and convection.

Not only is condensed matter a very broad field, it is also very interdisciplinary in nature. Biologists, chemists, engineers and mathematicians often collaborate with condensed matter physicists in order to better understand the dynamics of such systems as the cellular cytoskeleton, biological membranes, nanostructures, and electrical devices. Condensed matter is by far the largest subfield of physics, and research can range from mathematically abstract theoretical models to experimentation. New discoveries can also lead to new technologies and devices. Ideally, both experimentalists and theorists work in tandem to discover and formulate the understanding of previously unknown phenomena.

My Capstone project has consisted of an independent study in theoretical condensed matter, during which I have investigated the patterns and self-organization of liquid crystalline substances. A liquid crystal, as the name suggests, is a phase of matter that exhibits properties that are characteristic of both liquids and solids.

The liquid phase is characterized by rotational and translational disorder. If the local arrangement of the molecules in a liquid is either rotated or translated by an infinitesimal amount, then the new arrangement will also be disordered and will be essentially indistinguishable from the original system. Liquids are said to possess continuous rotational and translational symmetry. In contrast, the solid phase is characterized by order. The molecules align themselves into lattice arrangements. If the molecular arrangement in a solid were to be *locally* rotated or translated, then only very specific rotations or translations would leave the system unchanged. The continuous symmetry of the liquid phase is *broken* in the solid phase. Solids are rotationally and translationally ordered whereas liquids are rotationally and translationally disordered.

Liquid crystals are like liquids in that they too are translationally disordered. However, they are solid-like in that they are rotationally ordered. Equivalently, liquid crystals possess translational symmetry but have a broken rotational symmetry. Below is a picture of the molecular arrangement in a liquid crystal (the relevant diagram is the third from the left). As can be seen from the picture, the molecules tend to point in the same direction. If the arrangement was locally rotated in some direction, the material would appear markedly different and would display different macroscopic properties. On the other hand, the arrangement is translationally disordered. If the arrangement was locally translated in some direction, the resulting arrangement would be essentially identical to the original one.

I studied four different types of liquid crystals, and all four are composed of long, rod-like molecules. Nematic liquid crystals are the simplest liquid crystals I studied. In nematic materials, the cylindrical molecules tend to align themselves and give the material a macroscopic orientation. Polar liquid crystals are similar to nematics, except that in polar systems, the molecules align themselves in such a way so as to give the material's orientation a preferred direction. In nematics, opposite alignments are considered equivalent, for example, up-down is the same as down-up. In polar liquid crystals, these two configurations are different (hence the term polar).

An additional characterization of liquid crystals involves the consumption of energy. Generally, when one speaks of either nematic or polar liquid crystals, it is assumed that the substances are in thermodynamic equilibrium, and that energy is neither being consumed nor released. If the liquid crystals are in fact consuming energy, they are said to be active. For my project I studied both active and non-active nematic liquid crystals as well as both active and non-active polar liquid crystals.

The patterns that liquid crystalline substances assume depends upon the

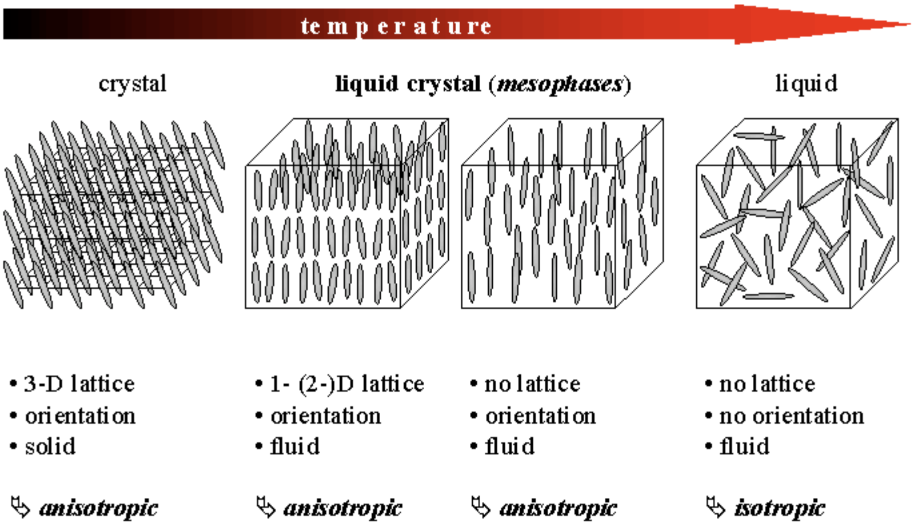

Figure 1.1: Liquid Crystal Phase. Image courtesy of http://www.physik.tu-berlin.de/institute/OI/lc/images/lcs_thermotropic_lcs.gif

geometry that the substances reside in. Are the liquid crystals confined by some shape? Is there a 2D sheet of liquid crystal material, or a 3D sample? It is also necessary to know the boundary conditions. An example of a boundary condition would be to stipulate that whenever a liquid crystal molecule comes into contact with the edge of its container, the molecule must meet the surface at some particular angle. I have studied these materials in a variety of different boundary conditions and geometries. It is generally simpler to treat inactive rather than active liquid crystals, and nematic rather than polar liquid crystals. Throughout my project, I have often begun by analyzing the simplest system, inactive nematic liquid crystals, and then working my way up to the more complicated active polar liquid crystals.

I have investigated a variety of liquid crystal systems, and my research has not at all progressed in a linear and predictable fashion. Certain systems were too mathematically intractable to analyze without resorting to numerical simulations, and some had already been investigated. The project initially began as a study of topological defects in nematic liquid crystals. Topological defects are closely related to certain types of patterns, and as the project progressed, we began to use the language of thermodynamics and energetics rather than that of topology. There are three main types of patterns we have investigated. Asters are star-like patterns in which the liquid crystals tend to arrange radially outward from some central point. In a vortex, the liquid crystal molecules tend to arrange themselves in concentric circles around a central point. Spirals are intermediate between aster and vortex patterns. In Figure 1.2 below, pictures b) through d) represent these patterns.

As the project progressed, Professor Cristina Marchetti joined Professor Bowick and I, and together we began to study biologically motivated liquid crystal systems (Prof. Marchetti is a biological physicist). She is particularly interested in the actin cytoskeleton, and we moved on to analyze liquid crystal models of this cytoskeleton.

This project has principally been a learning experience for me, and I benefitted tremendously from this research experience. Although my work has not led to any new insights concerning liquid crystals or the cellular cytoskeleton, the importance of a thorough theoretical understanding of these systems should be obvious. Liquid crystal displays are fast replacing cathode ray tubes in electrical devices, and a great deal of modern technology utilizes these interesting materials. Cytoskeletal networks may be found in all cells, and they are very important in a number of cellular functions. Understanding these systems can lead to advances in technology, biology, and medicine.

Physics generally involves a great deal of mathematics, and theoretical physics even more so. Much of my project has consisted of doing calculations, and after reading through a few pages of math scribbled in my handwriting, Prof. Bowick suggested that I type up my notes. LaTeX is a typesetting program that I learned how to use in the beginning of my project, and with it I have written up pages of annotated calculations, some which I include here. This document was written using LaTeX.

My thesis consists of a series of calculations that I did throughout my project. I have annotated my calculations to include descriptions and background information, and I have also tried to explain the physics behind the math. I try to accompany every step of my calculations with an explanation of what it is I am doing and why, and hopefully this format will allow the mathematical lay-person to follow the general logic behind my calculations, and to at least see the forest for the trees.

This project has been by far the singular most important activity I've been involved in as an undergraduate at Syracuse University. I began this effort in complete ignorance of the field of condensed matter. Throughout the duration of my research I have studied various kinds of liquid crystals, the cellular cytoskeleton, and active gels. I have also been introduced to a wide range of mathematics including group theory, topology, homotopy theory, complex analysis and Fourier Analysis. I have benefitted tremendously from weekly (and occasional biweekly) meetings with Professors Bowick and Marchetti. My research has also influenced my coursework; upon Bowick's advice I took his graduate class Phy 831: Statistical Theory of Fields during the fall semester of my senior year. This project has not only allowed me to learn about the physics of liquid crystals; I have also learned important theoretical techniques that may be applied to a wide range of condensed matter systems.

In addition to strengthening my mathematical abilities and improving my understanding of physics, this project has also been instrumental in my acceptance into graduate school. Next year I plan to enroll in the graduate program at the University of California at Santa Barbara. There I will pursue a Ph.D. in theoretical condensed matter physics. I am excited to have the opportunity to continue my education of the physical world, and I eventually hope to be able to contribute something of my own towards our collective understanding of the world.

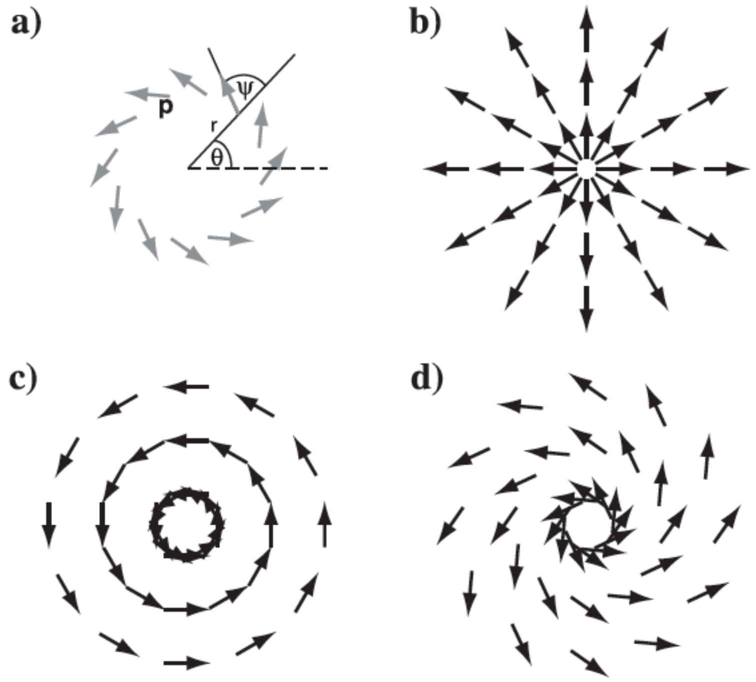

Fig. 1. Schematic representation of the geometry of point defects of topological charge one in two dimensions. (a) Description of a point defect in polar coordinates. Orientations of polarization vectors **p** for (b) aster, (c) vortex and (d) spiral.

Figure 1.2: Asters, Vortices, and Spirals. Image courtesy of Kruse et al, Asters, Vortices, and Rotating Spirals in Active Gels of Polar Filaments

Chapter 2

Spiral Patterns in Liquid Crystals

2.1 Initial Reading and Topological Defects

The project began with Prof. Bowick describing his idea for the project and giving me some background reading. Along with Chaikin and Lubensky's standard text *Principles of Condensed Matter Physics*, I was given a paper he had co-authored entitled *The Cosmological Kibble Mechanism in the Laboratory: String Formation in Liquid Crystals.* Prior to this project, I had worked on cosmology research, and I was fascinated to learn that ideas from the physics of the very largest distance and time scales, cosmology, could be applied to liquid crystals in the laboratory. The Cosmological Kibble Mechanism is a (now outdated) mechanism for producing topological line defects in the early universe. Along with his co-authors, Bowick took this mechanism and applied it to the formation of defects in samples of liquid crystals. In addition to introducing me to topological defects and the field of condensed matter, this paper was doubly interesting to me because I would later work on a research project studying a related type of cosmological strings during a summer research project at Cornell University.

I was also given the seminal paper *The topological theory of defects in ordered media* by David Mermin. In the paper's introduction, Mermin writes "The language, methods, and theorems of algebraic topology, particularly homotopy theory, have been used in the study of relativistic field theories for over a decade. Their systematic application to the study of defects in condensed matter physics is more recent ... At a minimum, homotopy theory provides *the* natural language for the description and classification of defects in a large class or ordered systems."

The aim of Mermin's article was to summarize the results of homotopy theory as applied to condensed matter physics. The theory is used to classify and describe topological defects in the order parameter field. Mermin's paper applies to a very broad range of condensed matter systems, and it is this generality which makes homotopy theory such a powerful tool. For the first few weeks of my Capstone project I worked through this paper and struggled to understand the main ideas. To do so, I had to teach myself the basics of group theory and topology. The work was rather slow and abstract, and as we moved on, our focus began to narrow. Rather than study comprehensive but abstract theories that describe a wide range of systems, we moved on to study specific physical systems. While I never fully understood Mermin's paper, working through it gave me an appreciation for the ability of abstract mathematics to describe physical systems. Since then, I have discovered that topology and group theory are crucial to an understanding of many different phenomena, and I hope to return to homotopy theory during graduate school. Since I began this project, I have learned a great deal of mathematics and physics, and hopefully when I encounter these ideas again, I'll be more mathematically equipped to understand them.

The aim of Mermin's paper is to describe the use homotopy theory in the study of defects in ordered media, as the title suggests. An ordered media is a substance which may be described by an order parameter field. At any given point within the substance, the order parameter is a quantity which describes some important local property. A classic example is magnetization. Throughout the interior of a magnet, one may draw little arrows, or vectors, which describe the local alignment of the magnetic dipoles. The local alignment of polar liquid crystal molecules are also described by a vector field. The order parameter field of nematic liquid crystals is similar to both magnets and polar liquid crystals, however for nematic materials the vectors are headless and do not point in a particular direction. For all materials, if the order parameter is everywhere the same, than the material is said to be uniform.

A defect is a region where it is impossible to assign an order parameter. A defect may be a point, a line or a plane where the order parameter cannot be defined. Defects are generally the cause of very interesting physics, and as Mermin says, homotopy theory provides the natural language for the study of defects.

From Mermin's pedagogical paper I moved on to study a research paper by Michael Deem entitled *Disclination asymmetry in two-dimensional nematic liquid crystals with unequal Frank constants.* Papers in physics will generally contain a series of relevant equations, and there is often a rather large gap between consecutive equations. My first task was to reproduce Deem's calculations and to re-derive some of his equations as I worked through his paper. From there I moved on to study spiral patterns in two-dimensional liquid crystal systems on my own.

2.2 Patterns in Nematic Liquid Crystals Obtained from Thermodynamic Considerations

Below is a great deal of math aimed at discovering the possible macroscopic configurations that a nematic liquid crystal may assume. I begin by reproducing some of Deem's equations, and then I move on to study the patterns formed by a sheet of nematic liquid crystal. In order to relay the logic behind the calculations, I'll briefly describe some of the general ideas. A liquid crystal is composed of an incredibly large number (around 10^{23}) of liquid crystal molecules. Because this system exists at some finite temperature, the individual molecules have thermal energy that causes them to vibrate and jiggle. The amount of vibrating and jiggling that occurs is related to the temperature of the system; at higher temperatures the jiggling becomes more violent, while at lower temperatures, the molecules are more tame and don't fidget as much. If the temperature is really extreme, thermal fluctuations will destroy any ordering of the molecules. Then the system will look like the liquid pictured in Figure 1.1. This phase is called the isotropic phase because all directions look the same. If the temperature is more reasonable, though, the molecules may order themselves as depicted in the third picture in Figure 1.1. They will still vibrate, but the vibrations will be gentle enough to preserve the molecule's order, and this is called the nematic phase.

In the nematic phase, the liquid crystals can be ordered. If one were to zoom in on a liquid crystal material in the nematic phase, one would find that, on average, a significant portion of the molecules were aligned along the same direction. This "zooming-in" process may be done throughout the whole material, and at any given point, the molecules should be fairly aligned. The alignment will not be perfect due to thermal fluctuations, but it wouldn't be too hard to see which direction most of the molecules were pointing in.

Suppose we may zoom in at any given point in the liquid crystal material enough to see which direction the majority of liquid crystals are pointing, but that we do not zoom in far enough to resolve individual molecules. This range is called mesoscopic, and is intermediate between the microscopic and macroscopic scales. At each "mesoscopic" point in the material, we may put an arrow pointing in the same direction as the local arrangement of the liquid crystal molecules. This is just a vector field–an arrow at each point. Keep in mind that each "mesoscopic" point actually contains a large number of liquid crystal molecules. We just agree not to zoom-in any further.

There is also a subtlety when dealing with nematic liquid crystals. Since the molecules have no distinguishable head or tail, the little arrows don't either. Our vector field is not a true vector field. It is called an orientation field.

In order to fully specify the state of a liquid crystal system, it is necessary to know the position and speed of each individual molecule. However, even if it were possible to have such detailed information, what sense could we possibly make of it? If there are 10^{23} molecules, and 3 position coordinates and 3 velocity coordinates for each molecule (3 because there is 1 coordinate for each dimension), then there are $6 * 10^{23}$ numbers to process! However, by examining the system from the mesoscopic scale and constructing an orientational field, we have enough information to describe the interesting details of the system, and we have also avoided a ridiculous overflow of information. This approach is called field theory, because the arrangement of a system is described by a field (in our case, an orientational field).

It should not be too much of a leap to suggest that the energy of a liquid crystal system depends upon the arrangement of liquid crystal molecules. If the molecules interact with one-another, certain configurations will be more energetically favorable than others. Rather than considering 10^{23} molecules and figuring out the energy-cost of different configurations, we can use our orientational field to calculate the energy of a given configuration. Let's denote our orientational field by $\vec{n}(x, y, z)$. At each point (x,y,z) in three dimensions, $\vec{n}$(x,y,z) returns three numbers which describe the little arrow that points along the local arrangement of molecules. $\vec{n}(x, y, z)$ returns three numbers because three numbers are needed to describe an arrow in three dimensions. The arrow sign is used to denoted a vector quantity.

At this point I should point out that the configuration of the liquid crystal is the same thing as our orientation field $\vec{n}(x, y, z)$. If we know $\vec{n}(x, y, z)$ for all points (x,y,z), then we know where, on average, the liquid crystal molecules are pointing. Based on symmetry considerations, one can write down an expression, called the Frank Free Energy (denoted below by the letter F), which describes the energy of a particular configuration. F is a function of $\vec{n}(x, y, z)$ (which is itself a function of the regular variables x, y, and z). Functions of this nature are called *functionals.*

In the calculation that follows, I find the particular orientation field $\vec{n}(x, y, z)$ (the liquid crystal configuration) that minimizes this free energy cost. It is a general physical principle that physical systems try to minimize their free energy–the same is true for liquid crystals. Therefore, what I am doing is finding the "energetically-cheapest" configuration, $\vec{n}(x, y, z)$. It is this configuration that we'd expect to find in nature.

Throughout my project, I have assumed that the liquid crystal sample is only two-dimensional. Our system consists of a thin sheet of liquid crystal material. In what follows, I examine the possible states for such a sample of liquid crystal material confined to a disk of radius R, as in a petri dish.

2.2.1 The Frank Free Energy

The Frank free energy for a three-dimensional sample of liquid crystal (LC) material is given by:

$$F = \frac{1}{2} \int d^2x \Big\{ k_1(\vec{\nabla} \cdot \vec{n})^2 + \ k_2(\vec{n} \cdot (\vec{\nabla} \times \vec{n}))^2 + \ k_3(\vec{n} \times (\vec{\nabla} \times \vec{n}))^2 \Big\} \tag{2.1}$$

where the integral is over the physical region of liquid crystalline material. The three elastic constants, k_1, k_2, k_3, represent the LC's resistance to splay, twist, and bend distortions, respectively. There are essentially three ways to distort a nematic liquid crystal, and each way has a different energy cost associated with it. These 3 constants describe this energy cost. Actually, the second constant, k_2 describes deformations that are only possible in 3 dimensions. Throughout my project I have restricted myself to only two dimensions, so I'll neglect the k_2 term. These deformations are pictured in below in Figure 2.1.

Here I would like to point out a correspondence between splay and bend deformations and aster and vortex patterns. In an aster, the liquid crystal orientation splays radially outward. An aster is a purely splay-type of deformation. Conversely, a vortex is a pure bend-type of deformation because the orientation bends around the vortex center without splaying outwards at all. Therefore, the two main patterns I deal with in my thesis are intrinsically related to the two main types of ways a 2D liquid crystal material may be deformed.

To describe the configuration of a nematic liquid crystal in two dimensions, a two-valued orientation field $\vec{n}(x, y)$ is needed. If we demand that the length of the orientation field is constant everywhere, and that this constant value is 1, than our field becomes a scalar field. To describe a vector in two dimensions, two numbers are needed, one that describes the length of the vector, and one number to give the angle that the vector makes with an arbitrary axis (we'll use the positive x-axis). By demanding that the length of vectors is constant, we only need to know the angle in order to specify the vector field throughout the liquid crystal material. We may replace the order parameter $\vec{n}(x, y)$ with an scalar field, $\theta(x, y)$. The orthogonal components of $\vec{n}(x, y)$ are related to $\theta(x, y)$ by: $n_x = |\vec{n}| \cos\theta = \cos\theta$, $n_y = |\vec{n}| \sin\theta = \sin\theta$.

Now that I have made the assumption that the orientation field has constant

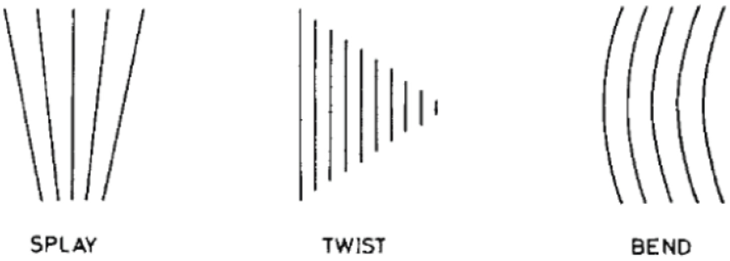

Figure 2.1: The three principal deformations in a liquid crystal. Image courtesy of S. Chandrasekhar and G. S. Ranganath, The structure and energetics of defects in liquid crystals.

length everywhere, I need to reformulate the Frank free energy in terms of θ, which I do term-by-term.

The Splay Term The splay term in the free energy may be written in terms of the θ field as:

$$\Big(\nabla \cdot \vec{n}\Big)^2 = \Big(\frac{\partial n_x}{\partial x} + \frac{\partial n_y}{\partial y}\Big)^2 = \theta_y^2 \cos^2\theta + \theta_x^2 \sin^2\theta - \theta_x\theta_y \sin 2\theta$$

The Twist Term The twist term in the free energy always vanishes in two dimensions, that is, $\vec{n} \cdot (\vec{\nabla} \times \vec{n}) = 0$. To explicitly show this, first calculate the curl of $\vec{n}$:

$$\vec{\nabla} \times \vec{n} = det \begin{pmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ n_x & n_y & n_z \end{pmatrix} = \Big(\frac{\partial n_y}{\partial x} - \frac{\partial n_x}{\partial y}\Big)\hat{k}.$$

The order parameter is restricted to the XY plane, $\vec{n} = (n_x, n_y, 0)$, $\vec{n}$ and its curl are orthogonal, and their dot product will always vanish:

$$\vec{n} \cdot (\vec{\nabla} \times \vec{n}) = 0$$

Therefore, LC materials restricted to thin planes are not subject to twist stresses.

The Bend Term

$$\Big(\vec{n} \times \Big(\vec{\nabla} \times \vec{n}\Big)\Big)^2 = \theta_x^2 \cos^2\theta + \theta_y^2 \sin^2\theta + \theta_x\theta_y \sin 2\theta$$

2.2.2 Reformulating the Free Energy in Terms of the Angular Order Parameter Field

First, we introduce two new constants, $J \equiv \frac{(k_1+k_3)}{2}$, and $\Delta \equiv \frac{(k_1-k_3)}{2}$. For two-dimensional samples, Δ represents a measure of the material's elastic anisotropy. Noting that $k_1 = (J+\Delta)$, $k_2 = (J-\Delta)$, We now rearrange the terms of the Frank free energy:

$$F = \frac{1}{2}\int d^2x\Big\{(J+\Delta)(\vec{\nabla}\cdot\vec{n})^2 + (J-\Delta)\big[\vec{n}\times(\vec{\nabla}\times\vec{n})\big]^2\Big\} \tag{2.2}$$

Substituting our results for the splay and bend terms, we obtain Deem's second equation:

$$F = \frac{J}{2}\int d^2x(\theta_x^2+\theta_y^2) + \frac{\Delta}{2}\int d^2x(\cos 2\theta)(\theta_y^2-\theta_x^2) - \Delta\int d^2x(\sin 2\theta)\theta_x\theta_y \tag{2.3}$$

2.2.3 Logarithmic Dependence of the Free Energy as $r \to \infty$

So far I have done my calculations in Cartesian coordinates. I'm free to use whichever coordinate system I like, but polar coordinates are a more natural coordinate system because of the geometry of the system. In the Appendix I perform the conversion from Cartesian to polar coordinates.

Rewrite $\vec{n}$, the order parameter field, in terms of the vectors $\hat{r}$ and $\hat{\phi}$.

$$\vec{n} = \cos\theta\hat{x} + \sin\theta\hat{y} = \cos(\theta-\phi)\hat{r} + \sin(\theta-\phi)\hat{\phi} = \cos\psi\hat{r} + \sin\psi\hat{\phi}$$

Where $\psi(r,\phi) \equiv \theta(r,\phi) + \phi$

We express the above free energy in terms of polar coordinates. This will allow me to easily exploit the fact that as sample sizes grow ($R \to \infty$), the θ-field must go to a constant for large r if the Frank free energy is to be both non-zero and non-singular. I now use polar coordinates to easily show that for large r the free energy has a logarithmic dependence on the system radius, R. Using the results contained in the Appendix, we may rewrite Deem's free energy in polar coordinates:

$$F = \frac{J}{2}\int dx^2(\theta_x^2+\theta_y^2) + \frac{\Delta}{2}\int dx^2(\cos 2\theta)(\theta_y^2-\theta_x^2) - \Delta\int dx^2(\sin 2\theta)\theta_x\theta_y$$

$$\begin{aligned} F &= \frac{J}{2}\int rdrd\phi(\theta_r^2+\frac{\theta_\phi^2}{r^2}) \\ &+ \frac{\Delta}{2}\int rdrd\phi(\cos 2\theta)\left[-(\cos 2\phi)\theta_r^2 + \frac{(\cos 2\phi)}{r^2}\theta_\phi^2 + \frac{2(\sin 2\phi)\theta_r\theta_\phi}{r}\right] \\ &- \Delta\int rdrd\phi(\sin 2\theta)\left[\frac{(\sin 2\phi)}{2}\theta_r^2 - \frac{(\sin 2\phi)}{2r^2}\theta_\phi^2 + \frac{(\cos 2\phi)}{r}\theta_r\theta_\phi\right] \end{aligned}$$

Now we impose the condition that $\theta(r,\phi) \sim \theta(\phi)$. We should expect this to hold for large r; at distances far from the origin, the θ-field should only vary with ϕ. This condition requires that $\theta_r \to 0$ as $r \to \infty$.

$$F \sim \int r dr d\phi \left\{ J\frac{\theta_\phi^2}{2r^2} + \Delta \cos 2\theta \frac{\cos 2\phi}{2r^2}\theta_\phi^2 + \Delta \sin 2\theta \frac{\sin 2\phi}{2r^2}\theta_\phi^2 \right\}$$

We may now integrate with respect to r. What are the limits of integration? The upper limit should represent the sample size, call it R. We would like to use 0 as our lower limit of r, but we risk extending beyond the regime where the order parameter is defined. The order parameter field describes the *local* orientation of the molecules at a given point, and so there is some cutoff distance of the molecular scale. Let us call this minimal distance a_0.

$$\begin{aligned} F &\sim \int_{a_0}^{R} \frac{dr}{r} \int_0^{2\pi} \frac{d\phi}{2} \left\{ J\theta_\phi^2 + \Delta \cos 2\theta \cos 2\phi \theta_\phi^2 + \Delta \sin 2\theta \sin 2\phi \theta_\phi^2 \right\} \\ &= \ln \frac{R}{a_0} \int_0^{2\pi} \left(\frac{d\phi}{2}\right) \theta_\phi^2 \left\{ J + \Delta \cos 2\theta \cos 2\phi + \Delta \sin 2\theta \sin 2\phi \right\} \end{aligned}$$

Making use of the angle addition formula $\cos(\alpha \pm \beta) = \cos\alpha \cos\beta \mp \sin\alpha \sin\beta$, and the fact that cosine is an even function, we obtain Deem's equations (3) and (4):

$$F \sim \left(\ln \frac{R}{a_0}\right) \int_0^{2\pi} \left(\frac{d\phi}{2}\right) \theta_\phi^2 \left\{ J + \Delta \cos \left[2\phi - 2\theta(\phi)\right] \right\} \tag{2.4}$$

2.2.4 The Search for Physical Solutions

Minimization of the Free Energy Functional (Cartesian)

We have succeeded in writing down the Free Energy in polar coordinates for the two-dimensional nematic system. Systems will naturally seek out states of minimal energy. Our next step is to compute the functional derivative of the Free Energy with respect to the order parameter field and set the resulting equation equal to 0. Functional differentiation may be defined in a few different ways. One is in terms of a limit and the Dirac delta function. For a functional, F, of a single-variable function, $\theta(x)$, the Functional derivative is defined as:

$$\frac{\delta F[\theta(x)]}{\delta \theta(y)} \equiv \lim_{\epsilon \to 0} \frac{F[\theta(x) + \epsilon \delta(x-y)] - F[\theta(x)]}{\epsilon} \tag{2.5}$$

Extended to functions of two variables, the functional derivative is defined:

$$\frac{\delta F[\theta(x,y)]}{\delta \theta(x',y')} \equiv \lim_{\epsilon \to 0} \frac{F[\theta(x,y) + \epsilon \delta(x-x')\delta(y-y')] - F[\theta(x,y)]}{\epsilon} \tag{2.6}$$

An equivalent way of computing the functional derivative involves the use of infinitesimal variations and δ notation. δ represents an infinitesimal variation of a function. The variation is constrained to be zero at the endpoints of a function. Barring a rigorous and dry mathematical definition, the variation can be a somewhat vague concept so I'll use an analogy to describe it. Think of a function, f, as a piece of string lying on the ground. The string has some sort of a configuration–it will have some particular curvy shape. If we use thumbtacks to pin down the ends of the string, and then gently tug on the string, the pattern will be slightly distorted. This new string configuration is the variation. Using the what is called the calculus of variations, the functional derivative bears great similarity to the ordinary derivative. Let f(x) be a function of the variable x, and let G[f(x)] be a functional of the function f. The derivative of f with respect to x is defined as:

$$\frac{df(x)}{dx} \equiv \lim_{h\to 0} \frac{f(x+h)-f(x)}{h}$$

And the functional derivative can be loosely defined as:

$$\frac{\delta G[f]}{\delta f} \equiv \lim_{\delta f\to 0} \frac{G[f+\delta f]-G[f]}{\delta f}$$

Here the limit is taking the variation (which is itself a function) to the zero function.

Below I calculate the functional derivative of the free energy using this method of variations, which will allow me to find the configurations that minimize the system's energy. I first perform the calculation for Cartesian coordinates, and then I convert it into polar coordinates.

In Cartesian coordinates:

$$F[\theta] = \frac{J}{2}\int d^2x(\theta_x^2+\theta_y^2) + \frac{\Delta}{2}\int d^2x(\cos 2\theta)(\theta_y^2-\theta_x^2) - \Delta\int d^2x(\sin 2\theta)\theta_x\theta_y$$

$$\begin{aligned}
F[\theta+\delta\theta]-F[\theta] &= \frac{J}{2}\int d^2x\Big[2\theta_x\delta\theta_x+(\delta\theta_x)^2+2\theta_y\delta\theta_y+(\delta\theta_y)^2\Big] \\
&+ \frac{\Delta}{2}\int d^2x\cos 2\theta\Big[2\theta_y\delta\theta_y+(\delta\theta_y)^2-2\theta_x\delta\theta_x-(\delta\theta_x)^2\Big] \\
&- \Delta\int d^2x\sin 2\theta\Big[\theta_y^2+2\theta_y\delta\theta_y+(\delta\theta_y)^2-\theta_x^2-2\theta_x\delta\theta_x-(\delta\theta_x)^2\Big]\delta\theta \\
&- \Delta\int d^2x\sin 2\theta\Big[\theta_x\delta\theta_y+\theta_y\delta\theta_x+\delta\theta_x\delta\theta_y\Big] \\
&- 2\Delta\int d^2x\cos 2\theta\Big[\theta_x\theta_y+\theta_x\delta\theta_y+\theta_y\delta\theta_x+\delta\theta_x\delta\theta_y\Big]\delta\theta
\end{aligned}$$

To first order in $\delta\theta$,

$$\begin{aligned}
F[\theta+\delta\theta]-F[\theta] &= \frac{J}{2}\int d^2x\Big[2\theta_x\delta\theta_x+2\theta_y\delta\theta_y\Big] \\
&+ \Delta\int d^2x\cos(2\theta)\Big[\theta_y\delta\theta_y-\theta_x\delta\theta_x-2\theta_x\theta_y\delta\theta\Big] \\
&- \Delta\int d^2x\sin(2\theta)\Big[\theta_y^2\delta\theta-\theta_x^2\delta\theta+\theta_x\delta\theta_y+\theta_y\delta\theta_x\Big]
\end{aligned}$$

Now we will use integration by parts to transfer the partial derivative acting on the δ-variation to instead act upon the whole term. In performing this step it is important to bring the derivative to the very forefront of the expression. It is also important to remember that integration by parts introduces a sign change.

$$\begin{aligned}
F[\theta+\delta\theta]-F[\theta] &= \int d^2x\Bigg\{-J\left[\frac{\partial}{\partial x}\theta_x+\frac{\partial}{\partial y}\theta_y\right] \\
&+ \Delta\Bigg[-\frac{\partial}{\partial y}\cos(2\theta)\theta_y+\frac{\partial}{\partial x}\cos(2\theta)\theta_x-2\cos(2\theta)\theta_x\theta_y \\
&- \sin(2\theta)\theta_y^2+\sin(2\theta)\theta_x^2+\frac{\partial}{\partial y}\sin(2\theta)\theta_x+\frac{\partial}{\partial x}\sin(2\theta)\theta_y\Bigg]\Bigg\}\delta\theta
\end{aligned}$$

We therefore arrive at Deem's equation number 6:

$$\frac{\delta F}{\delta\theta} = -J\big(\theta_{xx}+\theta_{yy}\big)+\Delta\sin 2\theta\big(\theta_y^2-\theta_x^2+2\theta_{xy}\big)+\Delta\cos 2\theta\big(\theta_{xx}-\theta_{yy}+2\theta_x\theta_y\big) \tag{2.7}$$

From this equation, one can see that the function $\theta =$ constant is a solution, since all the derivatives would then vanish. This constant solution corresponds to a uniform configuration of the liquid crystal – the liquid crystal molecules are on average all pointing in the same direction, and there is no spatial variation or interesting pattern. This solution is trivial and rather dull, and we would like to search for more complicated configurations that also minimize the free energy. Since we are using a disk geometry, our search would be made easier if we were to use polar coordinates. In the Appendix, I carry out the calculations necessary to convert this functional derivative into

2D polar coordinates. In polar coordinates, Deem's equation (6) becomes:

$$\begin{aligned}
&\frac{\delta F}{\delta\theta} = -J\Big(\psi_{rr} + \psi_{\phi\phi} + \frac{\psi_r}{r}\Big) \\
&+\Delta\sin(2s\phi + 2\psi)\Big[-\cos 2\phi(\psi_r)^2 + \frac{2\sin 2\phi}{r}(s+\psi_\phi)\psi_r + \frac{\cos 2\phi}{r^2}(s+\psi_\phi)^2 \\
&+\sin 2\phi\psi_{rr} - \frac{2\cos 2\phi}{r^2}(s+\psi_\phi) - \frac{\sin 2\phi}{r^2}\psi_{\phi\phi} + \frac{2\cos 2\phi}{r}\psi_{r\phi} - \frac{\sin 2\phi}{r}\psi_r\Big] \\
&+\Delta\cos(2s\phi + 2\psi)\Big[\cos 2\phi(\psi_{rr}) + \frac{2\sin\phi}{r^2}(s+\psi_\phi) - \frac{\cos 2\phi}{r^2}(\psi_{\phi\phi}) \\
&-\frac{2\sin 2\phi}{r}(\psi_{r\phi}) - \frac{\cos 2\phi}{r}(\psi_r) + \sin 2\phi(\psi_r)^2 + \frac{2\cos 2\phi}{r}(s+\psi_\phi)\psi_r \\
&-\frac{\sin 2\phi}{r^2}(s+\psi_\phi)^2\Big]
\end{aligned}$$

Where I have chosen to write θ as $s\phi + \psi(r,\phi)$. If we further specify the director field to have s=1, i.e. $\theta(r,\phi) = \phi + \psi(r,\phi)$ we obtain:

$$\begin{aligned}
\frac{\delta F}{\delta\theta} &= -J\Big(\psi_{rr} + \psi_{\phi\phi} + \frac{\psi_r}{r}\Big) + \Delta\cos(2\psi)\Big[\frac{2(1+\psi_\phi)\psi_r}{r} + \psi_{rr} - \frac{\psi_{\phi\phi}}{r^2} - \frac{\psi_r}{r}\Big] \\
&- \Delta\sin(2\psi)\Big[\psi_r^2 + \frac{(1+\psi_\phi)}{r^2} - \frac{2\psi_{r\phi}}{r}\Big] \qquad (2.8)
\end{aligned}$$

If ψ has no angular dependence, $\psi_\phi = 0$, and we obtain:

$$\frac{\delta F}{\delta\theta} = -\Big[J - \Delta\cos(2\psi)\Big]\Big[\frac{\psi_r}{r} + \psi_{rr}\Big] - \Delta\sin(2\psi)\Big[\psi_r^2 + \frac{1}{r^2}\Big] \qquad (2.9)$$

This is the equation we've been looking for. It is the functional derivative of the free energy with respect to the order parameter field. We expect that the configurations that the liquid crystal system should form in nature are ones that minimize this free energy, i.e, solutions of $\delta F/\delta\theta = 0$. We therefore search for functions (configurations) such that the above functional derivative vanishes.

Two obvious solutions are the constant solutions $\psi = 0, \pi$. Since these solutions are constant, the derivatives ψ_r all vanish, as well as the $\sin 2\psi$ term. What does it mean that ψ is constant with the above values? $\psi = 0, \pi$ corresponds to $\theta = \phi, \phi + \pi$, respectively. This implies that $\vec{n} = (\cos\phi, \sin\phi)$ or $-(\cos\phi, \sin\phi)$. These are aster patterns, and are depicted in Figure 1.2(b). At all points in the material, the liquid crystal orientation points radially outward ($\psi = 0$) or inward ($\psi = \pi$) from the center (remember that we are dealing with a disk geometry).

Another set of easy solutions is $\psi = \pm\pi/2$. This implies that $\theta = \pm\pi/2 + \phi$, and that $\vec{n} = (\sin\phi, -\cos\phi)$, or $(\sin\phi, \cos\phi)$. These solutions represent clockwise and counter-clockwise vortices, as depicted in Figure 1.2(c). At all points, the orientation points tangential to the circle of radius r centered at the origin.

We have therefore succeeded in discovering two interesting, non-uniform classes of solutions–that of asters and vortices.

2.3 Stability of Physical Solutions

2.3.1 Stability and Higher Functional Derivative

Systems naturally tend toward configurations of lower free energy, and we have found two configurations (asters and vortices) which minimize the free energy. But for a solution to be *physical*, we would expect that it is also stable. If a particular solution minimizes the free energy but quickly decays into a different configuration, than we might not ever see such a configuration in nature. We would therefore like to analyze the temporal stability of these solutions–will the system settle into a given configuration as time progresses? If a system starts out near an equilibrium point and survives small perturbations, then it is said to be stable. If the perturbations push the system away from the equilibrium point, then the configuration is unstable. The stability is analyzed by assuming that if θ were to be displaced from its equilibrium value, it would relax according to:

$$\gamma\frac{\partial\theta}{\partial t} = -\frac{\delta F}{\delta\theta}$$

Here γ is a positive phenomenological constant representing friction.

Solutions that minimize the free energy cause the first functional derivative to vanish. To evaluate perturbed equilibrium solutions, we introduce a time-dependent infinitesimal variation and Taylor expand the functional derivative around the equilibrium solution, that is, around $\theta = \theta_s + \delta\theta$ where θ_s is the equilibrium solution. If the perturbation grows in time, then the configuration will be unstable. If the perturbation diminishes with time, then the system will naturally relax back into the equilibrium solution, which will be stable.

$$\gamma\frac{\partial\theta}{\partial t} = \left[-\left.\frac{\delta F}{\delta\theta}\right|_{\theta_s} - \frac{1}{1!}\left.\frac{\delta^2 F}{\delta\theta^2}\right|_{\theta_s}[\delta\theta] - \frac{1}{2!}\left.\frac{\delta^3 F}{\delta\theta^3}\right|_{\theta_s}[\delta\theta]^2 - \quad \dots \quad \right]$$

Assuming that the second derivative term is non-zero and large enough to dominate the higher derivative terms, we can truncate the series there. By definition, the first term vanishes at the static solution, so we end up with:

$$\gamma \frac{\partial \delta\theta}{\partial t} = -\frac{\delta^2 F}{\delta\theta^2}\bigg|_{\theta_s} \delta\theta$$

Therefore, we need to find the second functional derivative of the free energy. To calculate the second derivative, we will simply use the same technique as before. Note that $\partial_t \theta = \partial_t(\theta_s + \delta\theta) = \partial_t \delta\psi$, and that $\delta\theta = \delta(\phi + \psi) = \delta\psi$. I will therefore use $\delta\theta$ and $\delta\psi$ interchangeably.

$$\begin{aligned}\frac{\delta F}{\delta\theta}[\psi + \delta\psi] &= -J\Big(\frac{\psi_r}{r} + \frac{\delta\psi_r}{r} + \psi_{rr} + \delta\psi_{rr}\Big) + \Delta\cos(2\psi)\Big(\frac{\psi_r}{r} + \frac{\delta\psi_r}{r} + \psi_{rr} + \delta\psi_{rr}\Big) \\ &\quad -2\Delta\delta\psi\sin(2\psi)\Big(\frac{\psi_r}{r} + \psi_{rr}\Big) - \Delta\sin(2\psi)\Big(\psi_r^2 + 2\psi_r\delta\psi_r + \frac{1}{r^2}\Big) \\ &\quad -2\Delta\delta\psi\cos(2\psi)\Big(\psi_r^2 + \frac{1}{r^2}\Big)\end{aligned}$$

$$\begin{aligned}&\frac{\delta F}{\delta\theta}[\psi + \delta\psi] - \frac{\delta F}{\delta\theta}[\psi] = -J\Big(\frac{\delta\psi_r}{r} + \delta\psi_{rr}\Big) + \Delta\cos(2\psi)\Big(\frac{\delta\psi_r}{r} + \delta\psi_{rr}\Big) \\ &-2\Delta\delta\psi\sin(2\psi)\Big(\frac{\psi_r}{r} + \psi_{rr}\Big) - 2\Delta\sin(2\psi)\Big(\psi_r\delta\psi_r\Big) \\ &-2\Delta\delta\psi\cos(2\psi)\Big(\psi_r^2 + \frac{1}{r^2}\Big)\end{aligned}$$

$$\frac{\delta^2 F}{\delta\theta^2}\delta\psi = \lim_{\delta\psi\to 0}\frac{1}{\delta\psi}\Big(\frac{\delta H}{\delta\theta}[\psi + \delta\psi] - \frac{\delta H}{\delta\theta}[\psi]\Big)\delta\psi$$

And we obtain an expression for the second functional derivative to first order in $\delta\psi$:

$$\begin{aligned}-\frac{\delta^2 F}{\delta\theta^2}\delta\psi &= J\Big(\frac{\delta\psi_r}{r} + \delta\psi_{rr}\Big) - \Delta\cos(2\psi)\Big(\frac{\delta\psi_r}{r} + \delta\psi_{rr}\Big) \\ &+ 2\Delta\delta\psi\sin(2\psi)\Big(\frac{\psi_r}{r} + \psi_{rr}\Big) + 2\Delta\sin(2\psi)\Big(\psi_r\delta\psi_r\Big) \\ &+ 2\Delta\delta\psi\cos(2\psi)\Big(\psi_r^2 + \frac{1}{r^2}\Big)\end{aligned} \tag{2.10}$$

2.3.2 Global Perturbations to Aster and Vortex Solution

Let us study the stability of two simple solutions, Asters and Vortices ($s = 1$) to global perturbations. Global perturbations are uniform throughout the material–at each point the orientation is shifted by some small angle, $\delta\psi$. The director field takes the form $\theta(r, \phi) = \phi + \psi$, where $\psi = 0, \pi$ for asters and $= \pm\frac{\pi}{2}$ for vortices. Using these conditions, we arrive at the stability equations for asters and vortices, respectively:

$$\gamma\frac{\partial \delta\psi}{\partial t} = (J - \Delta)\Big[\delta\psi_{rr} + \frac{\delta\psi_r}{r} + \frac{2\Delta}{(J - \Delta)}\frac{\delta\psi}{r^2}\Big] \tag{2.11}$$

$$\gamma\frac{\partial\delta\psi}{\partial t} = (J+\Delta)\Big[\delta\psi_{rr} + \frac{\delta\psi_r}{r} - \frac{2\Delta}{(J+\Delta)}\frac{\delta\psi}{r^2}\Big] \tag{2.12}$$

If we only consider global perturbations, that is $\delta\psi_r = 0$, the problem becomes substantially easier to solve.

$$\gamma\frac{\partial\delta\psi}{\partial t} = \frac{2\Delta\delta\psi}{r^2} \qquad \text{(Aster)}$$

$$\gamma\frac{\partial\delta\psi}{\partial t} = -\frac{2\Delta\delta\psi}{r^2} \qquad \text{(Vortex)}$$

These differential equations are easily solved, yielding exponential solutions. The stability of the Aster/Vortex solutions simply depends upon the exponent's coefficients.

$$\delta\psi(r,t) = \delta\psi_0 \exp\Big(\frac{2\Delta\delta\psi}{\gamma r^2}\Big) \qquad \text{(Aster)}$$

$$\delta\psi(r,t) = \delta\psi_0 \exp\Big(\frac{-2\Delta\delta\psi}{\gamma r^2}\Big) \qquad \text{(Vortex)}$$

We have analyzed the stability of aster and vortex solutions to *global* perturbations. We began by assuming that the perturbation, $\delta\psi$ was independent of r and ϕ, and we ended up with $\delta\psi$ as a function of both r and t. Therefore, we cannot place any faith in our analysis to global perturbations–our solution violates our initial assumptions.

Let us instead investigate the stability to global perturbations in the limit of a one dimensional system. We will fix the radius at a particular value, R, and study the stability of 1D asters and vortices. This system simply consists of a ring of liquid crystal material. A simple cartoon depicting this circular liquid crystal system is given below in Figure 2.2. Our above equations then become:

$$\delta\psi(r,t) = \delta\psi_0 \exp\Big(\frac{2\Delta\delta\psi}{\gamma R^2}\Big) \qquad \text{(Aster)}$$

$$\delta\psi(r,t) = \delta\psi_0 \exp\Big(\frac{-2\Delta\delta\psi}{\gamma R^2}\Big) \qquad \text{(Vortex)}$$

Δ negative implies that asters are stable and vortices are not. Δ positive implies that asters are not stable, and vortices are. These results makes sense since $\Delta < 0$ means that $k_1 < k_3$, and splay deformations are energetically favored, and we should expect asters to form. Conversely, $\Delta > 0$ means that $k_1 > k_3$, and bend deformations are energetically favored and we should expect vortices to form.

We now move on to study the more general case of local perturbations. The differential equation becomes much more complicated in this case since the spatial derivatives are no longer zero, and we turn to the famous Bessel functions in search of a solution.

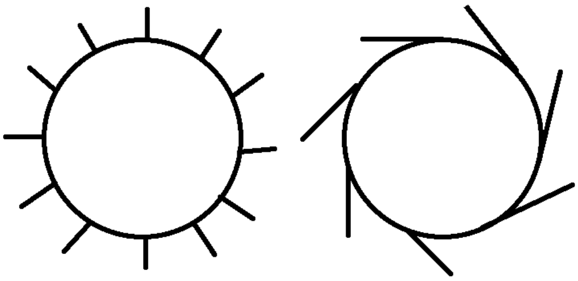

Figure 2.2: Asters and Vortices in a 1D Circular System

2.3.3 Local Perturbations to Aster and Vortex Solutions

To study stability against local perturbations, we will make use of a class of functions that are ubiquitous in the physical sciences. Bessel functions appear in heat conduction, modes of vibration on circular membranes, and diffusion problems.

Bessel Functions

Bessel functions arise when considering separable solutions to Laplace's equation in spherical coordinates:

$$\nabla^2\psi = 0 = \frac{\partial^2\psi}{\partial s^2} + \frac{1}{s}\frac{\partial\psi}{\partial s} + \frac{1}{s^2}\frac{\partial^2\psi}{\partial\phi^2} + \frac{\partial^2\psi}{\partial z^2}$$

If $\psi(s,\phi,z) = S(s)\Phi(\phi)Z(z)$, then plugging in and dividing by $S\Phi Z$ yields,

$$\nabla^2\psi = 0 = \frac{1}{S}\Big(\frac{\partial^2 S}{\partial s^2} + \frac{1}{s}\frac{\partial S}{\partial s}\Big) + \frac{1}{s^2\Phi}\frac{\partial^2\Phi}{\partial\phi^2} + \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}$$

Because each term except the last is independent of z, the last term must equal a constant, implying that $\frac{\partial^2 Z}{\partial z^2} = CZ$, where C is some constant. The third term is the only one dependent on ϕ, so it too must equal a constant: $\frac{\partial^2\Phi}{\partial\phi^2} = D\Phi$ Therefore,

$$0 = \frac{d^2S}{ds^2} + \frac{1}{s}\frac{dS}{ds} + \Big(\frac{D}{s^2} + C\Big)S$$

Letting $D = -\nu^2$ and $C = \kappa^2$,

$$0 = \frac{d^2S}{ds^2} + \frac{1}{s}\frac{dS}{ds} + \Big(\kappa^2 - \frac{\nu^2}{s^2}\Big)S$$

Changing variables so that $s = \frac{s'}{\kappa}$, we finally obtain Bessel's differential equation:

$$0 = \frac{d^2S}{ds'^2} + \frac{1}{s}\frac{dS}{ds'} + \Big(1 - \frac{\nu^2}{s'^2}\Big)S$$

Rewriting this equation to suite our current choice of notation, using primes to denote differentiation with respect to r:

$$\psi'' + \frac{1}{r}\psi' + \Big(1 - \frac{\nu^2}{r^2}\Big)\psi = 0 \tag{2.13}$$

Local Perturbations

These next few sections heavily follow notes made by Professor Marchetti.

In considering the more general case of local perturbations, we note that ψ may vary spatially. We have already assumed azimuthal symmetry, so the perturbations can only depend on r. Our goal is to solve the differential equations given by (13) and (14). Except for 2 exceptions, these equations resemble the Bessel Differential equation. The first difference is that these equations are not set equal to zero; they are equivalent to a time derivative. Secondly, they are missing the linear ψ term. However, let us ignore these obstacles for the moment and attempt to find solutions to the Bessel Differential equation that satisfy the boundary conditions of our current problem.

Bessel's Differential equation is solved by Bessel functions. There are many Bessel functions, each characterized by the constant ν. When ν is an integer, it is known as the order of the Bessel function. We write J_ν to represent the ν-th Bessel function, each of which contains an infinite number of zeroes which depend on the particular Bessel function in question. Let $\alpha_{\nu m}$ represent the m-th zero to the ν-th order Bessel function. We only consider solutions that have $\delta\psi(R) = 0$ for some R representing the radius of a two-dimensional circular sample of nematic material. We will modify the argument of the Bessel functions to represent this condition: $J_\nu(r) \to J_\nu(\alpha_{\nu m}\frac{r}{R})$.

We will make use of the orthogonality of Bessel functions of the same order:

$$\int_0^R rdr J_\nu(\alpha_{\nu m}\frac{r}{R})J_\nu(\alpha_{\nu n}\frac{r}{R}) = \begin{cases} 0 \text{ if } m \neq n \\ \frac{R^2}{2}\Big[J_\nu(\alpha_{\nu m}\frac{r}{R})\Big]^2 \text{if } m = n \end{cases} \tag{2.14}$$

We must solve a complicated differential equation, and we will make use of an important property of Bessel functions. The Bessel functions form a complete orthogonal set: any function can be represented as a linear combination of Bessel functions as long as they share the same boundary conditions. We hope to exploit the properties of Bessel functions to find an analytic solution to the coefficients; if we do so, then we will have arrived at an analytic solution to the differential equation.

The time dependence of the perturbation is manifested by allowing the

Bessel coefficients to vary with time. Our solution is of the form:

$$\delta\psi(r,t) = \sum_{m=1}^{\infty} C_{\nu m}(t) J_\nu(\alpha_{\nu m}\frac{r}{R}) \tag{2.15}$$

Next, we multiply by J_ν and integrate (in polar coordinates, so we pick up a rdr term) and exploit the orthogonality of the Bessel functions.

$$\begin{aligned}
\int \delta\psi(r,t) J_\nu(\alpha_{\nu m}\frac{r}{R}) rdr &= \int \Big[\sum_{m=1}^{\infty} C_{\nu m}(t) J_\nu(\alpha_{\nu m}\frac{r}{R}) J_\nu(\alpha_{\nu n}\frac{r}{R})\Big] rdr \\
&= \sum_{m=1}^{\infty} \Big[\int C_{\nu m}(t) J_\nu(\alpha_{\nu m}\frac{r}{R}) J_\nu(\alpha_{\nu n}\frac{r}{R}) rdr\Big] \\
&= C_{\nu m}(t)\frac{R^2}{2}\Big[J_\nu(\alpha_{\nu+1 m})\Big]^2
\end{aligned}$$

Therefore, the coefficients $C_{\nu m}$ are given by:

$$C_{\nu m}(t) = \frac{2}{R^2\big[J_\nu(\alpha_{\nu+1m})\big]^2}\int \delta\psi(r,t) J_\nu(\alpha_{\nu m}\frac{r}{R}) rdr \tag{2.16}$$

Let us first consider Aster solutions. Going back to equation (20) and plugging in the expression for $\delta\psi$:

$$\gamma\frac{\partial\delta\psi}{\partial t} = \sum_{m=1}^{\infty} \dot{C}_{\nu m}(t) J_\nu(\alpha_{\nu m}\frac{r}{R}) = (J-\Delta)\Big[\delta\psi_{rr} + \frac{\delta\psi_r}{r} + \frac{2\Delta}{(J-\Delta)}\frac{\delta\psi}{r^2}\Big]$$

Now the Bessel functions, $J_\nu(\alpha_{\nu m}\frac{r}{R})$ are solutions to the differential equation:

$$\frac{d^2\psi}{dr'^2} + \frac{1}{r'}\frac{d\psi}{dr'} + (1-\frac{\nu^2}{r'^2})\psi = 0$$

where $r' = \alpha_{\nu m}\frac{r}{R}$. Changing the variable back to r, and noting that $dr' = \frac{\alpha_{\nu m}}{R}dr$ we may rewrite the above equation as:

$$\frac{d^2\psi}{dr^2} + \frac{1}{r}\frac{d\psi}{dr} + (\frac{\alpha_{\nu m}^2}{R^2} - \frac{\nu^2}{r^2})\psi = 0$$

With $\nu^2 = -\frac{2\Delta}{J-\Delta} = \frac{2\Delta}{\Delta-J} = \frac{k_3-k_1}{k_3}$ we obtain a differential equation for the Bessel coefficients:

$$\begin{aligned}
\sum_{m=1}^{\infty} \dot{C}_{\nu m}(t) J_\nu(\alpha_{\nu m}\frac{r}{R}) &= (J-\Delta)\sum_{m=1}^{\infty}\Big[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{2\Delta}{(J-\Delta)}\frac{1}{r^2}\Big] J_\nu(\alpha_{\nu m}\frac{r}{R}) \\
&= -(J-\Delta)\frac{\alpha_{\nu m}^2}{R^2}\sum_{m=1}^{\infty} C_{\nu m}(t) J_\nu(\alpha_{\nu m}\frac{r}{R})
\end{aligned}$$

We can use the same orthogonality trick as before, multiplying each side of the equation by $J_\nu(\alpha_{\nu n}\frac{r}{R})$ and integrating with respect to r. We then find:

$$\dot{C}_{\nu m}(t) = -(J-\Delta)\frac{\alpha_{\nu m}^2}{R^2}C_{\nu m}(t)$$

This rather simple differential equation is solved by an exponential function:

$$C_{\nu m}(t) = C_{\nu m}(0)\exp[(\Delta - J)\frac{\alpha_{\nu m}^2}{R^2}t]$$

where $C_{\nu m}(0)$ represents the coefficient of the Bessel function $J_\nu(\alpha_{\nu m}\frac{r}{R})$ at time $t = 0$. $\Delta - J$ is the simply negative of the Frank constant for bend distortions, k_3, and our final expression for the local perturbation of an Aster pattern is:

$$\delta\psi(r,t) = \sum_{m=1}^{\infty} C_{\nu m}(0)\exp\Big(-k_3\frac{\alpha_{\nu m}^2}{R^2}t\Big)J_\nu(\alpha_{\nu m}\frac{r}{R}) \tag{2.17}$$

The vortex case is very similar. Here, $\nu^2 = \frac{2\Delta}{J+\Delta} = \frac{k_1-k_3}{k_3}$ and the $-(J-\Delta)$ factor in the exponential is replaced by $-(J+\Delta) = -k_1$.

$$\delta\psi(r,t) = \sum_{m=1}^{\infty} C_{\nu m}(0)\exp\Big(-k_1\frac{\alpha_{\nu m}^2}{R^2}t\Big)J_\nu(\alpha_{\nu m}\frac{r}{R}) \tag{2.18}$$

The Bessel roots, the $\alpha_{\nu m}^2$ are real when $\nu^2 > 0$ Therefore, we again obtain the intuitive stability conditions: Aster solutions are stable for $k_3 > k_1$ and Vortex solutions are stable for $k_1 > k_3$. Having $\nu^2 < 0$ entails that some of the Bessel roots will be imaginary. An imaginary Bessel root will cause that particular coefficient to not exponentially decay, but to exponentially grow instead. Thus, a single imaginary root cause the perturbation to destroy the initial aster/vortex solution. Our final results in the anisotropic case $k_1 \neq k_3$ are as follows:

Aster solutions stable for $k_3 > k_1$, and unstable for $k_1 > k_3$.

Vortex solutions stable for $k_1 > k_3$, and unstable for $k_3 > k_1$.

2.4 Spiral Solutions in the Isotropic Approximation

We consider strength s=1 solutions that minimize the system's free energy when the two Frank constants are equal, $k_1 = k_3 = K$. This is known as the isotropic approximation because it implies that the liquid crystal resists bend and splay deformations equally. This section follows entirely from Professor Marchetti's notes. When $\Delta = 0$, $J = K$, and my equation (16) for the first functional derivative of the free energy is:

$$\gamma \frac{\delta H}{\delta \theta} = -K\nabla^2\theta$$

For order parameter fields of the form $\theta(r,\phi) = \phi + \psi(r,\phi)$, we have:

$$\gamma \frac{\partial \psi}{\partial t} = -\frac{\delta H}{\delta \theta} = K\nabla^2\psi$$

If we search for stationary solutions, $\frac{\partial \psi}{\partial t} = 0$, we have

$$0 = K\left[\frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial \psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial \psi}\right]$$

We may obtain an interesting set of solutions by making a variable change

$$\frac{\partial}{\partial r} = \frac{1}{r}\frac{\partial}{\partial \ln r}$$

Our equation then takes the form:

$$\nabla^2\psi = \frac{\partial \psi^2}{\partial \ln^2 r} + \frac{\partial^2\psi}{\partial^2\phi} = 0$$

Making the variable change $x = \frac{\ln(\frac{r}{r_0})}{\phi}$, we find that

$$\left(\frac{\partial \psi}{\partial r}\right)_\phi = f'\frac{\partial x}{\partial r} = \frac{1}{r\phi}f'$$

$$\left(\frac{\partial^2\psi}{\partial r^2}\right)_\phi = -\frac{1}{r^2\phi}f' + (\frac{1}{r\phi})^2 f''$$

$$\left(\frac{\partial \psi}{\partial \phi}\right)_r = -\frac{x}{\phi}f'$$

$$\left(\frac{\partial^2\psi}{\partial \phi^2}\right)_r = \frac{2x}{\phi^2}f' + \frac{x^2}{\phi^2}f''$$

substituting we find:

$$\frac{2x}{r^2\phi^2}f' + \frac{x^2}{r^2\phi^2}f'' - \frac{1}{r^2\phi}f' + \frac{1}{r^2\phi^2}f'' + \frac{1}{r^2\phi}f' = 0$$

$$(1+x^2)f'' + 2xf' = 0$$

Letting $u = (1+x^2)f'$,

$$\frac{du}{dx} = (1+x^2)f'' + 2xf' = 0$$

Since $\frac{du}{dx} = 0$, we know that u(x) must be a constant, call it C_1.

$$f' = \frac{u(x)}{1+x^2} = \frac{C_1}{1+x^2}$$

which gives us a solution for f(x):

$$f(x) = C_0 + C_1 arccot(x)$$

We therefore obtain the following solution

$$\psi(r,\phi) = C_0 + C_1 arccot\Big(\frac{\ln(r/r_0)}{\phi}\Big)$$

C_0 is an arbitrary angle, which we set equal to zero. C_1 specifies $\psi(r = r_0, \phi)$ at the molecular cut-off distance. If we look for solutions that begin as vortices with $\psi = \pm\frac{\pi}{2}$ near the center, then we may set $C_1 = \pm 1$ because $\psi(r_0, \phi) = \pm\frac{\pi}{2}$. Noting that as $r \to \infty$, $\psi \to 0$, we see that these solutions asymptotically become asters. Our order parameter field takes the form

$$\theta(r,\phi) = \phi \pm arccot\Big(\frac{\ln(r/r_0)}{\phi}\Big) \tag{2.19}$$

With C_1 set to $\pm\frac{\pi}{2}$, these solutions take the form of vortices at the cut-off distance r_0, and asters as $r \gg r_0$. The constant C_0 here merely represents an overall rotation of the system, and does not affect the structure of the solutions. C_1 controls the order parameter orientation at $r = r_0$. For $\psi(r = r_0, \phi) = 0$, the solution is exactly that of an aster. For all other values of C_1, our solution represents a pattern that begins as a vortex near the cut-off distance, and spirals into an aster solution at larger values of r. We have therefore found a steady-state spiral pattern for the isotropic approximation.

2.5 Spiral Patterns induced by Boundary Conditions

2.5.1 Review of D. R. M. Williams' Work

In **Nematic liquid crystals between antagonistic cylinders: Spirals with bend-splay director undulations**, Phys. Rev. E **50** 1686(1994), D. Williams examines spiral patterns that arise when the director is constrained to certain boundary conditions. The LC is constrained to lie between two concentric cylinders, and the director field is additionally constrained to be perpendicular to the cylindrical axis. Following our earlier convention and letting ψ denote the angle between the radial unit vector and the orientation of the director, we may write the order parameter field in cylindrical coordinates as $\vec{n}(r, \phi, z) = (\cos\psi, \sin\psi, 0)$. Therefore, a value of $\psi = 0, \pi$ will yield a radial orientation, while $\psi = \pm\frac{\pi}{2}$ will yield a tangential orientation. We consider a setup such that ψ is radial along the surface of the inner cylindrical wall, and makes some non-zero angle α with the outer wall. We will also assume cylindrical symmetry. Letting r_1, r_2 denote the inner and outer cylindrical radii, respectively, our free energy looks like:

$$H = \int_0^{2\pi} d\phi \int_{r_1}^{r_2} rdr \Big[(J - \Delta)\psi_r^2 - 2\Delta\frac{\psi^2}{r^2}\Big]$$

We then make the useful variable change $t = \ln(r/r_1)$. Noting that

$$\frac{d\psi}{dr} = \frac{d\psi}{dt}\frac{dt}{dr} = \frac{1}{r}\frac{d\psi}{dt}$$

$$dr = rdt$$

We may use the chain rule and integrate over ϕ to obtain:

$$H \propto \int_{\ln r_1}^{\ln r_2} dt \Big[\dot{\psi}^2 - \frac{2\Delta}{J - \Delta}\psi^2\Big] = \int_{\ln r_1}^{\ln r_2} dt \Big[\dot{\psi}^2 - \frac{k_1 - k_3}{k_3}\psi^2\Big] \tag{2.20}$$

Where the dot indicates differentiation with respect to time, as usual. This equation is similar to the action of a particle in a parabolic potential well. The action $\mathcal{S}$ is a functional of the Lagrangian $\mathcal{L}$ for a system with generalized coordinates q_i:

$$\mathcal{S}[q_i(t)] \equiv \int_{t_1}^{t_2} \mathcal{L}[q_i(t), \dot{q}_i(t), t]dt$$

where $\mathcal{L} \equiv T - V$, with T and V the kinetic and potential energy terms, respectively. If we consider a particle with one generalized coordinate, ψ, subject to a potential of the form $V(\psi) = \frac{mk}{2}\psi^2$, k being a positive constant and m being the particle's mass, then we find that:

$$\mathcal{L} = \frac{1}{2}m\dot{\psi}^2 - \frac{mk}{2}\psi^2$$

We then minimize the free energy and search for solutions to the Euler-Lagrange equation:

$$\frac{\partial \mathcal{L}}{\partial \psi} = \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{\psi}} \implies -k\psi = \ddot{\psi}$$

Letting $k = \frac{k_1 - k_3}{k_3}$, we note that the expression for the action of a particle trapped in a parabolic potential well is the same as (29). Therefore, we search for solutions for ψ that satisfy

$$\ddot{\psi} = -k\psi = -\Big(\frac{k_1 - k_3}{k_3}\Big)\psi$$

The solution depends on the relative strengths of the Frank constants. We have three cases to consider.

Case 1: $k_1 = k_3$, the isotropic case We have the easy differential equation to solve:

$$\ddot{\psi} = 0 \Longrightarrow \psi(t) = C_1 t + C_2$$

where the C's are constants of integration. Changing variables back to r, we find

$$\psi(r) = C_1 \ln(r/r_1) + C_2$$

Dropping the constant rotation term C_2, and fixing C_1 so that ψ fits our boundary conditions, $\psi(r_1) = 0$, $\psi(r_2) = \alpha$,

$$\psi(r) = \alpha \frac{\ln(r/r_1)}{\ln(r_2/r_1)} \tag{2.21}$$

Case 2: $k_1 > k_3$ Here k is a positive constant, and our differential equation is solved by sinusoidal solutions:

$$\psi(t) = C_1 \cos(\sqrt{k}t) + C_2 \sin(\sqrt{k}t)$$

Noting that $t = 0$ and $t = \ln(r_2/r_1)$ correspond to $r = r_1$ and $r = r_2$, respectively, we may solve for the constants

$$\psi(t = 0) = 0 \Longrightarrow C_1 = 0$$

$$\psi\big(t = \ln(r_2/r_1)\big) = C_2 \sin\left(\sqrt{k}\ln(r_2/r_1)\right) = \alpha \Longrightarrow C_2 = \frac{\alpha}{\sin\left(\sqrt{k}\ln(r_2/r_1)\right)}$$

Then our final solution is of the form:

$$\psi(r) = \alpha \frac{\sin\left(\sqrt{k}\ln(r/r_1)\right)}{\sin\left(\sqrt{k}\ln(r_2/r_1)\right)} \tag{2.22}$$

Case 3: $k_3 > k_1$ Now k is negative, and our solution will be comprised of exponentials:

$$\psi(t) = C_1 \exp(\sqrt{-k}t) + C_2 \exp(-\sqrt{-k}t)$$
$$\psi(t = 0) = C_1 + C_2 = 0 \Longrightarrow C_1 = -C_2$$

$$\begin{aligned}
\psi\big(t = \ln(r_2/r_1)\big) &= C_1\Big(\exp\left[\sqrt{-k}\ln(r_2/r_1)\right] - \exp\left[-\sqrt{-k}\ln(r_2/r_1)\right]\Big) \\
&= 2C_1 \sinh\left[\sqrt{-k}\ln(r_2/r_1)\right] = \alpha \Longrightarrow \\
& C_1 = \frac{\alpha}{2\sinh\left[\sqrt{-k}\ln(r_2/r_1)\right]}
\end{aligned}$$

And we find

$$\psi(r) = \alpha \frac{\sinh\left[\sqrt{-k}\ln(r/r_1)\right]}{\sinh\left[\sqrt{-k}\ln(r_2/r_1)\right]} \tag{2.23}$$

The argument of the sine function for the second case is: $\sqrt{k}\ln(r/r_1)$. If we consider t-space, then these solutions have an angular frequencies $\sqrt{k}$ which only depend on the relative strengths of the bend and splay Frank constants. If the maximum value of the argument, $\sqrt{k}\ln(r_2/r_1)$, exceeds 2π, then the director will have made one or more complete oscillations. Letting $\lfloor x \rfloor$ denote the floor function, also known as the greatest integer function, then the number of complete oscillations, n, made by the director field is given by:

$$n = \left\lfloor \frac{\sqrt{k}\ln(r_2/r_1)}{2\pi} \right\rfloor$$

With the ansatz that the angles made by the director at the boundary of each cylindrical wall are non-equal, $\psi(r_1) \neq \psi(r_2)$, we have ensured that

$$n = \left\lfloor \frac{\sqrt{k}\ln(r_2/r_1)}{2\pi} \right\rfloor \neq \frac{\sqrt{k}\ln(r_2/r_1)}{2\pi}$$

that is, the director is prevented from integral number of oscillations.
The director orientation in the two cases of unequal Frank constants is depicted below in Figure 2.2.

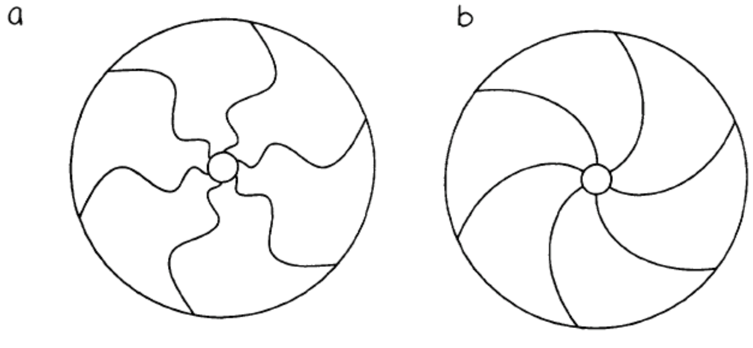

FIG. 2. The director orientation between the cylinder in the two cases. (a) $K_s/K_b = 26 > 1$, so the bends to escape splay. (b): $K_s/K_b = 0.5 < 1$; there are no oscillations. We have chosen $r_2/r_1 = 10$ and the anchoring angle $\alpha = 1$, to make the oscillations clear. The director is tangent to the curves at each point.

Figure 2.3: The three principal deformations in a liquid crystal. Image and caption courtesy of D.R.M. Williams, Nematic liquid crystals between antagonistic cylinders: Spirals with bend-splay director undulations.

2.5.2 Extension of Williams' work to Polar Liquid Crystals

We are interested in examining the behavior of polar liquid crystals when subjected to the same conditions as in Williams' work on nematic liquid crystals. The free energy per length functional for a polar substance in two dimensions is the same as that of a nematic material with the exception of an additional term representing spontaneous splay. To emphasize the fact that our order parameter now describes polar materials, we use $\hat{p}$ to describe the director field:

$$H = \frac{1}{2}\int d^2x\Big\{k_1(\nabla\cdot\hat{p})^2 + \ k_3[\hat{p}\times(\nabla\times\hat{p})]^2 + k(\nabla\cdot\hat{p})\Big\} \tag{2.24}$$

We will use the same order parameter formulation used in the nematic case. The cylindrical symmetry of the problem naturally suggests the use of cylindrical coordinates: $\hat{p} = \hat{r}\cos\psi + \hat{\phi}\sin\psi$. We also note that $\frac{\partial\psi}{\partial\phi} = \psi_\phi$, the angular derivative of ψ, must be zero if the configuration is to exhibit cylindrical symmetry. We also make the assumption that $\psi << 1$. Let us now search for solutions which minimize the free energy.

$$\begin{aligned}\nabla\cdot\hat{p} &= \frac{1}{r}\frac{\partial}{\partial r}(r\cos\psi) + \frac{1}{r}\frac{\partial}{\partial\phi}(\sin\psi)\\ &= \frac{1}{r}\frac{\partial}{\partial r}(r\psi_r\cos\psi)\end{aligned}$$

$$(\nabla\cdot\hat{p})^2 = \frac{\cos^2\psi}{r^2} + \psi_r^2\sin^2\psi - \frac{\psi_r}{r}\sin 2\psi$$

$$\nabla\times\hat{p} = \frac{\hat{z}}{r}\Big[\frac{\partial}{\partial r}(r\sin\psi) - \frac{\partial}{\partial\phi}(\cos\psi)\Big] = \frac{\hat{z}}{r}\Big[\sin\psi + r\cos\psi\Big]$$

$$\hat{p}\times(\nabla\times\hat{p}) = det\begin{pmatrix}\hat{r} & \hat{\phi} & \hat{z}\\ \cos\psi & \sin\psi & 0\\ 0 & 0 & \frac{\sin\psi}{r} + \psi_r\cos\psi\end{pmatrix}$$

$$= \hat{r}\Big[\frac{\sin^2\psi}{r} + \psi_r\sin\psi\cos\psi\Big] - \hat{\phi}\Big[\frac{\sin\psi\cos\psi}{r} + \psi_r\cos^2\psi\Big]$$

$$= \Big[\frac{\sin\psi}{r} + \psi_r\cos\psi\Big]\Big(\hat{r}\sin\psi - \hat{\theta}\cos\psi\Big)$$

$$\big[\hat{p}\times(\nabla\times\hat{p})\big]^2 = \frac{\sin^2\psi}{r^2} + \frac{\psi_r}{r}\sin 2\psi + \psi_r^2\cos^2\psi$$

We may now write a general expression for the free energy using the scalar field ψ and it's first derivatives:

$$\begin{aligned}H[\psi] &= \frac{1}{2}\int drd\phi\Bigg\{k_1\Bigg[\frac{\cos^2\psi}{r} + r\psi_r^2\sin^2\psi - \psi_r\sin 2\psi\Bigg] + k\frac{\partial}{\partial r}\Bigg[r\cos\psi\Bigg]\\ &+ \ k_3\Bigg[\frac{\sin^2\psi}{r} + \psi_r\sin 2\psi + r\psi_r^2\cos^2\psi\Bigg]\Bigg\}\end{aligned}$$

We may integrate out the spontaneous splay term since it is a total derivative:

$$\begin{aligned} H[\psi] &= \pi \int dr \Bigg\{ k_1 \left[\frac{\cos^2 \psi}{r} + r\psi_r^2 \sin^2 \psi - \psi_r \sin 2\psi \right] \\ &+ k_3 \left[\frac{\sin^2 \psi}{r} + \psi_r \sin 2\psi + r\psi_r^2 \cos^2 \psi \right] \Bigg\} + \pi k \Big[r_2 \cos \alpha - r_1 \Big] \end{aligned}$$

We now compute the functional derivative:

$$\begin{aligned} \delta H[\psi] &= \frac{1}{2} \int dr d\phi \Bigg\{ k_1 \Bigg[- \frac{\sin 2\psi \delta\psi}{r} + 2r\psi_r \sin^2 \psi \delta\psi_r + r\psi_r^2 \sin 2\psi \delta\psi \\ &- 2\psi_r \cos 2\psi \delta\psi - \sin 2\psi \delta\psi_r \Bigg] \\ &+ k_3 \Bigg[\frac{\sin 2\psi \delta\psi}{r} + 2\psi_r \cos 2\psi \delta\psi + \sin 2\psi \delta\psi_r \\ &+ 2r\psi_r \cos^2 \psi \delta\psi_r - r\psi_r^2 \sin 2\psi \delta\psi \Bigg] \Bigg\} \end{aligned}$$

Integrating by parts, we find:

$$\begin{aligned} \frac{\delta H}{\delta \psi} &= k_1 \left[- \frac{\sin 2\psi}{r} - 2r\psi_{rr} \sin^2 \psi - 2\psi_r \sin^2 \psi - r\psi_r^2 \sin 2\psi \right] \\ &+ k_3 \left[\frac{\sin 2\psi}{r} - 2\psi_r \cos^2 \psi - 2r\psi_{rr} \cos^2 \psi + r\psi_r^2 \sin 2\psi \right] \end{aligned}$$

We are interested in solutions that minimize the free energy, that is, functions $\psi(r)$ that satisfy the following differential equation:

$$\begin{aligned} 0 &= k_1 \left[- \frac{\sin 2\psi}{r} - 2r\psi_{rr} \sin^2 \psi - 2\psi_r \sin^2 \psi - r\psi_r^2 \sin 2\psi \right] \\ &+ k_3 \left[\frac{\sin 2\psi}{r} - 2\psi_r \cos^2 \psi - 2r\psi_{rr} \cos^2 \psi + \frac{r\psi_r^2}{2} \sin 2\psi \right] \end{aligned}$$

If we make the assumption that both $\psi << 1$, and $r\psi_r << 1$, then to $O(\psi^3)$:

$$\left(\frac{k_3 - k_1}{k_3} \right) \frac{\psi}{r} - \Big(\psi_r + r\psi_{rr} \Big) = 0 \tag{2.25}$$

With boundary conditions, $\psi(r_1) = 0, \psi(r_2) = \alpha$.

Divergence Theorem

This problem may be analyzed from a different perspective. The spontaneous splay term may be manipulated through the use of the divergence theorem. I will show that the additional term does not affect the form of the free energy functional. Therefore, the minimization of the nematic and polar free energies will be equivalent. Letting H_{ss} denote the free energy due solely to the spontaneous splay term, we have:

$$H_{ss} = \frac{k}{2}\int_S \Big(\nabla \cdot \vec{p}\Big) da = \frac{k}{2}\int_{\partial S} \vec{p} \cdot d\vec{s} \qquad \text{(Divergence Theorem)}$$

where S is the region enclosed by the annulus, and ∂S is the region's boundary, the circles centered at the origin of radius r_1 and r_2, and $d\vec{s} = \hat{r} r d\phi$ is a radial line element pointing to the normal of the bounding lines.

$$\begin{aligned} H_{ss} &= \frac{k}{2}\int_S \Big(\nabla \cdot \vec{p}\Big) da = \left[\frac{k}{2}\int_0^{2\pi} r d\phi \cos\psi\right]\Bigg|_{r_2} - \left[\frac{k}{2}\int_0^{2\pi} r d\phi \cos\psi\right]\Bigg|_{r_1} \\ &= k\pi\Big[r_2 \cos\psi(r_2) - r_1 \cos\psi(r_1)\Big] = k\pi\Big[r_2\cos\alpha - r_1\Big] \end{aligned}$$

Therefore, the spontaneous splay contribution to the free energy is simply a constant. Since the zero of free energy is arbitrary, translating the free energy by a constant does not affect the physics of the system, and we find that both nematic and polar liquid crystals obey the same differential equation when constrained to lie in the plane of an annulus.

2.6 Active Systems

2.6.1 Active Asters and Vortices

We now move into the more complicated physical realm of non-equilibrium processes. Outside of thermal equilibrium, it does not make sense to define a Hamiltonian, so to be precise we must technically start from scratch. However if we consider systems relatively close to equilibrium, we would expect that the general form of the behavior would be very similar to equilibrium behavior. We propose that the order parameter obeys the following equation, substituting our earlier result from the functional derivative of the Hamiltonian, even though the Hamiltonian no longer exists.

$$\gamma\frac{\partial \vec{n}}{\partial t} = -\frac{\delta H}{\delta \vec{n}} - \beta\big(\vec{n} \cdot \nabla\big)\vec{n} \tag{2.26}$$

Here $\vec{n}$ is the order parameter in vector form. The new term distinguishes the equilibrium system from the active one, and effectively describes convection. I have already reformulated the original equation in terms of the angular order parameters, $\theta(r,\phi)$ and $\psi(r,\phi)$, and I wish to do the same thing for the new convective term. For now, let's only consider this new term, adding on the old functional derivative term at the end. We really have two equations, one for each of the vector components. After playing around with each separately and then recombining them, we can reduce these two equations into one useful one. We're about to enter a jungle of trigonometry, so beware...

$$\vec{n} = \hat{x}\cos\theta + \hat{y}\sin\theta = \hat{r}\cos(\theta-\phi) + \hat{\phi}\sin(\theta-\phi)$$

$$\vec{n}\cdot\nabla = \cos\theta\partial_x + \sin\theta\partial_y$$

$$\Big(\vec{n}\cdot\nabla\Big)\vec{n} = -\hat{x}\Big(\theta_x\cos\theta\sin\theta + \theta_y\sin^2\theta\Big) + \hat{y}\Big(\theta_x\cos^2\theta + \theta_y\sin\theta\cos\theta\Big)$$

Earlier in these notes I wrote out expressions for converting unit vectors and derivatives in Cartesian coordinates into polar coordinates, and here I make use of these conversions:

$$\begin{aligned}
\Big(\vec{n}\cdot\nabla\Big)\vec{n} &= -\Big(\hat{r}\cos\phi - \hat{\phi}\sin\phi\Big)\Bigg(\theta_r\cos\theta\sin\theta\cos\phi + \theta_r\sin^2\theta\sin\phi \\
&+ \frac{\theta_\phi}{r}\sin^2\theta\cos\phi - \frac{\theta_\phi}{r}\cos\theta\sin\theta\sin\phi\Bigg) \\
&+ \Big(\hat{r}\sin\phi + \hat{\phi}\cos\phi\Big)\Bigg(\theta_r\cos^2\theta\cos\phi + \theta_r\sin\theta\cos\theta\sin\phi \\
&+ \frac{\theta_\phi}{r}\sin\theta\cos\theta\cos\phi - \frac{\theta_\phi}{r}\cos^2\theta\sin\phi\Bigg)
\end{aligned}$$

We can split the above vector equation into R- and Φ-component equations, which we can manipulate separately.

$$\begin{aligned}
&\Big[\big(\vec{n}\ \cdot\nabla\big)\vec{n}\Big]_r \\
&= \theta_r\Bigg(-\cos\theta\sin\theta\cos^2\phi - \sin^2\theta\sin\phi\cos\phi + \cos^2\theta\cos\phi\sin\phi + \sin\theta\cos\theta\sin^2\phi\Bigg) \\
&+ \frac{\theta_\phi}{r}\Bigg(\sin\theta\cos\theta\cos\phi\sin\phi + \cos\theta\sin\theta\sin\phi\cos\phi - \sin^2\theta\cos^2\phi - \cos^2\theta\sin^2\phi\Bigg) \\
&= -\theta_r\sin(\theta-\phi)\Bigg(\cos\theta\cos\phi - \sin\theta\sin\phi\Bigg) + \frac{\theta_\phi}{r}\sin(\theta-\phi)\Bigg(\sin\phi\cos\theta - \sin\theta\cos\phi\Bigg) \\
&= -\theta_r\sin(\theta-\phi)\cos(\theta-\phi) - \frac{\theta_\phi}{r}\sin^2(\theta-\phi)
\end{aligned}$$

Similarly for ϕ,

$$\begin{aligned}
&\Big[(\vec{n} \ \ \cdot\nabla)\vec{n}\Big]_\phi \\
= \ & \theta_r\Bigg(\cos\theta\sin\theta\cos\phi\sin\phi+\cos\theta\sin\theta\cos\phi\sin\phi+\sin^2\theta\sin^2\phi+\cos^2\theta\cos^2\phi\Bigg) \\
+ \ & \frac{\theta_\phi}{r}\Bigg(-\sin\theta\cos\theta\sin^2\phi+\sin^2\theta\sin\phi\cos\phi-\cos^2\theta\cos\phi\sin\phi+\cos\theta\sin\theta\cos^2\phi\Bigg) \\
= \ & \theta_r\cos(\theta-\phi)\Bigg(\cos\theta\cos\phi+\sin\theta\sin\phi\Bigg)+\frac{\theta_\phi}{r}\sin(\theta-\phi)\Bigg(\cos\theta\cos\phi+\sin\theta\sin\phi\Bigg) \\
= \ & \theta_r\cos^2(\theta-\phi)+\frac{\theta_\phi}{r}\sin(\theta-\phi)\cos(\theta-\phi)
\end{aligned}$$

Finally we come back to our original vector equation, which we have now separated into two parts

$$\gamma\frac{\partial\vec{n}}{\partial t}=-\beta\big(\vec{n}\cdot\nabla\big)\vec{n}$$

$$\textbf{R:} \qquad \gamma\frac{\partial}{\partial t}\cos(\theta-\phi)=\beta\Bigg[\cos(\theta-\phi)\sin(\theta-\phi)\theta_r+\frac{\sin^2(\theta-\phi)}{r}\theta_\phi\Bigg]$$

$$\boldsymbol{\Phi}\textbf{:} \qquad \gamma\frac{\partial}{\partial t}\sin(\theta-\phi)=-\beta\Bigg[\cos^2(\theta-\phi)\theta_r+\frac{\sin(\theta-\phi)\cos(\theta-\phi)}{r}\theta_\phi\Bigg]$$

Next multiply the R-equation by $-\sin(\theta-\phi)$, the Φ-equation by $\cos(\theta-\phi)$, and add them together. The $\dot{\theta}$ trig terms combine to just 1, leaving

$$\begin{aligned}
\gamma\dot{\theta} \ &= \ -\beta\Bigg[\cos(\theta-\phi)\sin^2(\theta-\phi)\theta_r+\frac{\sin^3(\theta-\phi)}{r}\theta_\phi\Bigg] \\
&- \ \ \beta\Bigg[\cos^3(\theta-\phi)\theta_r+\frac{\sin(\theta-\phi)\cos^2(\theta-\phi)}{r}\theta_\phi\Bigg] \\
&\qquad\qquad \text{and} \\
\gamma\dot{\theta} \ &= \ -\beta\Bigg[\cos(\theta-\phi)\theta_r+\frac{\sin(\theta-\phi)}{r}\theta_\phi\Bigg]
\end{aligned}$$

Then substituting $\psi=\theta-s\phi$, and also that $s=1$,

$$\gamma\dot{\psi}=-\beta\Bigg[\cos\psi(\psi_r)+\frac{\sin\psi}{r}(\psi_\phi+1)\Bigg]$$

Now we combine this result for the convective term with our earlier equation for the minimization of the first functional derivative (setting $\psi_\phi = 0$):

$$\begin{aligned}
\gamma\frac{\partial\vec{n}}{\partial t} &= -\frac{\delta H}{\delta\vec{n}} - \beta\big(\vec{n}\cdot\nabla\big)\vec{n} \quad \Longrightarrow \\
\gamma\frac{\partial\psi}{\partial t} &= \Big[J - \Delta\cos(2\psi)\Big]\Big[\frac{\psi_r}{r} + \psi_{rr}\Big] + \Delta\sin(2\psi)\Big[\psi_r^2 + \frac{1}{r^2}\Big] \\
&- \beta\Big[\cos\psi(\psi_r) + \frac{\sin\psi}{r}\Big] \qquad (2.27)
\end{aligned}$$

Let's check to see if Asters and Vortices, which have $\psi = 0, \pi$ or $\pm\pi/2$ and $\psi_r = 0$, are still steady-state solutions. Plugging these numbers in, Asters are still solutions satisfying $\dot{\psi} = 0$, but Vortices are not! The new term causes Vortices to not be steady state solutions. **Asters are steady-state solutions, Vortices are not!**

2.6.2 The Stability of 1D Asters Against Global Perturbations

Before investigating the more general case of local perturbations, we first study stability of 1D solutions to global perturbations. Again, we make our system one dimensional by fixing the radius to some particular value, R, and only consider a ring geometry. To derive the equation governing the growth of small perturbations, we can simply add a new convective term to the old equilibrium equation. I'll calculate the new convective term and then tack on the results to our old equations. For small perturbations, the convective term contributes the following:

$$\begin{aligned}
&-\beta\Big(\hat{n}\cdot\nabla\Big)\hat{n}\Big|_{\psi+\delta\psi} - \beta\Big(\hat{n}\cdot\nabla\Big)\hat{n}\Big|_{\psi} \\
&= -\beta\Big[\cos(\psi+\delta\psi)(\psi_r+\delta\psi_r) + \frac{\sin(\psi+\delta\psi)}{r}(\psi_\phi+\delta\psi_\phi+1) \\
&- \Big(\cos\psi\psi_r + \frac{\sin\psi}{r}(\psi_\phi+1)\Big)\Big] \\
&= -\beta\Big[\cos\psi\cos\delta\psi(\psi_r+\delta\psi_r) - \sin\psi\sin\delta\psi(\psi_r+\delta\psi_r)\Big] \\
&- \beta\Big[\frac{\sin\psi\cos\delta\psi}{r}(\psi_\phi+\delta\psi_\phi+1) + \frac{\sin\delta\psi\cos\psi}{r}(\psi_\phi+\delta\psi_\phi+1)\Big] \\
&+ \beta\Big[\cos\psi\psi_r + \frac{\sin\psi}{r}(\psi_\phi+1)\Big] \\
&= -\beta\Big[\cos\psi\Big((\delta\psi_r) + \frac{\delta\psi(\psi_\phi+1)}{r}\Big) + \sin\psi\Big(\frac{(\delta\psi_\phi)}{r} - (\delta\psi)\psi_r\Big)\Big] + O(\delta\psi^2)
\end{aligned}$$

Considering only radially-dependent perturbations, we impose that $\delta\psi_\phi = 0$:

$$= -\beta\Big[\cos\psi\Big(\delta\psi_r + \frac{\delta\psi}{r}\Big) - \sin\psi(\delta\psi)\psi_r\Big]$$

Tacking on this new term to our previous stability equation for asters (13), and evaluating the expression at the ring radius R, we arrive at the stability equations for asters in 1D active polar liquid crystal systems:

$$\gamma\frac{\partial\delta\psi}{\partial t} = (J-\Delta)\Big[\delta\psi_{rr} + \frac{\delta\psi_r}{R} + \frac{2\Delta}{(J-\Delta)}\frac{\delta\psi}{R^2}\Big] \mp \beta\Big[\delta\psi_r + \frac{\delta\psi}{R}\Big] \qquad \text{(Asters)}$$

The treatment of convection introduces a new term which may be either positive or negative. The negative β sign comes from evaluating the above new term with $\psi = 0$, and the positive β sign comes from evaluating the expression with $\psi = \pi$. The sign signifies whether asters are pointing radially outward or inward. $\psi = 0$ corresponds to outward-pointing asters while $\psi = \pi$ corresponds to inward-pointing asters. Since the β term began with a negative sign, note that in the above equation, a negative β term corresponds to outward-pointing asters.

For global perturbations, the radial derivatives vanish:

$$\gamma\frac{\partial\delta\psi}{\partial t} = 2\Delta\frac{\delta\psi}{R^2} \pm \beta\frac{\delta\psi}{R} = \delta\psi\Big(\frac{2\Delta \pm \beta R}{R^2}\Big)$$

This equation is solved by:

$$\delta\psi(t) = \delta\psi_0 \exp\Big(\frac{2\Delta \pm \beta R}{\gamma R^2}\Big)$$

Compared to the case of ordinary polar and nematic liquid crystals, in order to analyze the stability of one-dimensional asters in active liquid crystals, we need to know the sign and magnitude of β in addition to the sign of δ. Remembering that Δ is negative for $k_3 > k_1$, the sign of β can have some interesting consequences. If it is negative, it can allow asters to be stable beyond some minimal radius, even if the ratio of Frank constants are not favorable to aster patterns. If β is positive, it can destroy the stability of asters beyond some minimal radius. In these two cases, this special radius is given by:

$$R^* = \frac{2|\Delta|}{\beta}$$

2.6.3 Stability of Asters against Local Perturbations

Let's consider the stability of asters against local perturbations, while still restricting ourselves to only radial perturbations ($\delta\psi_\phi = 0$).

$$\gamma\frac{\partial\delta\psi}{\partial t} = (J-\Delta)\Big[\delta\psi_{rr} + \frac{\delta\psi_r}{r} + \frac{2\Delta}{(J-\Delta)}\frac{\delta\psi}{r^2}\Big] \mp \beta\Big[\delta\psi_r + \frac{\delta\psi}{r}\Big]$$

This is a partial differential equation for a function describing the time and space dependence of a perturbation to the initial aster pattern, and we begin by searching for separable solutions: $\delta\psi(r,t) = R(r)\cdot T(t)$ Denoting spacial and temporal differentiation by primes and dots, respectively:

$$\gamma R\dot{T} = (J-\Delta)T\Big[R'' + \frac{R'}{r} + \frac{2\Delta}{(J-\Delta)}\frac{R}{r^2}\Big] \mp \beta T\Big[R' + \frac{R}{r}\Big]$$

Then divide by $R(r)T(t)$:

$$\gamma\frac{\dot{T}}{T} = (J-\Delta)\frac{R''}{R} + \Big(\frac{J-\Delta}{r} \mp \beta\Big)\frac{R'}{R} + \Big(\frac{2\Delta}{r^2} \mp \frac{\beta}{r}\Big)$$

Since each side of the equation is a function or either only t or only r, we can be sure that they are independent of each other and must equal a constant, which we denote as -E. Then solve each ODE separately. The time-equation is particularly simple:

$$\gamma\frac{\dot{T}}{T} = -E \Longrightarrow T(t) = A\exp\Big(-\frac{Et}{\gamma}\Big)$$

Now the spatial equation is a bit tougher:

$$(J-\Delta)\frac{R''}{R} + \Big(\frac{J-\Delta}{r} \mp \beta\Big)\frac{R'}{R} + \Big(\frac{2\Delta}{r^2} \mp \frac{\beta}{r}\Big) = -E$$

$$(J-\Delta)R'' + \Big(\frac{J-\Delta}{r} \mp \beta\Big)R' + \Big(E + \frac{2\Delta}{r^2} \mp \frac{\beta}{r}\Big)R = 0$$

Let us now pause and examine the constants and dimensionality involved in this equation. Denote length by l, time by t, energy by e:

$$[J] = [\Delta] = e, \quad [\gamma] = e\cdot t\cdot l^{-2}, \quad [\beta] = e\cdot l^{-1}, \qquad [E] = e\cdot l^{-2}$$

I am free to measure time in units of γ/E and length in units of $(J-\Delta)/\beta$. Then the previously solved equation for T(t) becomes under $t \longrightarrow t'$ (I'll just drop the prime and use the original variable, t):

$$T(t) = A\exp\big(-t\big)$$

And as $r \longrightarrow r'$, our differential equation for R(r) becomes :

$$\frac{\beta^2}{J-\Delta}R'' + \frac{\beta^2}{J-\Delta}\left(\frac{1}{r} \mp 1\right)R' + \left(E + \frac{2\Delta\beta^2}{(J-\Delta)^2 r^2} \mp \frac{\beta^2}{(J-\Delta)r}\right)R = 0$$

Now let $\beta^2/(J-\Delta) \equiv k$:

$$R'' + \Big(\frac{1}{r} \mp 1\Big)R' + \Big(\frac{E}{k} \mp \frac{1}{r} + \frac{2\Delta}{(J-\Delta)r^2}\Big)R = 0$$

At this point let's note that this is a linear 2nd order homogenous ODE for R(r) of the form $R'' + f(r)R' + g(r)R = 0$. Avoiding for now the task of finding an exact solution, let's explore the solution in the asymptotic limit $r >> 1, \quad r^2 >> 2\Delta/(J - \Delta)$. In this limit our equation becomes:

$$R'' \mp R' + \frac{E}{k}R = 0$$

Even in this simplified case, our solution depends on whether the aster is pointing inwards or outwards, and upon the ratio E/k. E originally appeared in the argument of the exponential solution for T(t). Firstly, note that if E is negative, then the perturbations do not decay in time and are therefore not stable. So we may restrict ourselves to positive values of E. As $E \to \infty$ the perturbation decays away very rapidly. As $E \to 0$, the perturbation does not decay and remains constant. Of course, E does not appear alone in the exponential argument, γ is also present, but I propose that with these redefined units, the ratio E/k is something of a measure of how "stiff" the system is. Also note that the sign of E/k depends on the relative strength of the Frank constants.

This equation is simply that of the damped, undriven harmonic oscillator.

2.7 Modeling the Cellular Cytoskeleton as a Liquid Crystal

The cellular cytoskeleton is an important structure that is present in all cells. In Eukaryotic cells it is composed of networks of three different kinds of protein filaments–actin filaments, intermediate filaments, and microtubules. The cytoskeleton is responsible for the physical shape and structural stability of the cell, and is also important in crucial cellular functions such as motility and intracellular transport. The protein filaments that constitute the cytoskeleton bear a resemblance to liquid crystals; they are long, rod-like molecules. Inert protein filaments may be modeled as nematic liquid crystals. Chemically active protein filaments may be modeled as active polar liquid crystals. Protein filaments are polymers, long molecules composed of smaller molecular building blocks called monomers.

These protein filaments are very active players within the cellular environment. The move throughout the cell, and they form dynamic networks with each other through smaller molecules known as molecular motors. These motors may attach themselves to protein filaments and "walk" along their length. They may also move the filaments relative to one another. Networks of protein filaments attached through molecular motors are known as active gels. The protein filaments are also dynamic in another sense; they grow. The filaments are composed of monomers, and these monomer building blocks are diffused throughout the cell. During a phenomena known as treadmilling, the monomers spontaneously detach from one end of the filament, and spontaneously attach at the opposite end. Treadmilling causes the filaments to have a preferred orientation (the growing end behaves differently than the disintegrating end), and therefore treadmilling filaments may be modeled as active liquid crystals. A complete description of the cellular cytoskeleton would necessarily include all three types of filaments, molecular motors, and the tremendous variety of chemical components that exist within the cell. However, simplified liquid crystal models of the cytoskeleton can be very useful in capturing the relevant physics, and can lead to a more thorough understanding of cytoskeleton dynamics.

In the sections that follow, I describe our most recent line of investigation. I have analyzed and compared the approaches of two different groups of physicists in modeling the cytoskeleton as a liquid crystal. Each group makes different simplifying assumptions, and after I analyze the two, I attempt to extend their work into a more accurate description of the cytoskeleton. Below I've borrowed two figures (and their captions) from Thomas Risler's *Cytoskeleton and Cell Motility.*

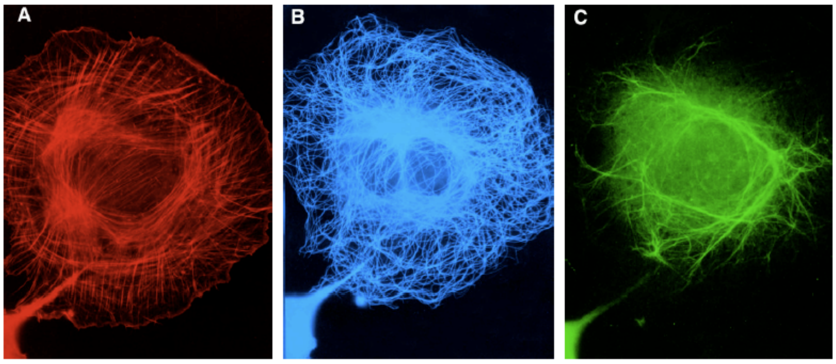

FIG. 7: The three-polymer system of a fibroblast cytoskeleton, as seen in the fluorescence microscope after fixation and labelling with specific probes. A, the actin cytoskeleton; B, the microtubule cytoskeleton; C, the intermediate-filament cytoskeleton, here where the intermediate-filament protein vimentin has been stained. Source: http://cellix.imba.oeaw.ac.at/cytoskeleton (taken from Herzog et al., 1994: see web-site).

Figure 2.4: Cytoskeleton, courtesy of T. Risler

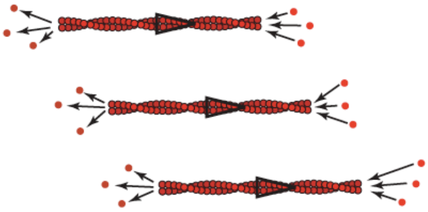

FIG. 9: Schematic representation of a treadmilling actin filament. The arrows indicate the polarity of the filaments. Monomers are added to the plus end and removed from the minus end at the same rate, such that while the filament's length remains constant, its center of mass is advancing. Top to bottom shows three subsequent times. Source: courtesy of Karsten Kruse.

Figure 2.5: Treadmilling, courtesy of T. Risler

2.7.1 Aranson and Tsimring

In their paper **Theory of self-assembly of microtubules and motors** [Physical Review E **74** 031915 (2006)], Aranson and Tsimring (henceforth AT) study the formation of aster and vortex patterns in systems of microtubules and molecular motors. It would be interesting to compare their work on asters and vortices with our own analysis, as well as with the approach taken by Voituriez et al (done in the following section). AT model the microtubule network as a polar liquid crystal.

The most relevant equation in their paper is (62). This equation assumes uniform density and describes the time-evolution of the amplitude of the orientation vector for microtubules in solution. Rather than working with a two-dimensional vector, they have chosen to write their equations in terms of a complex scalar. After rescaling, their equation (62) is:

$$\begin{aligned}\partial_t A &= D_1\Big(\partial_r^2 + r^{-1}\partial_r - r^{-2}\Big)A + D_2\Big(\partial_r^2 + r^{-1}\partial_r - r^{-2}\Big)A^* \\ &+ (1-|A|^2)A + H\left[a_1 A Re(\partial_r + r^{-1})A + a_2\partial_r A Re A + \frac{i a_2 A Im A}{r}\right]\end{aligned} \tag{2.28}$$

They then chose to write A(r) as $A(r) = \Phi(r)\exp(i\varphi(r))$. Plugging this into the above equation, we find:

$$\begin{aligned}
\partial_t \ln\Phi \;&+\; i\partial_t\varphi = D_1\Big[\frac{\Phi''}{\Phi} + i\varphi'\frac{\Phi'}{\Phi} + i\varphi'' - (\varphi')^2 + \frac{\Phi'}{\Phi r} + i\frac{\varphi'}{r} - \frac{1}{r^2}\Big] \\
&+\; D_2\Big[\frac{\Phi''}{\Phi} - i\varphi'\frac{\Phi'}{\Phi} - i\varphi'' - (\varphi')^2 + \frac{\Phi'}{\Phi r} - i\frac{\varphi'}{r} - \frac{1}{r^2}\Big]\exp(-2i\varphi) + \Big[1 - \Phi^2\Big]\Phi \\
&+\; H\Bigg\{a_1\Big[\Phi'\cos\varphi - \varphi'\Phi\sin\varphi + \frac{\Phi\cos\varphi}{r}\Big] + a_2\Big[\Phi' + i\Phi\varphi'\Big]\cos\varphi + \frac{ia_2\sin\varphi}{r}\Bigg\}
\end{aligned} \tag{2.29}$$

Because the above equation is complex, we can reduce it into a imaginary and a real part.

$$\begin{aligned}
\textbf{Im:}\quad \dot\varphi \;&=\; \Big[D_1 - D_2\cos 2\varphi\Big]\Big[\frac{\varphi'\Phi'}{\Phi} + \varphi'' + \frac{\varphi'}{r}\Big] \\
&+\; D_2\sin 2\varphi\Big[(\varphi')^2 + \frac{1}{r^2} - \frac{\Phi''}{\Phi} - \frac{\Phi'}{r}\Big] + Ha_2\Phi\Big(\varphi'\cos\varphi + \frac{\sin\varphi}{r}\Big)
\end{aligned} \tag{2.30}$$

$$\begin{aligned}
\textbf{Re:}\quad \partial_t\ln\Phi \;&=\; \Big[D_1 + D_2\cos 2\varphi\Big]\Big[(\varphi')^2 + \frac{1}{r^2} - \frac{\Phi''}{\Phi} - \frac{\Phi'}{\Phi r}\Big] \\
&+\; D_2\sin 2\varphi\Big[\frac{\varphi'\Phi'}{\Phi} + \varphi'' + \frac{\varphi'}{r}\Big] + \Big[\Phi^2 - 1\Big] \\
&+\; H\Bigg\{a_1\Big[\Phi\varphi'\sin\varphi - \Phi'\cos\varphi - \frac{\Phi\cos\varphi}{r}\Big] - a_2\Phi'\cos\varphi\Bigg\}
\end{aligned} \tag{2.31}$$

If $\Phi(r) = \textit{const.}$, then the imaginary equation reduces to our earlier equation (29), which for reference I've included immediately below the reduced Aranson and Tsimring (AT) equation:

$$\dot\varphi = \Big[D_1 - D_2\cos 2\varphi\Big]\Big[\varphi'' + \frac{\varphi'}{r}\Big] + D_2\sin 2\varphi\Big[(\varphi')^2 + \frac{1}{r^2}\Big] + Ha_2\Big(\varphi'\cos\varphi + \frac{\sin\varphi}{r}\Big) \tag{AT}$$

$$\gamma\dot\psi = \Big[J - \Delta\cos(2\psi)\Big]\Big[\psi_{rr} + \frac{\psi_r}{r}\Big] + \Delta\sin(2\psi)\Big[\psi_r^2 + \frac{1}{r^2}\Big] - \beta\Big[\cos\psi(\psi_r) + \frac{\sin\psi}{r}\Big] \tag{our eq. 29}$$

However, the real AT equation constrains the possible solutions, and we find that in AT's formulation, steady-state, uniform aster solutions are not permitted. For constant polarization amplitude Φ and $\varphi = 0, \pi$, the real equation becomes:

$$0 = \Big[D_1 + D_2\Big]\frac{1}{r^2} \mp Ha_1\frac{\Phi}{r} + \Big[\Phi^2 - 1\Big]$$

From our initial assumption of constant polarization amplitude Φ and $\varphi = 0, \pi$, the fact that this equation is not satisfied by a range of r values implies that no such solutions exist.

AT analyzed the full equation for complex amplitude A numerically, and found aster and vortex-like patterns with spatially varying polarization amplitude. They also investigated the dynamics of such solutions.

2.7.2 Voituriez et al

In their paper **Spontaneous flow transition in active polar gels** [Europhysics Letters **70** 404 (2005)], Voituriez, Joanny, and Prost (henceforth Voituriez et al) model the cytoskeleton as an polar liquid crystal immersed in a liquid capable of flowing. The active dynamics lead to a flow velocity field, while the filamentary nature of the cytoskeleton proteins lead to an orientation field similar to my earlier approaches.

Voituriez et al deal with a quasi-1D geometry and neglect the effects of activity on the orientation of the rods, and only treat activity in terms of the velocity flow field. In my analysis, I have switched to polar coordinates and have incorporated the effect of activity on the polarization (hence the β-term in the below equation). We start with two main equations, one for the polarization vector p (in the beginning of this paper I called the same vector field n), and one for the hydrodynamic stress tensor.

$$\frac{Dp_i}{Dt} \equiv \Big(\partial_t + v_j\partial_j\Big)p_i + \omega_{ij}p_j = \frac{1}{\gamma}h_i + \lambda\Delta\mu p_i - \nu u_{ij}p_j - \beta\Big(\vec{p}\cdot\nabla\Big)\vec{p} \quad (2.32)$$

$$2\eta u_{ij} = \sigma_{ij} + \zeta\Delta\mu p_i p_j - \frac{\nu}{2}\Big(p_i h_j + p_j h_i\Big) + \frac{1}{2}\Big(p_i h_j - p_j h_i\Big) + \bar{\zeta}\Delta\mu\delta_{ij} \quad (2.33)$$

Here $\Delta\mu$ is the chemical potential difference between ATP and its hydrolysis products, $\vec{p} = \hat{x}\cos\theta + \hat{y}\sin\theta$, D/DT is the corotational time derivative. u_{ij} and ω_{ij} are the strain rate tensor and vorticity tensor, respectively, and are given below. h_i is the molecular field, and is also given below. $h_{||}$ is a Lagrange multiplier, which is invoked in order to constrain p to be of constant magnitude.

$$h_i \equiv \left(\frac{\delta F}{\delta p_i}\right) = h_{||}p_i + K_1\partial_i\Big(\nabla\cdot\vec{p}\Big) + K_3\Big(\nabla^2 p_i - \partial_i\nabla\cdot\vec{p}\Big) + w\nabla\rho \quad (2.34)$$

$$u_{ij} = \frac{1}{2}\Big(\partial_i v_j + \partial_j v_i\Big), \quad \omega_{ij} = \frac{1}{2}\Big(\partial_i v_j - \partial_j v_i\Big)$$

I will only consider order parameter fields of the form $\theta(r,\phi) = \phi + \psi(r)$. I will assume constant density ρ, and velocity fields of the form $\vec{v}(r,\phi) = \hat{\phi}v(r)$, which follows directly from incompressibility. After imposing these assumptions and converting to polar coordinates, we then obtain two equations, one determining $\partial_t\psi$ and one that determines the velocity field.

$$\begin{aligned}\gamma\partial_t\psi = &\Big[J - \Delta\cos 2\psi\Big]\Big[\psi'' + \frac{\psi'}{r}\Big] + \Delta\sin 2\psi\Big[\psi'^2 + \frac{1}{r^2}\Big] \\ &-\beta\gamma\Big[\psi'\cos\psi + \frac{\sin\psi}{r}\Big] + \frac{\gamma}{2}\Big[\frac{dv(r)}{dr} - \frac{v(r)}{r}\Big]\Big[1 - \nu\cos 2\psi\Big] \qquad (2.35)\end{aligned}$$

This equation is very similar to my earlier eq. (29).

2.8 Conclusions and Future Directions

The previous section is incomplete, and I am still in the process of deriving the relevant equations and analyzing this system. I plan to continue working on this project until graduation, as well as during the summer (after a well deserved break, of course). I have spent a great deal of time and effort learning about liquid crystal physics, and our eventual goal is to obtain a significant research result of our own, and to publish the result in a scientific journal.

This research has been the most influential academic experience of my undergraduate career, and I am deeply indebted to Professors Bowick and Marchetti for the tremendous amount of time and effort they have devoted towards my education. This project has benefitted me far more than other individual, and I am very lucky to have worked so closely with two such excellent physicists. I would like to end this Capstone project with an expression of my deepest gratitude for their guidance and instruction.

Chapter 3

Appendix

3.1 Conversion to Polar Coordinates

There are a few different ways to calculate the free energy in polar coordinates. One would be to functionally differentiate the polar free energy, as we did with the Cartesian free energy. Or, we could simply take the result we have already calculated and convert it to polar coordinates. I'll chose the second method. First, we need to know how the partial derivatives involved in the above expression translate to polar coordinates.

$$\frac{\partial \theta}{\partial x} = \frac{\partial \theta}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial \theta}{\partial \phi}\frac{\partial \phi}{\partial x}$$

$$\frac{\partial \theta}{\partial y} = \frac{\partial \theta}{\partial r}\frac{\partial r}{\partial y} + \frac{\partial \theta}{\partial \phi}\frac{\partial \phi}{\partial y}$$

We can use the identities $r^2 = x^2 + y^2$ and $\phi = \arctan(\frac{y}{x})$ to determine what θ_x and θ_y are in terms of θ_r and θ_ϕ

$$\frac{\partial r}{\partial x} = \cos\phi, \qquad \frac{\partial r}{\partial y} = \sin\phi$$

$$\frac{\partial \phi}{\partial x} = -\frac{\sin\phi}{r}, \qquad \frac{\partial \phi}{\partial y} = \frac{\cos\phi}{r}$$

We obtain the conversion from Cartesian to Polar partial derivatives:

$$\frac{\partial}{\partial x} = (\cos\phi)\frac{\partial}{\partial r} - (\frac{\sin\phi}{r})\frac{\partial}{\partial \phi}$$

$$\frac{\partial}{\partial y} = (\sin\phi)\frac{\partial}{\partial r} + (\frac{\cos\phi}{r})\frac{\partial}{\partial \phi}$$

Operating on $\theta(x, y)$, we have:

$$\theta_x = (\cos\phi)\theta_r - (\frac{\sin\phi}{r})\theta_\phi \tag{3.1}$$

$$\theta_y = (\sin\phi)\theta_r + (\frac{\cos\phi}{r})\theta_\phi \tag{3.2}$$

Using the above results we can solve for various expressions that we will later use:

$$\theta_x^2 = (\cos^2\phi)\theta_r^2 + (\frac{\sin^2\phi}{r^2})\theta_\phi^2 - \frac{\sin 2(\phi)}{r}\theta_r\theta_\phi$$

$$\theta_y^2 = (\sin^2\phi)\theta_r^2 + (\frac{\cos^2\phi}{r^2})\theta_\phi^2 + \frac{\sin 2(\phi)}{r}\theta_r\theta_\phi$$

$$(\theta_x^2 + \theta_y^2) = (\cos^2\phi + \sin^2\phi)\theta_r^2 + (\frac{\cos^2\phi + \sin^2\phi}{r^2})\theta_\phi^2$$

$$(\theta_x^2 + \theta_y^2) = \theta_r^2 + \frac{\theta_\phi^2}{r^2}$$

$$(\theta_y^2 - \theta_x^2) = -(\cos^2\phi - \sin^2\phi)\theta_r^2 + \frac{(\cos^2\phi - \sin^2\phi)}{r^2}\theta_\phi^2 + \frac{2(\sin 2\phi)\theta_r\theta_\phi}{r}$$

$$(\theta_y^2 - \theta_x^2) = -(\cos 2\phi)\theta_r^2 + \frac{(\cos 2\phi)}{r^2}\theta_\phi^2 + \frac{2(\sin 2\phi)\theta_r\theta_\phi}{r}$$

$$\theta_x\theta_y = \cos\phi\sin\phi\theta_r^2 + \frac{cos^2\phi}{r}\theta_r\theta_\phi - \frac{sin^2\phi}{r}\theta_r\theta_\phi - \frac{\cos\phi\sin\phi}{r^2}\theta_\phi^2$$

$$\theta_x\theta_y = \frac{(\sin 2\phi)}{2}\theta_r^2 - \frac{(\sin 2\phi)}{2r^2}\theta_\phi^2 + \frac{(\cos 2\phi)}{r}\theta_r\theta_\phi$$

Now if our director field happens to be of the form, $\theta(r,\phi) = s\phi + \psi(r,\phi)$, then we may find a more specific expression for the above derivates. These are used in the :

$$\theta_x = \cos\phi(\psi_r) - \frac{\sin\phi}{r}(s + \psi_\phi)$$

$$\theta_y = \sin\phi(\psi_r) + \frac{\cos\phi}{r}(s + \psi_\phi)$$

$$\theta_x^2 = \cos^2\phi(\psi_r^2) - \frac{2\sin\phi\cos\phi}{r}(s + \psi_\phi)\psi_r + \frac{\sin^2\phi}{r^2}(s + \psi_\phi)^2$$

$$\theta_y^2 = \sin^2\phi(\psi_r^2) + \frac{2\sin\phi\cos\phi}{r}(s + \psi_\phi)\psi_r + \frac{\cos^2\phi}{r^2}(s + \psi_\phi)^2$$

$$\theta_x\theta_y = \frac{\sin 2\phi}{2}(\psi_r^2) + \frac{\cos 2\phi}{r}(s + \psi_\phi)\psi_r - \frac{\sin 2\phi}{2r^2}(s + \psi_\phi)^2$$

$$\theta_{xx} = \cos^2\phi(\psi_{rr}) + \frac{2\sin\phi\cos\phi}{r^2}(s + \psi_\phi) + \frac{\sin^2\phi}{r^2}(\psi_{\phi\phi}) - \frac{2\cos\phi\sin\phi}{r}(\psi_{r\phi}) + \frac{\sin^2\phi}{r}(\psi_r)$$

$$\theta_{yy} = \sin^2\phi(\psi_{rr}) - \frac{2\cos\phi\sin\phi}{r^2}(s + \psi_\phi) + \frac{\cos^2\phi}{r^2}(\psi_{\phi\phi}) + \frac{2\cos\phi\sin\phi}{r}(\psi_{r\phi}) + \frac{\cos^2\phi}{r}(\psi_r)$$

$$\theta_{xy} = \frac{\sin 2\phi}{2}(\psi_{rr}) - \frac{\cos 2\phi}{r^2}(s + \psi_\phi) - \frac{\sin 2\phi}{2r^2}(\psi_{\phi\phi}) + \frac{\cos 2\phi}{r}(\psi_{r\phi}) - \frac{\sin 2\phi}{2r}(\psi_r)$$

Chapter 4

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