ON LANDAU–DE GENNES ENERGY MINIMIZERS SURROUNDING GENERALIZED COLLOID PARTICLES

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BY

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To

my wonderful partner Brooke,

my loving mother Mary Kay

and my encouraging grandparents Walter & Vera.

Abstract

We consider the interaction between a single colloid particle of generalized shape and nematic liquid crystal in the framework of Landau–de Gennes theory. At the particle surface, general strong or weak uniaxial anchoring conditions are applied as well as uniform uniaxial forcing at infinity. In this context, it is found that the field-free Landau–de Gennes functional with surface energy admits uniformly continuous minimizers. We then study two examples of non-spherical colloids in a limiting regime known as the 'small particle limit'. Explicit solutions to the small particle limit are found in the case of a prolate and oblate spheroidal colloid with 'almost homeotropic' strong anchoring. From there, a Saturn ring defect is numerically observed in both cases.

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Contents

1 Introduction

Generally speaking, a material that is classified as 'liquid crystal' is one in which properties of both isotropic liquid and solid crystal are observed at the molecular level. The term isotropic liquid corresponds exactly to the general definition of 'liquid' we are familiar with. In this case, all of the molecules constituting the given material are randomly oriented throughout the entire sample.

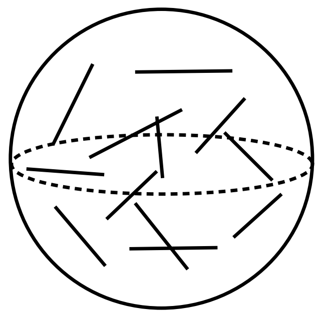

Figure 1: Sample of isotropic liquid molecules

The complete opposite is true for solid crystal. In this state, a material's molecular structure is highly ordered. Although there are many types of structuring orders for solid crystal, a typical visualization one can refer to is that of a lattice.

Much like other types of matter, liquid crystal can attain and be classified by different 'phases' which generally depend on the material, temperature, etc. [6]. In each of these phases, the liquid crystal exhibits a characteristic ordering and response to certain external factors. For our case, we will be considering the *nematic* phase.

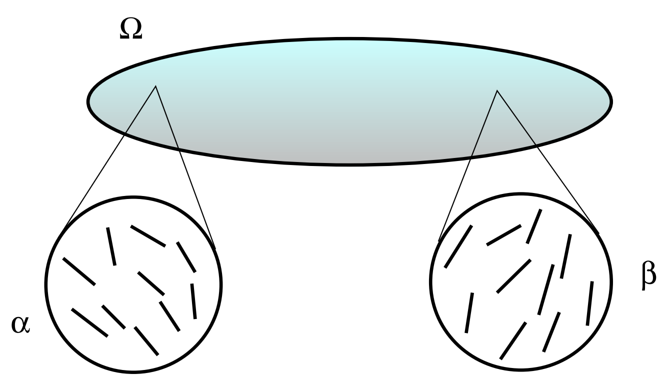

Figure 2: Subsamples α & β of nematic liquid crystal Ω.

The visual characteristics of nematic liquid crystal are best described when viewed from a global and local sense. In the general global view, molecules in this phase are free to flow throughout the sample just as a liquid may. However, when restricting the focus to a sufficiently small subsample, it is apparent that there is a preferred direction of molecular orientation and alignment. That is, locally, molecular orientation is not random. This property is depicted in Figure 2 above.

In the context of nematic liquid crystal, there are two main non-random orientation states that occur. The first of these states is called *uniaxial*. A sample of nematic liquid crystal is said to be in the uniaxial state when there is one distinct direction of preferred alignment. Associated to this state is a vector called the *director* which gives this direction.

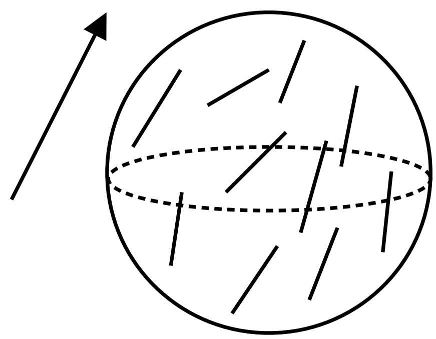

Figure 3: Uniaxial nematic liquid crystal with director.

The second state is called *biaxial* and is much harder to visualize. A nematic liquid crystal in the biaxial state amounts to having preferred alignment directions in multiple planes for a given subsample. A visual of this state can be found in [6].

There are several mathematical models available which aim to study nematic liquid crystal. These models are particularly useful when information about molecular configuration is desired. Two primary theories used to do this are the Oseen–Frank model and the Landau–de Gennes model.

In the Oseen–Frank theory, the nematic liquid crystal is assumed to be uniaxial and is described by a unit vector field $n(x) \in \mathbb{S}^2$ defined on the sample [10]. Of course, a major drawback to this model is that the case of biaxiality is not considered. However, a more subtle flaw is in the representation $n \in \mathbb{S}^2$ itself. By representing the liquid crystal as a vector field, there is an inherent imposed distinction between the 'head' and 'tail' of any given molecule in the sample. But in reality, most molecules that comprise nematic liquid crystal have indistinguishable head and tail. To fix these issues, we introduce the richer Landau–de Gennes theory and is what we will use in this work.

In the Landau–de Gennes framework, nematic liquid crystal is represented by a real 3×3 symmetric, traceless matrix-valued function called a Q-tensor. This model allows for isotropic, uniaxial and biaxial states and are characterized by the eigenvalues and eigenvectors of the Q-tensor. Furthermore, this model describes orientation relative to $\mathbb{R}P^2$ rather than $\mathbb{S}^2$ which takes care of the head-tail problem as seen in the Oseen–Frank model [3]. The Landau–de Gennes model also provides us with an energy functional $\mathcal{F}$ which acts on the space of Q-tensors. By minimizing this functional over an appropriate class of Q-tensors, we obtain a means to find energy minimizing configurations of nematic liquid crystal by observing the eigenvectors of the minimizer.

In this paper, we are interested in showing the existence of a minimizer for $\mathcal{F}$ in a very particular setting. We consider a sample of nematic liquid crystal occupying all space outside some colloid particle. At the particle's surface, we impose that the liquid crystal be uniaxial in the sense of Robin and Dirichlet boundary conditions (also known in the physics literature as *weak* and *strong anchoring* respectively). Far away from the colloid ($|x| \to \infty$) we also impose uniform uniaxial conditions such that the director is parallel to the vertical 'z-direction'.

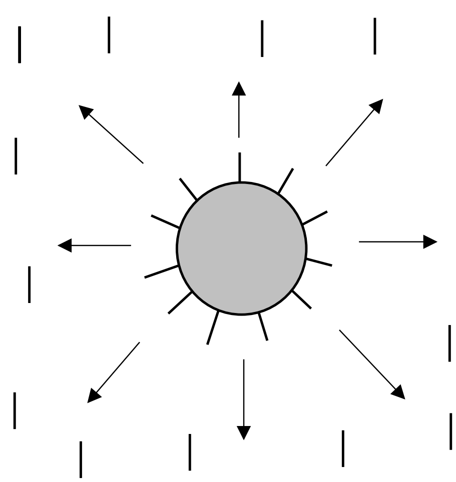

Figure 4: General setup of colloid anchoring and uniform uniaxial conditions at ∞.

The existence of a minimizer for $\mathcal{F}$ in the specific case of a spherical colloid with homeotropic boundary conditions (where the molecules lay perpendicular to the particle's surface, as shown in Figure 4) is proved in [1]. Extending this result for a general colloid shape with general uniaxial anchoring conditions is one of the main goals of our present work. We note that results on multiple particle systems [14], different colloid structures [13] and applied electric fields [9] in similar setups have also been studied, but is not the focus of this paper.

Another interesting topic that is studied in [1] is that of the 'small particle limit'. The authors consider minimizers of the spherical colloid case and a limiting regime which, in a sense, allows one to view minimizing configurations as the particle size tends to zero. In this limit, the authors show the existence of a 'Saturn ring' defect about the colloid (a circle for which the liquid crystal abruptly becomes uniaxial). With this, the other goal of our present work is to consider the same setup but in two different examples. In one example, we take a prolate spheroidal colloid with 'almost homeotropic' boundary conditions and an oblate spheroidal colloid with the same boundary conditions. We calculate the small particle limit in both cases and show also a Saturn ring defect can be obtained.

The paper begins with a 'Preliminaries' section. Here, we discuss definitions, notation and the necessary foundation needed to use the Landau–de Gennes model. In section 3, we construct the general domains and colloid particles we wish to consider. From there, we define the space over which we would like to minimize the Landau–de Gennes energy functional and then perform nondimensionalization. In section 4, we prove the existence of minimizers in our generalized setting. The Euler–Lagrange equations are constructed and then used to show regularity results of said minimizers. Finally, in section 5 we derive the equations used to calculate the 'small particle solution' that corresponds to the small particle limit in general. We end by explicitly calculating the small particle solutions for the case of a prolate spheroidal colloid and an oblate spheroidal colloid and qualitatively examine their Saturn ring defects.

2 Preliminaries

2.1 Definitions & Notations

Points & Sets

We restrict ourselves to subsets of $\mathbb{R}^3 = \mathbb{R} \times \mathbb{R} \times \mathbb{R}$. A point $x \in \mathbb{R}^3$ has coordinates (x_1, x_2, x_3) and

$$|x| := \sqrt{x_1^2 + x_2^2 + x_3^2}$$

will denote the standard Euclidean norm on $\mathbb{R}^3$. As usual, a *domain* $X \subseteq \mathbb{R}^3$ is an open, connected subset of $\mathbb{R}^3$ and its *complement* is defined by $X^c := \mathbb{R}^3 \setminus X$. The *interior*, *closure* and *boundary* of a set X will be denoted X°, $\overline{X}$ and ∂X respectively. Using the typical notation,

$$B_r(x_0) := \left\{x \in \mathbb{R}^3 : |x - x_0| < r\right\}$$

will represent the *open ball* of radius $r > 0$ centred at $x_0 \in \mathbb{R}^3$.

Quite often, we will also use the quantity

$$\operatorname{diam}(X) := \sup\{|x - y| : x, y \in X\}$$

called the *diameter* of a set X.

Finally, we say a subset $U \subset X$ is *compactly contained* in X if $\overline{U} \subset X$ and $\overline{U}$ is compact. This will be denoted by $U \Subset X$.

Matrices & Matrix-Valued Function Spaces

Let $M_3(\mathbb{R})$ be the set of all 3×3 real matrices $Q = (Q_{ij})$ and let I be the 3×3 identity matrix. The standard operations of *trace* and *transpose* acting on elements of $M_3(\mathbb{R})$ will be denoted via

$$\operatorname{tr}(Q) = \sum_{i=1}^{3} Q_{ii} \qquad \text{and} \qquad Q^T = (Q_{ij})^T = (Q_{ji})$$

respectively. When paired with the operation

$$Q_1 \cdot Q_2 = \operatorname{tr}(Q_2^T Q_1), \qquad Q_1, Q_2 \in M_3(\mathbb{R}) \tag{1}$$

the set $M_3(\mathbb{R})$ forms an inner product space. From this, a natural norm on $M_3(\mathbb{R})$ can be obtained by defining

$$|Q| := (Q \cdot Q)^{1/2}. \tag{2}$$

For the remainder of this work, we will be restricting ourselves to the subspace $\mathcal{S}_0 \subset M_3(\mathbb{R})$ defined by

$$\mathcal{S}_0 := \left\{ Q \in M_3(\mathbb{R}) : Q = Q^T,\ \operatorname{tr}(Q) = 0 \right\}.$$

That is, $\mathcal{S}_0$ is the set of symmetric, traceless 3×3 matrices. The reason for this restriction will be explained in section 2.2 below. We endow $\mathcal{S}_0$ with the same inner product (1) as above. When this is done, it is easy to see that $\mathcal{S}_0$ takes on some very desirable properties. For example, the pairing $(\mathcal{S}_0, |\cdot|)$ where $|\cdot|$ is the naturally induced norm (2), forms a Banach space. Even more, since each $Q \in \mathcal{S}_0$ is symmetric, the norm $|\cdot|$ takes the simple form

$$|Q| = \left(\sum_{i,j=1}^{3} Q_{ij}^2 \right)^{1/2}.$$

Let $C^k(X; \mathcal{S}_0)$ denote the set of k-times continuously differentiable $\mathcal{S}_0$-valued maps $Q : X \to \mathcal{S}_0$, where $k \geq 0$. By this, we mean $Q(x)$ is k-times continuously differentiable if each $Q_{ij} : X \to \mathbb{R}$ are k-times continuously differentiable in all variables. If $k = 0$, we will agree to define $C^0(X; \mathcal{S}_0)$ as the set of continuous (not necessarily differentiable) $\mathcal{S}_0$-valued functions. For $k = \infty$, we will say $C^\infty(X; \mathcal{S}_0)$ is the set of infinitely differentiable $\mathcal{S}_0$-valued functions. Finally, the set $C_0^k(X; \mathcal{S}_0)$ will denote the space of k-times continuously differentiable $\mathcal{S}_0$-valued functions with compact support in X.

The *gradient* of a $\mathcal{S}_0$-valued function can be defined via $\nabla Q = (\nabla Q_{ij})$ with the multiplication convention

$$(\nabla A \nabla B)_{ij} = \sum_{k=1}^{3} \nabla A_{ik} \cdot \nabla B_{kj}$$

where " $\cdot$ " denotes the standard Euclidean dot product in this context.

With this, note that we may then write

$$|\nabla Q| = \left(\sum_{i,j,k=1}^{3} \left(\frac{\partial Q_{ij}}{\partial x_k} \right)^2 \right)^{1/2}.$$

The typical definitions of L^p-spaces may also be extended for matrix-valued functions. We say a measurable function $Q : X \to \mathcal{S}_0$ belongs to $L^p(X; \mathcal{S}_0)$ if

$$\|Q\|_{L^p(X)} := \begin{cases} \left(\int_X \sum_{i,j=1}^{3} |Q_{ij}(x)|^p \, dx \right)^{1/p} & \text{if } 1 \leq p < \infty, \\ \sum_{i,j=1}^{3} \inf\{C \geq 0 : |Q_{ij}(x)| \leq C \text{ a.e. in } X\} & \text{if } p = \infty \end{cases}$$

is finite. That is, $Q \in L^p(X; \mathcal{S}_0)$ if $Q_{ij} \in L^p(X; \mathbb{R})$ for every $1 \leq i, j \leq 3$. From here, we can define the Sobolev spaces

$$W^{k,p}(X; \mathcal{S}_0) := \{Q \in L^p(X; \mathcal{S}_0) : D^\alpha Q_{ij} \in L^p(X) \; \forall 1 \leq i, j \leq 3 \text{ and } \forall |\alpha| \leq k\}$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ is a multi-index such that $|\alpha| = \alpha_1 + \alpha_2 + \alpha_3 \leq k \in \mathbb{N}$ and

$$D^\alpha Q_{ij} := \frac{\partial^{|\alpha|} Q_{ij}}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \partial x_3^{\alpha_3}}$$

exists in the weak sense. The norm we impose on $W^{k,p}(X; \mathcal{S}_0)$ is given by

$$\|Q\|_{W^{k,p}(X)} := \begin{cases} \left(\int_X \sum_{i,j=1}^{3} \sum_{0 \leq |\alpha| \leq k} |D^\alpha Q_{ij}(x)|^p \, dx \right)^{1/p} & \text{if } 1 \leq p < \infty, \\ \sum_{i,j=1}^{3} \left(\max_{0 \leq |\alpha| \leq k} \inf\{C \geq 0 : |D^\alpha Q_{ij}(x)| \leq C \text{ a.e. in } X\} \right) & \text{if } p = \infty \end{cases}.$$

In the special case where $k = 1$ and $p = 2$, $H^1(X; \mathcal{S}_0) := W^{1,2}(X; \mathcal{S}_0)$ becomes a Hilbert space with inner product

$$\langle Q_1, Q_2 \rangle_{H^1(X)} = \int_X (Q_1 \cdot Q_2 + \nabla Q_1 \cdot \nabla Q_2) \, dx$$

and induced norm

$$\|Q\|_{H^1(X)} = \left(\int_X \left(|Q|^2 + |\nabla Q|^2 \right) dx \right)^{1/2}.$$

To broaden this definition, we can define the space of local H^1-functions $H^1_{loc}(X;\mathcal{S}_0)$ by stating $Q \in H^1_{loc}(X;\mathcal{S}_0)$ if $Q \in H^1(U;\mathcal{S}_0)$ for all $U \Subset X$.

2.2 Landau–de Gennes Theory

In the body of this work, a great deal of interest is paid to molecular configurations and associated minimal energies of nematic liquid crystal. An approach to understanding both of these topics and how they are related can be found via the Landau–de Gennes model. We partition this subsection into two categories that deal with these subjects separately.

The Space of Q-Tensors

As discussed in the introduction, we are interested in studying nematic liquid crystal while allowing for the uniaxial, biaxial and isotropic states to be considered. Finding an efficient model that accommodates these conditions is what lies at the heart of Landau–de Gennes theory. To start, suppose X is a domain representing a space occupied by nematic liquid crystal. The model tells us to consider the space of Q*-tensors*

$$\mathcal{S}_0 = \left\{ Q \in M_3(\mathbb{R}) : Q = Q^T,\ \mathrm{tr}(Q) = 0 \right\}$$

as defined in section 2.1. By observing the microscopic molecular orientation distributions at each $x \in X$, a mapping $Q : X \to \mathcal{S}_0$ can be constructed so that the eigenvalues λ_i of $Q(x)$ determine whether the state is uniaxial, biaxial or isotropic. The characterization of these states is as follows:

Uniaxial Q-tensors

The uniaxial state is given when the eigenvalues of $Q(x)$ satisfy any of the conditions

$$\lambda_i = \lambda_j \neq \lambda_k \ ; \quad i,j,k \in \{1,2,3\} \quad \text{with} \quad \lambda_i = \lambda_j \neq 0.$$

That is, the uniaxial state is characterized by $Q(x)$ having two equal non-zero eigenvalues. In this way, we obtain a direction of preferred molecular alignment by observing the largest eigenvalue and its associated eigenvector called the *director*. It is worth while to note here that uniaxial Q-tensors can be written in the form

$$Q = s\left(n \otimes n - \frac{1}{3}I\right); \quad s \in \mathbb{R} \setminus \{0\},\ n \in \mathbb{S}^2$$

as shown in [10].

Biaxial Q-tensors

Representation of nematic liquid crystal in the biaxial state is given when the eigenvalues of $Q(x)$ satisfy

$$\lambda_i < \lambda_j < \lambda_k \ ; \quad i, j, k \in \{1, 2, 3\}.$$

This state does not admit a classic director, but taking the largest of the three distinct eigenvalues and observing the corresponding eigenvector can be used as an approximate director.

Isotropic Q-tensors

In this final case, the only option we are left with is to have all eigenvalues equal. However, the traceless condition from $\mathcal{S}_0$ allows us to easily conclude that

$$\lambda_1 = \lambda_2 = \lambda_3 = 0.$$

In fact, since any Q-tensor can also always be written in a distinct form which is given by

$$Q = s\left(n \otimes n - \frac{1}{3}I\right) + r\left(m \otimes m - \frac{1}{3}I\right); \quad s, r \in \mathbb{R}$$

where n, m are orthonormal eigenvectors of Q and s, r are piecewise linear combinations of the eigenvalues of Q, [10, Proposition 1], we obtain that Q is isotropic when $Q = 0$. In a physical sense, this condition given by the equal eigenvalues indicates that there is no preferred direction of alignment, and thus coincides with our typical view of traditional 'liquid' material at the particle level.

Stepping away from the physics momentarily, it will be convenient to shed light on a useful basis for $\mathcal{S}_0$. We begin by considering the standard cylindrical coordinate system given by the equations

$$x_1 = \rho\cos(\theta), \quad x_2 = \rho\sin(\theta), \quad x_3 = z$$

where $\rho \in [0, \infty)$, $\theta \in [0, 2\pi)$ and $z \in (-\infty, \infty)$.

Observing the orthonormal frame (e_ρ, e_θ, e_z) where

$$e_\rho = (\cos(\theta), \sin(\theta), 0), \quad e_\theta = (-\sin(\theta), \cos(\theta), 0), \quad e_z = (0, 0, 1),$$

it can be shown that the set of matrices $\{E_j(\theta)\}_{j=1}^5$ given by

$$\begin{aligned} E_1(\theta) &= \sqrt{\frac{3}{2}}\left(e_z \otimes e_z - \frac{1}{3}I\right), & E_2(\theta) &= \frac{1}{\sqrt{2}}\left(e_\rho \otimes e_\rho - e_\theta \otimes e_\theta\right), \\ E_3(\theta) &= \frac{1}{\sqrt{2}}\left(e_\rho \otimes e_z + e_z \otimes e_\rho\right), & E_4(\theta) &= \frac{1}{\sqrt{2}}\left(e_\theta \otimes e_z + e_z \otimes e_\theta\right), \\ E_5(\theta) &= \frac{1}{\sqrt{2}}\left(e_\theta \otimes e_\rho + e_\rho \otimes e_\theta\right) \end{aligned} \tag{3}$$

form an orthonormal basis for $\mathcal{S}_0$. That is, $\mathcal{S}_0 = \operatorname{span}\{E_j(\theta)\}_{j=1}^5$ with $E_i \cdot E_j = \delta_{ij}$. This basis is extensively used in [1] and will be used in this work to compute x_3-axially symmetric solutions to some variational problems.

Landau–de Gennes Energy Functionals

In addition to the space of Q-tensors, the Landau–de Gennes model provides us with a nonlinear functional $\mathcal{F}$ defined on $\mathcal{S}_0$ describing the energy of a physical system containing nematic liquid crystal. This functional may take into account elastic energy, possible surface energy coming from particle-boundary interactions, electric and magnetic fields and other forms of energy related to the system. Our objective here is to study a field-free functional that includes particle-boundary surface energy and will be in the form of an integral taken over an unbounded domain Ω. The technicalities and restrictions we impose on such domains will be discussed in section 3.1. For now, it is enough to know that Ω will be defined so that its complement Ω^c could be physically interpreted as a colloid particle (some solid body) about the origin. The associated energy components we will be using are the following:

Elastic Energy

The elastic energy is given by the standard Dirichlet integral

$$F_E[Q] := \frac{L}{2}\int_\Omega |\nabla Q|^2 \, dx \tag{4}$$

where $L > 0$ is a material-dependent elastic constant with units given in energy per unit length.

The elastic density term $|\nabla Q|^2$ is a means to penalize spatial inhomogeneities within the liquid crystal [10].

Bulk Energy

To account for bulk effects of the liquid crystal, a bulk energy is defined by

$$F_B[Q] := \int_\Omega f_B(Q)\ dx \tag{5}$$

where

$$f_B(Q) := -\frac{a}{2}\operatorname{tr}(Q^2) - \frac{b}{3}\operatorname{tr}(Q^3) + \frac{c}{4}\left(\operatorname{tr}(Q^2)\right)^2 \tag{6}$$

is the bulk energy density. The parameter $a = a(T) \geq 0$ is a material and temperature-dependent constant with units of energy per volume times temperature. The positive parameters b and c are material-dependent constants with units of energy per volume [12]. As done in [1], our purposes allow us to fix $a = a(T_0)$ where T_0 is the critical nematic-isotropic transition temperature. The constant a will now have units of energy per volume.

It is apparent that f_B is a fourth-order polynomial in the entries of Q and the reasoning behind this choice of bulk density is noted in [10]. The authors claim that f_B as shown in (6) is the simplest form of the bulk density that admits a first-order nematic-isotropic phase transition and multiple local minima.

A global minimum of f_B can also be achieved. A useful fact proven in [8] that will be used a great deal is that f_B attains this global minimum on a special set of uniaxial Q-tensors given by

$$\mathcal{U}_* := \left\{ Q \in \mathcal{S}_0 : Q = s_* \left(n \otimes n - \frac{1}{3} I \right) \right\} \tag{7}$$

where $n \in \mathbb{S}^2$ is the director and $s_* := (b + \sqrt{b^2 + 24ac})/4c > 0$. With this, we can then define a modified bulk potential

$$\tilde{f}_B(Q) := f_B(Q) - \min_{Q \in \mathcal{S}_0} f_B(Q)$$

so that $\tilde{f}_B(Q) \geq 0$ for all $Q \in \mathcal{S}_0$ and $\tilde{f}_B(Q) = 0$ if and only if $Q \in \mathcal{U}_*$. Since this is a convenient definition, we will relabel $\tilde{f}_B$ as f_B and use this convention for the remainder of the paper.

Surface Energy

The final component we consider is that which describes the energy at the particle's surface. Recall that the domain Ω is defined so that Ω^c can be physically interpreted as a particle. Therefore, the surface of the particle is given by $\partial\Omega$ and we define the energy

$$F_S[Q] := \frac{W}{2}\int_{\partial\Omega} |Q_s - Q|^2 \, dA. \tag{8}$$

Here, we take Q_s to be a boundary condition of the form

$$Q_s(x) = s_* \left(n(x) \otimes n(x) - \frac{1}{3} I \right)$$

where $n : \partial\Omega \to \mathbb{S}^2$ is smooth. The constant $W > 0$ has units of energy per area and is called the *anchoring strength*. We allow W to assume values from the interval $(0, +\infty]$. For finite W, we say that Q has *weak anchoring* at the particle surface and it will be discussed in section 4.2 that this corresponds to the Robin boundary condition

$$\frac{L}{W}\frac{\partial Q}{\partial \nu} = Q_s - Q \quad \text{on } \partial\Omega$$

where ν is the outward unit normal to $\partial\Omega$. When $W = +\infty$, we say that Q has *strong anchoring* at the particle surface and this case corresponds to the Dirichlet boundary condition

$$Q = Q_s \quad \text{on } \partial\Omega.$$

The technicalities of this case will be discussed in section 4.2. Thus, the surface energy F_S is a means to force a particular configuration that the liquid crystal must satisfy on the surface of the particle.

Adding the energies (4), (5) and (8), we arrive at the quantity

$$\mathcal{F}_\Omega[Q] := \int_\Omega \left(\frac{L}{2}|\nabla Q|^2 + f_B(Q) \right) dx + \frac{W}{2}\int_{\partial\Omega} |Q_s - Q|^2 \, dA \tag{9}$$

called the *Landau–de Gennes energy.* The functional $\mathcal{F}_\Omega$ is represents the total energy of the system we wish to consider and it is this energy we wish to minimize later on.

3 Mathematical Framework

As stated in the introduction, a primary goal of this work is to study energy minimizing configurations of nematic liquid crystal about some colloid particle. In particular, the liquid crystal is to satisfy a given configuration at the particle's surface and uniform alignment parallel to the x_3-axis at infinity. In terms of the energy (9) from section 2.2 and previously discussed terminology, this amounts to observing the eigenvectors of some Q_* satisfying the variational problem

$$\mathcal{F}_\Omega[Q_*] = \inf_{Q \in Y} \mathcal{F}_\Omega[Q] \tag{10}$$

for a suitable class of domains Ω and function space Y. The space Y should be defined so that the pointwise condition of a solution Q_* to (10) satisfies

$$\lim_{|x| \to \infty} Q_*(x) = Q_\infty := s_* \left(e_z \otimes e_z - \frac{1}{3} I \right). \tag{11}$$

Indeed, since e_z is the director corresponding to Q_∞, uniform alignment along the x_3-axis will occur at infinity if (11) is enforced.

Besides the general existence of a solution Q_* to (10), there are already several issues one must contemplate. The first concern is effectively modelling the physical space in which we'll be working. In section 3.1, we will be giving a detailed mathematical description of 'colloid particle' and the corresponding domain Ω. The next issue is choosing the appropriate function space Y, which in general is a fairly challenging task. Section 3.2 will be dedicated to defining a space with the desired properties discussed above.

Recall also from the introduction that we are interested in observing minimizing configurations in the small particle limit. To make sensible comparisons using this limit, the functional $\mathcal{F}_\Omega$ must be nondimensionalized and will be done in section 3.3.

3.1 Colloid Particles & External Domains

To model our problem appropriately, we need to define a class of domains which possess sufficiently nice mathematical properties and physically meaningful geometry in the sense of liquid crystal-particle interaction. To do this, we will describe a 'colloid particle' as an element of the set

$$\mathcal{K} := \left\{ K \subset \mathbb{R}^3 : K \text{ is compact, star-convex with respect to } 0 \in K^\circ \text{ and } \partial K \in C^\infty \right\}. \tag{12}$$

The condition that $0 \in K^\circ$ is for technical reasons that will be seen later, while star-convexity ensures reasonable boundary behaviour. Since our problem is to consider liquid crystal occupying all space about some colloid particle, the domains of interest are subsets from the collection

$$\mathcal{ED} := \{\Omega \subset \mathbb{R}^3 : \Omega = K^c \text{ for } K \in \mathcal{K}\} \tag{13}$$

which we will call the set of *external domains*. That is, $\mathcal{ED}$ is defined as the collection of sets which are exterior to sets belonging to $\mathcal{K}$.

A simple example of a domain $\Omega \in \mathcal{ED}$ is to take $K = \overline{B_1(0)} \in \mathcal{K}$ as the closed unit ball centred at the origin and define $\Omega = \overline{B_1(0)}^c$.

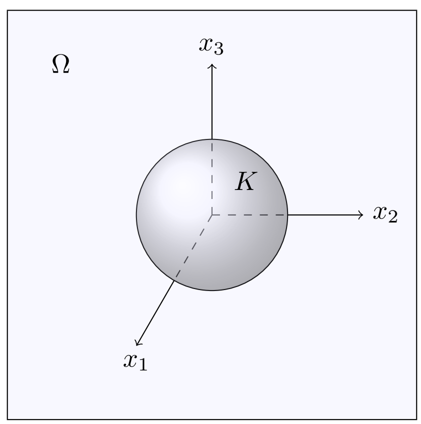

Figure 5: Example of an External Domain $\Omega = K^c = \overline{B_1(0)}^c$.

Since every external domain is unbounded, it may be difficult to work with $\Omega \in \mathcal{ED}$ directly in certain circumstances. However, results involving unbounded domains can often be shown using some 'approximating' sequence of bounded open sets. For this reason, we will construct such a sequence for $\Omega \in \mathcal{ED}$. In particular, we will build a sequence $\{\Omega_n\}_{n=1}^\infty$ of bounded open sets for $\Omega \in \mathcal{ED}$ such that

$$\begin{cases} \Omega_n \subset \Omega_{n+1} \quad \forall n \in \mathbb{N}, \\ \Omega_n \Subset \Omega \quad \forall n \in \mathbb{N}, \\ \bigcup_{n=1}^{\infty} \Omega_n = \Omega \end{cases} . \tag{14}$$

To do this, we consider first an extension of a set $K \in \mathcal{K}$. Since ∂K is smooth, the outward normal $\nu(x)$ is a smooth function of $x \in \partial K$. At each point $x_0 \in \partial K$, define the normal line segment

$$\ell_n(x_0) := \left\{ x_0 + \frac{t}{n}\nu(x_0) \in \mathbb{R}^3 : 0 \leq t \leq 1,\ n \in \mathbb{N} \text{ fixed} \right\}$$

and let

$$K_n := K \bigcup \left(\bigcup_{x_0 \in \partial K} \ell_n(x_0) \right).$$

With this, note that $\{K_n\}_{n=1}^{\infty}$ is a decreasing sequence of sets in $\mathcal{K}$ (i.e., $K_{n+1} \subset K_n$ for all $n \in \mathbb{N}$) and

$$\bigcap_{n=1}^{\infty} K_n = K.$$

Let $r_n = \text{diam}(K_1) + n$ and consider the open ball $B_{r_n}(0)$. By our choice of r_n, K_n is strictly contained in $B_{r_n}(0)$ for each $n \geq 1$ and of course $\{B_{r_n}(0)\}_{n=1}^{\infty}$ is an increasing sequence (i.e., $B_{r_n}(0) \subset B_{r_{n+1}}(0)$ for all $n \in \mathbb{N}$) satisfying $\cup_{n=1}^{\infty} B_{r_n}(0) = \mathbb{R}^3$. Define the bounded open set

$$\Omega_n := B_{r_n}(0) \setminus K_n. \tag{15}$$

Given $\{B_{r_n}(0)\}_{n=1}^{\infty}$ is increasing and $\{K_n\}_{n=1}^{\infty}$ is decreasing with $K_n \subset B_{r_n}(0)$, it is obvious that $\{\Omega_n\}_{n=1}^{\infty}$ is increasing. Also,

$$\bigcup_{n=1}^{\infty} \Omega_n = \bigcup_{n=1}^{\infty} (B_{r_n}(0) \setminus K_n) = \mathbb{R}^3 \setminus K = K^c =: \Omega \in \mathcal{ED}.$$

By construction we also have $\Omega_n \Subset \Omega$ for all $n \in \mathbb{N}$. Thus, $\{\Omega_n\}_{n=1}^{\infty}$ is a sequence of bounded open sets satisfying the desired properties (14). Since this process can be done for any $K \in \mathcal{K}$, we obtain that every $\Omega \in \mathcal{ED}$ can be given as a countable union of sets of the form (15). A simple example of this construction can be seen again by considering $\Omega = K^c = \overline{B_1(0)}^c$. Here, we have

$$K_n = B_{1+\frac{1}{n}}(0), \quad r_n = \text{diam}(K_1) + n = 4 + n, \quad \Omega_n = B_{r_n}(0) \setminus K_n.$$

3.2 Minimizing Sets

Recall that we are interested in finding a function space Y such that the variational problem (10) is satisfied by some $Q_* \in Y$ with $\lim_{|x|\to\infty} Q_*(x) = Q_\infty$. Fortunately, such a space has been carefully constructed in [1] for the special case where $\Omega = \overline{B_1(0)}^c$.

The authors of [1] start by replacing the pointwise condition (11) by the integrability condition

$$\int_{\overline{B_1(0)}^c} \frac{|Q - Q_\infty|^2}{|x|^2}\, dx < \infty$$

and claim that (11) can be recovered by resorting to estimates using the Euler–Lagrange equations associated to $\mathcal{F}_\Omega$. From here, they define the affine Hilbert space $\mathcal{H}_\infty$

$$\mathcal{H}_\infty := \mathcal{H} + Q_\infty$$

$$\mathcal{H} := \left\{ Q \in H^1_{loc}(\overline{B_1(0)}^c; \mathcal{S}_0) : \int_{\overline{B_1(0)}^c} \frac{|Q|^2}{|x|^2}\, dx + \int_{\overline{B_1(0)}^c} |\nabla Q|^2\, dx < \infty \right\}.$$

With this, the authors then prove the existence of some $Q_B \in \mathcal{H}_\infty$ that satisfies

$$\mathcal{F}_{B_1(0)}[Q_B] = \inf_{Q \in \mathcal{H}_\infty} \mathcal{F}_{B_1(0)}[Q]$$

and condition (11) [1, Proposition 3].

Using this construction as a guideline, we can consider a generalization for arbitrary external domains. To do this, let $\Omega \in \mathcal{ED}$ and define the Hilbert space

$$\mathcal{H}^\Omega := \left\{ Q \in H^1_{loc}(\Omega; \mathcal{S}_0) : \int_\Omega \frac{|Q|^2}{|x|^2}\, dx + \int_\Omega |\nabla Q|^2\, dx < \infty \right\}$$

with associated inner product

$$\langle Q_1, Q_2 \rangle_{\mathcal{H}^\Omega} := \int_\Omega \frac{Q_1 \cdot Q_2}{|x|^2}\, dx + \int_\Omega (\nabla Q_1 \cdot \nabla Q_2)\, dx$$

and induced norm

$$\|Q\|_{\mathcal{H}^\Omega} := \langle Q, Q \rangle^{1/2}_{\mathcal{H}^\Omega} = \left(\int_\Omega \frac{|Q|^2}{|x|^2}\, dx + \int_\Omega |\nabla Q|^2\, dx \right)^{1/2}.$$

Again as in [1], we define the affine Hilbert space

$$\mathcal{H}^{\Omega}_{\infty} := \mathcal{H}^{\Omega} + Q_{\infty}.$$

Since any element of $Q \in \mathcal{H}^{\Omega}_{\infty}$ is of the form $Q = \widetilde{Q} + Q_{\infty}$ for $\widetilde{Q} \in \mathcal{H}^{\Omega}$, we can rearrange to obtain $\widetilde{Q} = Q - Q_{\infty}$ and

$$\int_{\Omega} \frac{|Q - Q_{\infty}|^2}{|x|^2}\, dx = \int_{\Omega} \frac{|\widetilde{Q}|^2}{|x|^2}\, dx < \infty \tag{16}$$

is satisfied by definition of $\mathcal{H}^{\Omega}$. Thus, the integrability condition (16) is an inherent property of the set $\mathcal{H}^{\Omega}_{\infty}$ and as in [1], we claim that (16) will be enough to recover the pointwise condition (11). This will be shown later in section 4.3 and follows from observing the Euler–Lagrange equations associated to $\mathcal{F}_{\Omega}$. With this and results from 4.1, it will be clear that $\mathcal{H}^{\Omega}_{\infty}$ is an appropriate choice of function space.

The idea behind imposing condition (16) is due to the inherent unboundedness of external domains $\Omega \in \mathcal{ED}$. Indeed, for Ω unbounded we no longer have the useful results of Poincaré's inequality or particular compactness theorems. By imposing (16), the definition of $\mathcal{H}^{\Omega}$ is such that *Hardy's inequality* can be implemented and thus acts as a compromise for our unbounded setting. For a thorough reference on Hardy's inequality, one can see [2]. We end this subsection with a useful fact about $\mathcal{H}^{\Omega}$. It is presented in the following lemma and will be needed later for proving existence to the variational problem (10):

Lemma 3.1. *Suppose $\Omega \in \mathcal{ED}$ and let $\{Q_n\}_{n=1}^{\infty}$ be a sequence of functions in $\mathcal{H}^{\Omega}$ such that $Q_n \rightharpoonup Q$ weakly in $\mathcal{H}^{\Omega}$ for some $Q \in \mathcal{H}^{\Omega}$. Then, up to a suitable subsequence, $Q_n(x) \to Q(x)$ pointwise almost everywhere in Ω.*

Proof of Lemma 3.1. Let $\{\Omega_n\}_{n=1}^{\infty}$ be an approximating sequence for Ω where each Ω_n is of the form (15) as constructed in section 3.1. Given $Q_n \rightharpoonup Q$ in $\mathcal{H}^{\Omega}$, we have $Q_n \rightharpoonup Q$ in $\mathcal{H}^{\Omega_1}$ since $\Omega_1 \subset \Omega$. Using the fact that $\Omega_1 \Subset \Omega$, the definition of $\mathcal{H}^{\Omega} \subset H^1_{loc}(\Omega; \mathcal{S}_0)$ implies $Q_n \rightharpoonup Q$ in $H^1(\Omega_1; \mathcal{S}_0)$. Thus, there exists a subsequence of $\{Q_n\}_{n=1}^{\infty}$ (denoted by $\{Q_{n,1}\}_{n=1}^{\infty}$) such that $Q_{n,1}(x) \to Q(x)$ pointwise almost everywhere in Ω_1. But since $\{Q_{n,1}\}_{n=1}^{\infty}$ is a subsequence of $\{Q_n\}_{n=1}^{\infty}$, the uniqueness of weak limits gives $Q_{n,1} \rightharpoonup Q$ in $\mathcal{H}^{\Omega}$. Applying the same procedure with this subsequence, $Q_{n,1} \rightharpoonup Q$ in $\mathcal{H}^{\Omega}$ implies $Q_{n,1} \rightharpoonup Q$ in $\mathcal{H}^{\Omega_2}$ since $\Omega_2 \subset \Omega$. Again, using the fact that $\Omega_2 \Subset \Omega$, the definition of

$\mathcal{H}^\Omega$ gives $Q_{n,1} \rightharpoonup Q$ in $H^1(\Omega_2; \mathcal{S}_0)$. As before, there exists a subsequence of $\{Q_{n,1}\}_{n=1}^\infty$ (denoted by $\{Q_{n,2}\}_{n=1}^\infty$) such that $Q_{n,2}(x) \to Q(x)$ pointwise almost everywhere in Ω_2. By the uniqueness of weak limits, $Q_{n,2} \rightharpoonup Q$ in $\mathcal{H}^\Omega$. Continuing in this way, we obtain subsequences $\{Q_{n,k}\}_{n=1}^\infty$ so that $Q_{n,k}(x) \to Q(x)$ pointwise almost everywhere in Ω_k with $Q_{n,k} \rightharpoonup Q$ in $\mathcal{H}^\Omega$.

Next, we claim that the subsequence $\{Q_{n,n}\}_{n=1}^\infty$ satisfies $Q_{n,n}(x) \to Q(x)$ pointwise almost everywhere in all of Ω. From above, we know that the subsequence $\{Q_{n,N_0}\}_{n=1}^\infty$ satisfies $Q_{n,N_0}(x) \to Q(x)$ pointwise almost everywhere in Ω_{N_0}. By the nature of $\{\Omega_n\}_{n=1}^\infty$, we may choose any $x \in \Omega$ so that for some $N \in \mathbb{N}$, $x \in \Omega_n$ for all $n \geq N$. Thus, choose $x_0 \in \Omega$ so that for $N_0 = N \in \mathbb{N}$ large enough, $x_0 \in \Omega_n$ for all $n \geq N$ and $Q_{n,N}(x_0) \to Q(x_0)$ pointwise in Ω_N. By construction, $\{Q_{n,n}\}_{n=1}^\infty$ is a subsequence of $\{Q_{n,N}\}_{n=1}^\infty$ when $n \geq N$. In particular, $Q_{n,n}(x_0) \to Q(x_0)$ in Ω_n for all $n \geq N$. Since this may be done for almost any $x_0 \in \Omega$, we conclude that $Q_{n,n}(x) \to Q(x)$ pointwise almost everywhere in Ω. □

3.3 Nondimensionalization

Closely following the methods of [1] and [12, Appendix A], we nondimensionalize the functional $\mathcal{F}_\Omega$. To begin, let μ represent a natural length scale of the domain $\Omega \in \mathcal{ED}$. For our case, μ in some way should characterize the relative size of the colloid particle. As an example, if $\Omega = \overline{B_r(0)}^c$ then one can take $\mu = r$ as done in [1]. For $x \in \Omega$, define $\hat{x} := x/\mu$ so that $\hat{x}$ is nondimensional and let $\hat{\Omega} = \{x/\mu : x \in \Omega\}$. By change of variables, $dx = \mu d\hat{x}$ and

$$\frac{1}{\mu^3}\mathcal{F}_{\hat{\Omega}} = \int_{\hat{\Omega}} \left(\frac{L}{2\mu^2}|\nabla \hat{Q}|^2 + f_B(\hat{Q}) \right) dx + \frac{W}{2\mu} \int_{\partial\hat{\Omega}} |\hat{Q}_s - \hat{Q}|^2 \, dA$$

where $Q(x) = \hat{Q}(\hat{x})$ and each term now has units of energy per volume. Using the parameter $a = a(T_0)$ as a reference energy (as defined in section 2.2), dividing through by a we obtain

$$\hat{\mathcal{F}}_{\hat{\Omega}} = \int_{\hat{\Omega}} \left(\frac{\hat{L}}{2}|\nabla \hat{Q}|^2 + \hat{f}_B(\hat{Q}) \right) dx + \frac{\hat{W}}{2} \int_{\partial\hat{\Omega}} |\hat{Q}_s - \hat{Q}|^2 \, dA$$

where $\hat{\mathcal{F}}_{\hat{\Omega}}$ is now nondimensional, $\hat{f}_B$ is simply f_B with parameters a, b, c normalized by a and

$$\hat{L} = \frac{L}{\mu^2 a}, \qquad \hat{W} = \frac{W\mu a}{L}.$$

Relabeling $\hat{\mathcal{F}}_{\hat{\Omega}}$ as $\mathcal{F}_\Omega$, we now assume $\mathcal{F}_\Omega$ has been nondimensionalized from now on.

4 Minimizers

With the proper mathematical framework in place, the variational problem (10) can be presented more specifically. Taking $\Omega \in \mathcal{ED}$ and $Y = \mathcal{H}^{\Omega}_{\infty}$, problem (10) now takes the form

$$\mathcal{F}_{\Omega}[Q_*] = \inf_{Q \in \mathcal{H}^{\Omega}_{\infty}} \mathcal{F}_{\Omega}[Q]$$

where the hope is to find a solution $Q_* \in \mathcal{H}^{\Omega}_{\infty}$. In section 4.1, an exact formulation of this problem will be given, along with its existence result. The Euler–Lagrange equations (to be derived in 4.2) will then be used in section 4.3 to show regularity results of the solution $Q_* \in \mathcal{H}^{\Omega}_{\infty}$ and that (11)

$$\lim_{|x| \to \infty} Q_*(x) = Q_{\infty}.$$

is satisfied.

4.1 Existence of Minimizing Solutions

The following proposition expands the existence result found in [1, Proposition 3] for general external domains Ω.

Proposition 4.1. *Let $L > 0$, $W \in (0, +\infty]$ and suppose $\Omega \in \mathcal{ED}$. Then there exists $Q_* \in \mathcal{H}^{\Omega}_{\infty}$ such that*

$$\mathcal{F}_{\Omega}[Q_*] = \inf_{Q \in \mathcal{H}^{\Omega}_{\infty}} \mathcal{F}_{\Omega}[Q]. \tag{17}$$

Proof of Proposition 4.1. This result follows from the direct method of the calculus of variations [5]. We proceed by confirming that the following three steps hold:

Step 1: $\mathcal{F}_{\Omega}$ is bounded below and is finite for some $Q \in \mathcal{H}^{\Omega}_{\infty}$;

Step 2: Any minimizing sequence of $\mathcal{F}_{\Omega}$ admits a weak limit (up to a subsequence);

Step 3: $\mathcal{F}_{\Omega}$ is lower semicontinuous.

Step 1:

It is trivial that $\mathcal{F}_{\Omega} \geq 0$ since the elastic energy F_E, bulk energy F_B and surface energy F_S are non-negative on $\mathcal{H}^{\Omega}_{\infty}$. To show $\mathcal{F}_{\Omega}$ admits finite energy, the cases where $W < +\infty$ and $W = +\infty$

will be considered separately. In the case of weak anchoring, let $Q = Q_\infty + \Phi$ where $\Phi \in C_0^\infty(\overline{\Omega}; \mathcal{S}_0)$ is arbitrary. Denote the support of Φ by X_Φ and notice that $Q_\infty \in \mathcal{U}_*$. Therefore, $f_B(Q_\infty) = 0$ and we can write

$$\begin{aligned}\mathcal{F}_\Omega[Q] &= \int_{\Omega \setminus X_\Phi} + \int_{X_\Phi} \left[\frac{L}{2} \left|\nabla(Q_\infty + \Phi)\right|^2 + f_B(Q_\infty + \Phi)\right] dx + \frac{W}{2}\int_{\partial\Omega} \left|Q_s - (Q_\infty + \Phi)\right|^2 \, dA \\ &= \int_{X_\Phi} \left(\frac{L}{2}\left|\nabla\Phi\right|^2 + f_B(Q_\infty + \Phi)\right) dx + \frac{W}{2}\int_{\partial\Omega} \left|Q_s - (Q_\infty + \Phi)\right|^2 \, dA.\end{aligned}$$

Since X_Φ is of finite measure and Φ is smooth, the first integral above is finite. By definition, the surface matrix Q_s and boundary $\partial\Omega$ are smooth and so we also obtain finite surface energy. Thus, there exists $Q \in \mathcal{H}_\infty^\Omega$ for which $\mathcal{F}_\Omega[Q] < \infty$. In the case of strong anchoring, we consider maps $Q \in \mathcal{H}_\infty^\Omega$ for which $Q = Q_s$ on $\partial\Omega$ in the trace sense. As before, define $Q = Q_\infty + \Phi$ but now take $\Phi \in C_0^\infty(\overline{\Omega}; \mathcal{S}_0)$ such that $\Phi = Q_s - Q_\infty$ on $\partial\Omega$. Then

$$\int_{\partial\Omega} \left|Q_s - Q\right|^2 \, dA = 0$$

and we have $\mathcal{F}_\Omega[Q] < \infty$ by the same arguments used in the weak anchoring case.

<u>Step 2</u>:

Let

$$m := \inf_{Q \in \mathcal{H}_\infty^\Omega} \mathcal{F}_\Omega[Q]$$

and let $\{Q_n\}_{n=1}^\infty$ be a minimizing sequence in $\mathcal{H}_\infty^\Omega$ with $W < +\infty$. By definition, there exists $N \in \mathbb{N}$ such that

$$m + 1 \geq \mathcal{F}_\Omega[Q_n] = \int_\Omega \left(\frac{L}{2}|\nabla Q_n|^2 + f_B(Q_n)\right) dx + \frac{W}{2}\int_{\partial\Omega} |Q_s - Q_n|^2 \, dA$$

for all $n \geq N$. In particular, the non-negativity of f_B and F_S allows us to write

$$m + 1 \geq \mathcal{F}_\Omega[Q_n] \geq \int_\Omega \frac{L}{2}|\nabla Q_n|^2 \, dx \implies \frac{4(m+1)}{L} \geq 2\int_\Omega |\nabla Q_n|^2 \, dx.$$

Recall that since $Q_n \in \mathcal{H}_\infty^\Omega$, we have the representation $Q_n = Q_\infty + \widetilde{Q_n}$ where $\widetilde{Q_n} \in \mathcal{H}^\Omega$. Using this and invoking Hardy's inequality,

$$2\int_\Omega |\nabla Q_n|^2 \, dx = 2\int_\Omega |\nabla \widetilde{Q_n}|^2 \, dx \geq \int_\Omega |\nabla \widetilde{Q_n}|^2 \, dx + C\int_\Omega \frac{|\widetilde{Q_n}|^2}{|x|^2} \, dx$$

where $C > 0$ is a constant independent of n.

If $C \geq 1$, then

$$\frac{4(m+1)}{L} \geq \int_\Omega |\nabla \widetilde{Q_n}|^2 \, dx + \int_\Omega \frac{|\widetilde{Q_n}|^2}{|x|^2} \, dx = \|\widetilde{Q_n}\|^2_{\mathcal{H}^\Omega}.$$

If $C < 1$, then

$$\frac{4(m+1)}{L} \geq C\int_\Omega |\nabla \widetilde{Q_n}|^2 \, dx + C\int_\Omega \frac{|\widetilde{Q_n}|^2}{|x|^2} \, dx = C\|\widetilde{Q_n}\|^2_{\mathcal{H}^\Omega}.$$

In both situations, the sequence $\{\widetilde{Q_n}\}_{n=1}^\infty$ is uniformly bounded in $\mathcal{H}^\Omega$. Since $\mathcal{H}^\Omega$ is a Hilbert space, there exists a subsequence (still denoted $\{\widetilde{Q_n}\}_{n=1}^\infty$) such that $\widetilde{Q_n} \rightharpoonup \widetilde{Q_*}$ in $\mathcal{H}^\Omega$ for some $\widetilde{Q_*} \in \mathcal{H}^\Omega$. Defining

$$Q_* := \widetilde{Q_*} + Q_\infty,$$

we obtain that $Q_* \in \mathcal{H}^\Omega_\infty$ is the weak limit of the minimizing subsequence

$$\{Q_n\}_{n=1}^\infty = \{\widetilde{Q_n} + Q_\infty\}_{n=1}^\infty.$$

In the case where $W = +\infty$, let $\{Q_n\}_{n=1}^\infty$ be a minimizing sequence such that $Q_n = Q_s$ on $\partial\Omega$ in the trace sense for each $n \in \mathbb{N}$. Applying the same arguments as in the weak anchoring case, we obtain a subsequence $\{Q_n\}_{n=1}^\infty \subset \mathcal{H}^\Omega_\infty$ with weak limit $Q_* \in \mathcal{H}^\Omega_\infty$.

Step 3:

By Lemma 3.1, we may assume that the minimizing subsequence $\{Q_n\}_{n=1}^\infty$ satisfies $Q_n(x) \to Q_*(x)$ pointwise almost everywhere in Ω. Consider the sequence $\{f_B(Q_n)\}_{n=1}^\infty$ and define

$$f(x) := \lim_{n\to\infty} f_B(Q_n(x)), \quad x \in \Omega.$$

Since f_B is continuous,

$$f_B(Q_*(x)) = \lim_{n\to\infty} f_B(Q_n(x)) = f(x)$$

almost everywhere in Ω. Applying Fatou's lemma,

$$\int_\Omega f_B(Q_*)\ dx \leq \liminf_{n\to\infty} \int_\Omega f_B(Q_n)\ dx.$$

Using the convexity of the remaining energy terms in $\mathcal{F}_\Omega$, we have

$$m \leq \mathcal{F}_\Omega[Q_*] \leq \liminf_{n\to\infty} \mathcal{F}_\Omega[Q_n] = m \implies \mathcal{F}_\Omega[Q_*] = m.$$

Thus, the direct method gives the existence of a minimizer $Q_* \in \mathcal{H}^\Omega_\infty$ to the problem (17). □

4.2 Euler–Lagrange Equations

The main focus of this section deals primarily with deriving the Euler–Lagrange equations as shown in the following proposition. The equations will be used to show regularity results in section 4.3.

Proposition 4.2. *Suppose $Q \in \mathcal{H}^\Omega_\infty$ is a minimizer of $\mathcal{F}_\Omega$. Then Q weakly satisfies the system of semilinear partial differential equations*

$$L\Delta Q = -aQ - b\left(Q^2 - \frac{1}{3}|Q|^2 I\right) + c|Q|^2 Q \tag{18}$$

in Ω and weakly satisfies the boundary conditions

$$\begin{cases} \dfrac{L}{W}\dfrac{\partial Q}{\partial \nu} = Q_s - Q & \text{if } W < +\infty \\ Q = Q_s & \text{if } W = +\infty \end{cases}$$

on $\partial\Omega$ where the Dirichlet boundary condition can be interpreted in the trace sense.

Before committing our efforts to deriving (18), it will be worth while to note a subtlety from the previous section. By using $\mathcal{H}^\Omega_\infty$ as our minimizing space, we are directly imposing that any minimizing solution Q_* of $\mathcal{F}_\Omega$ will satisfy the trace condition $\mathrm{tr}\,(Q_*) = 0$. On the other hand, there is nothing inherent about the functional $\mathcal{F}_\Omega$ which imposes this traceless constraint in general. Therefore, without reference to $\mathcal{H}^\Omega_\infty$, an arbitrary solution Q_* to the Euler–Lagrange equations constructed from $\mathcal{F}_\Omega$ does not necessarily have to satisfy $\mathrm{tr}(Q_*) = 0$. However, modifications to the Lagrangian

$$\mathcal{L}(x, Q, \nabla Q) := \frac{L}{2}|\nabla Q|^2 + f_B(Q)$$

can be made to rectify this issue.

To start, consider the technique used in [8] to show that f_B attains its minimum on the set of uniaxial Q-tensors $\mathcal{U}_*$. The first realization is that f_B can be recast in terms of the eigenvalues of Q. Indeed, suppose $\lambda_1, \lambda_2, \lambda_3$ are the eigenvalues of Q. Then since $\operatorname{tr}(Q^n) = \sum_{i=1}^3 \lambda_i^n$, one has

$$f_B(Q) = f_B(\lambda_1, \lambda_2, \lambda_3) := -\frac{a}{2}\sum_{i=1}^3 \lambda_i^2 - \frac{b}{3}\sum_{i=1}^3 \lambda_i^3 + \frac{c}{4}\left(\sum_{i=1}^3 \lambda_i^2\right)^2.$$

Via the method of Lagrange multipliers, we minimize $f_B(\lambda_1, \lambda_2, \lambda_3)$ subject to the constraint $g(\lambda_1, \lambda_2, \lambda_3) := \sum_{i=1}^3 \lambda_i = 0$. Proceeding as usual, define the auxiliary function

$$\tilde{f}(\lambda_1, \lambda_2, \lambda_3) := f_B(\lambda_1, \lambda_2, \lambda_3) - \delta g(\lambda_1, \lambda_2, \lambda_3)$$

where δ is the associated Lagrange multiplier. As given in [8], for each $i = 1, 2, 3$

$$\frac{\partial \tilde{f}}{\partial \lambda_i} = 0 \iff -a\lambda_i - b\lambda_i^2 + c\left(\sum_{j=1}^3 \lambda_j^2\right)\lambda_i = \delta.$$

Also, $\partial\tilde{f}/\partial\lambda_i = 0$ for each $i = 1, 2, 3 \implies \sum_{i=1}^3 \partial\tilde{f}/\partial\lambda_i = 0$ and so

$$-a\sum_{i=1}^3 \lambda_i - b\sum_{i=1}^3 \lambda_i^2 + c\left(\sum_{j=1}^3 \lambda_j^2\right)\sum_{i=1}^3 \lambda_i = 3\delta.$$

Imposing the condition $\sum_{i=1}^3 \lambda_i = 0$, we are left with

$$-a \cdot 0 - b\sum_{i=1}^3 \lambda_i^2 + c\left(\sum_{j=1}^3 \lambda_j^2\right) \cdot 0 = 3\delta \implies \delta = -\frac{b}{3}\sum_{i=1}^3 \lambda_i^2.$$

Resorting back to the original notation, we have found that the appropriate Lagrange multiplier is given by $\delta = -(b/3)\operatorname{tr}\left(Q^2\right)$. Therefore, by taking $\delta = -(b/3)\operatorname{tr}\left(Q^2\right)$, the function $\tilde{f}$ is a modification of f_B which enforces the traceless constraint. With the same logic, it is easy to see that the Lagrangian

$$\widetilde{\mathcal{L}}(x, Q, \nabla Q) := \frac{L}{2}|\nabla Q| + f_B(Q) - \lambda \operatorname{tr}(Q)$$

is a modification of $\mathcal{L}$ which enforces the traceless condition if we take $\lambda = -(b/3)\operatorname{tr}\left(Q^2\right)$. Notice also that if we define $\widetilde{\mathcal{F}_\Omega}[Q] = \int_\Omega \tilde{\mathcal{L}}(x, Q, \nabla Q)\, dx + F_S[Q]$, then there is $Q_* \in \mathcal{H}_\infty^\Omega$ such that

$$\mathcal{F}_\Omega\left[Q_*\right] = \inf_{Q \in \mathcal{H}^\Omega_\infty} \mathcal{F}_\Omega[Q] = \inf_{Q \in \mathcal{H}^\Omega_\infty} \widetilde{\mathcal{F}_\Omega}[Q] = \widetilde{\mathcal{F}_\Omega}\left[Q_*\right]$$

since $\mathcal{L} = \widetilde{\mathcal{L}}$ over $\mathcal{H}^\Omega_\infty$. Thus, a minimizer of $\mathcal{F}_\Omega$ will at least weakly satisfy the Euler–Lagrange equations derived from $\widetilde{\mathcal{F}_\Omega}$. Using this and the fact that $\widetilde{\mathcal{L}}$ incorporates the traceless condition directly, it will make more sense for us to construct the Euler–Lagrange equations from $\widetilde{\mathcal{F}_\Omega}$ as opposed to $\mathcal{F}_\Omega$. This way, solutions to the Euler–Lagrange equations will automatically satisfy the traceless constraint, regardless of reference to the minimizing space $\mathcal{H}^\Omega_\infty$.

We now derive the Euler–Lagrange equations (18) via the first variation of $\widetilde{\mathcal{F}_\Omega}$.

Proof of Proposition 4.2. Let $Q \in \mathcal{H}^\Omega_\infty$ be a minimizer of

$$\widetilde{\mathcal{F}_\Omega}[Q] = \int_\Omega \left(\frac{L}{2}|\nabla Q| + f_B(Q) - \lambda \mathrm{tr}(Q) \right) + \frac{W}{2} \int_{\partial\Omega} |Q_s - Q|^2 \; dA$$

where $\lambda = -(b/3)\mathrm{tr}\left(Q^2\right)$ is the associated Lagrange multiplier accounting for tracelessness. The first variation of $\widetilde{\mathcal{F}_\Omega}$ is given by

$$\left. \frac{d}{d\varepsilon} \widetilde{\mathcal{F}_\Omega}[Q + \varepsilon\Phi] \right|_{\varepsilon=0} = 0$$

where $\Phi \in C^\infty_0(\overline{\Omega}; \mathcal{S}_0)$ is a smooth, compactly supported matrix-valued function on $\overline{\Omega}$ and $\varepsilon \neq 0$ is a scalar. We calculate this quantity in a number of steps, starting with the elastic energy term.

$$\begin{aligned}
\frac{d}{d\varepsilon} \int_\Omega \frac{L}{2} \left|\nabla(Q + \varepsilon\Phi)\right|^2 dx &= \int_\Omega \left(\frac{L}{2} \frac{d}{d\varepsilon} \sum_{i,j=1}^{3} \left|\nabla Q_{ij} + \varepsilon \nabla \Phi_{ij}\right|^2 \right) dx \\
&= \int_\Omega \left(\frac{L}{2} \frac{d}{d\varepsilon} \sum_{i,j,k=1}^{3} \left(\frac{\partial Q_{ij}}{\partial x_k} + \varepsilon \frac{\partial \Phi_{ij}}{\partial x_k} \right)^2 \right) dx \\
&= \int_\Omega \left(L \sum_{i,j,k=1}^{3} \left(\frac{\partial Q_{ij}}{\partial x_k} + \varepsilon \frac{\partial \Phi_{ij}}{\partial x_k} \right) \frac{\partial \Phi_{ij}}{\partial x_k} \right) dx.
\end{aligned}$$

Setting $\varepsilon = 0$ gives

$$\begin{aligned}
\left. \left(\frac{d}{d\varepsilon} \int_\Omega \frac{L}{2} \left|\nabla(Q + \varepsilon\Phi)\right|^2 dx \right) \right|_{\varepsilon=0} &= \int_\Omega \left(L \sum_{i,j,k=1}^{3} \frac{\partial Q_{ij}}{\partial x_k} \frac{\partial \Phi_{ij}}{\partial x_k} \right) dx \\
&= \int_\Omega L \nabla Q \cdot \nabla \Phi \; dx.
\end{aligned}$$

Recognizing that $Q \in H^1_{loc}(\Omega)$ and using $\Phi \in C_0^\infty(\overline{\Omega}; \mathcal{S}_0)$, we can integrate by parts to obtain

$$\left(\frac{d}{d\varepsilon}\int_\Omega \frac{L}{2}\left|\nabla(Q+\varepsilon\Phi)\right|^2 dx\right)\Bigg|_{\varepsilon=0} = -\int_\Omega LQ\cdot\Delta\Phi\ dx + \int_{\partial\Omega} LQ\cdot\frac{\partial\Phi}{\partial\nu}\ dA. \tag{19}$$

Next we calculate

$$\left(\frac{d}{d\varepsilon}\int_\Omega f_B(Q+\varepsilon\Phi)\ dx\right)\Bigg|_{\varepsilon=0}$$

by first individually computing each of the terms

(a) $\displaystyle \frac{d}{d\varepsilon}\int_\Omega -\frac{a}{2}\,\mathrm{tr}\left((Q+\varepsilon\Phi)^2\right)dx$

(b) $\displaystyle \frac{d}{d\varepsilon}\int_\Omega -\frac{b}{3}\,\mathrm{tr}\left((Q+\varepsilon\Phi)^3\right)dx$

(c) $\displaystyle \frac{d}{d\varepsilon}\int_\Omega \frac{c}{4}\,\mathrm{tr}\left((Q+\varepsilon\Phi)^2\right)^2 dx$

and then taking $\varepsilon = 0$. For the sake of organization, we define the matrix $G(\varepsilon) = Q + \varepsilon\Phi$ so that $G_{ij}(0) = Q_{ij}$ and $G'_{ij}(\varepsilon) = \Phi_{ij}$.

(a)

$$\frac{d}{d\varepsilon}\int_\Omega -\frac{a}{2}\mathrm{tr}\left(G^2\right)dx = \int_\Omega -\frac{a}{2}\frac{d}{d\varepsilon}|G|^2\ dx = \int_\Omega\left(-a\sum_{i,j=1}^3 G_{ij}(\varepsilon)G'_{ij}\right)dx.$$

Taking $\varepsilon = 0$,

$$\left(\frac{d}{d\varepsilon}\int_\Omega -\frac{a}{2}\mathrm{tr}\left(G^2\right)dx\right)\Bigg|_{\varepsilon=0} = \int_\Omega\left(-a\sum_{i,j=1}^3 Q_{ij}\Phi_{ij}\right)dx = \int_\Omega\left(-aQ\cdot\Phi\right)dx.$$

(b)

First, we recognize that $\mathrm{tr}(G^3) = \sum_{j=1}^5 P_j(\varepsilon)$ where

$$P_1 = G_{11}^3 + G_{22}^3 + G_{33}^3, \quad P_2 = 3G_{12}^2\left(G_{11}+G_{22}\right),$$

$$P_3 = 3G_{13}^2\left(G_{11}+G_{33}\right), \quad P_4 = 3G_{23}^2\left(G_{22}+G_{33}\right),$$

$$P_5 = 6G_{12}G_{13}G_{23}.$$

Then

$$\frac{d}{d\varepsilon}\int_\Omega -\frac{b}{3}\operatorname{tr}\left(G^3\right)dx = \int_\Omega \left(-\frac{b}{3}\sum_{j=1}^{5} P_j'(\varepsilon)\right)dx$$

and we calculate

$$\begin{aligned}
\frac{1}{3}P_1'(0) &= Q_{11}^2\Phi_{11} + Q_{22}^2\Phi_{22} + Q_{33}^2\Phi_{33}\\
\frac{1}{3}P_2'(0) &= Q_{12}^2(\Phi_{11}+\Phi_{22}) + 2Q_{12}\Phi_{12}(Q_{11}+Q_{22})\\
\frac{1}{3}P_3'(0) &= Q_{13}^2(\Phi_{11}+\Phi_{33}) + 2Q_{13}\Phi_{13}(Q_{11}+Q_{33})\\
\frac{1}{3}P_4'(0) &= Q_{23}^2(\Phi_{22}+\Phi_{33}) + 2Q_{23}\Phi_{23}(Q_{22}+Q_{33})\\
\frac{1}{3}P_5'(0) &= 2\Phi_{12}Q_{13}Q_{23} + 2Q_{12}\Phi_{13}Q_{23} + 2Q_{12}Q_{13}\Phi_{23}.
\end{aligned}$$

Summing the above and factoring with respect to Φ_{ij}, it straightforward to check

$$\frac{1}{3}\sum_{j=1}^{5} P_j'(0) = Q^2\cdot\Phi$$

and therefore

$$\left(\frac{d}{d\varepsilon}\int_\Omega -\frac{b}{3}\operatorname{tr}\left(G^3\right)dx\right)\Bigg|_{\varepsilon=0} = \int_\Omega \left(-bQ^2\cdot\Phi\right)dx.$$

(c)

It is convenient to recognize

$$\frac{d}{d\varepsilon}\operatorname{tr}(G^2)^2 = \frac{d}{d\varepsilon}\left(\sum_{i,j=1}^{3} G_{ij}^2\right)^2 = 2\left(\sum_{i,j=1}^{3} G_{ij}^2\right)\sum_{i,j=1}^{5}\frac{d}{d\varepsilon}G_{ij}^2.$$

Setting $\varepsilon = 0$ and referring to the calculations done in (a), we obtain

$$2\left(\sum_{i,j=1}^{3} G_{ij}(0)^2\right)\sum_{i,j=1}^{5}\frac{d}{d\varepsilon}G_{ij}^2\Bigg|_{\varepsilon=0} = 2|Q|^2(2Q\cdot\Phi) = 4(|Q|^2 Q\cdot\Phi).$$

Therefore

$$\left(\frac{d}{d\varepsilon}\int_\Omega \frac{c}{4}\operatorname{tr}\left(G^2\right)^2 dx\right)\Bigg|_{\varepsilon=0} = \int_\Omega c|Q|^2 Q\cdot\Phi\ dx.$$

Adding parts (a), (b) and (c),

$$\left(\frac{d}{d\varepsilon} \int_\Omega f_B(Q + \varepsilon\Phi)\ dx \right)\Big|_{\varepsilon=0} = \int_\Omega \left(-aQ - bQ^2 + c|Q|^2 Q \right) \cdot \Phi\ dx. \tag{20}$$

Next,

$$\frac{d}{d\varepsilon} \lambda \operatorname{tr}(Q + \varepsilon\Phi) = \lambda \sum_{i=1}^{3} \Phi_{ii} = \lambda I \cdot \Phi$$

and so

$$\left(\frac{d}{d\varepsilon} \lambda \operatorname{tr}(Q + \varepsilon\Phi) \right)\Big|_{\varepsilon=0} = \int_\Omega \lambda I \cdot \Phi\ dx = \int_\Omega \left(-\frac{1}{3} |Q|^2 I \cdot \Phi \right) dx. \tag{21}$$

Finally, using a similar calculation as done in (a)

$$\left(\frac{d}{d\varepsilon} \frac{W}{2} \int_{\partial\Omega} |Q_s - (Q + \varepsilon\Phi)|^2\ dA \right)\Big|_{\varepsilon=0} = -W \int_{\partial\Omega} (Q_s - Q) \cdot \Phi\ dA. \tag{22}$$

Summing (19), (20), (21) and (22), the first variation of $\widetilde{\mathcal{F}_\Omega}$ is given by

$$-\int_\Omega LQ \cdot \Delta\Phi\ dx + \int_\Omega \left(-aQ - b\left(Q^2 - \frac{1}{3}|Q|^2 I \right) + c|Q|^2 Q \right) \cdot \Phi\ dx$$
$$+ \int_{\partial\Omega} LQ \cdot \frac{\partial\Phi}{\partial\nu}\ dA - W \int_{\partial\Omega} (Q_s - Q) \cdot \Phi\ dA = 0.$$

In the special case where $\Phi \in C_0^\infty(\Omega; \mathcal{S}_0)$, then

$$\int_{\partial\Omega} LQ \cdot \frac{\partial\Phi}{\partial\nu}\ dA = W \int_{\partial\Omega} (Q_s - Q) \cdot \Phi\ dA = 0$$

and we are left with

$$-\int_\Omega LQ \cdot \Delta\Phi\ dx + \int_\Omega \left(-aQ - b\left(Q^2 - \frac{1}{3}|Q|^2 I \right) + c|Q|^2 Q \right) \cdot \Phi\ dx = 0$$

holding for all $\Phi \in C_0^\infty(\Omega; \mathcal{S}_0)$. That is, Q weakly satisfies (18)

$$L\Delta Q = -aQ - b\left(Q^2 - \frac{1}{3}|Q|^2 I \right) + c|Q|^2 Q.$$

Now, for general $\Phi \in C_0^\infty(\overline{\Omega}; \mathcal{S}_0)$, Q still weakly satisfies (18) but we now have the extra condition

$$\int_{\partial\Omega} LQ \cdot \frac{\partial\Phi}{\partial\nu}\ dA - W \int_{\partial\Omega} (Q_s - Q) \cdot \Phi\ dA = 0$$

forced by definition of the first variation. In other words,

$$\frac{L}{W}\frac{\partial Q}{\partial \nu} = Q_s - Q \tag{23}$$

weakly on $\partial\Omega$.

We can now see how the anchoring strength W dictates the boundary condition at the particle surface. In the case of weak anchoring ($W < +\infty$), the Robin boundary condition (23) is left as is. For the case of strong anchoring ($W = +\infty$), observe that in the weak formulation

$$\int_{\partial\Omega} (Q_s - Q) \cdot \Phi \, dA = \frac{L}{W} \int_{\partial\Omega} Q \cdot \frac{\partial \Phi}{\partial \nu} \, dA = 0$$

for all $\Phi \in C_0^\infty(\overline{\Omega}, \mathcal{S}_0)$. Since Q_s and $\partial\Omega$ are smooth and $Q \in H^1_{loc}(\Omega; \mathcal{S}_0)$, the trace theorem implies that we may think of $Q = Q_s$ in the trace sense for $W = +\infty$. $\square$

4.3 Regularity

In general, a minimizer $Q \in \mathcal{H}^\Omega_\infty$ of $\mathcal{F}_\Omega$ is dependent on the parameters L and W. To indicate this, one may write $Q = Q_{L,W}$ for particular L and W. However, solutions to (18) have the nice property that they are bounded, *independent* of L and W.

Lemma 4.3. *Let $\Omega \in \mathcal{ED}$ and suppose $Q \in \mathcal{H}^\Omega_\infty$ solves (18). Then $\|Q\|_{L^\infty(\Omega)} \leq \gamma$ for some $\gamma = \gamma(\Omega, Q_s, a, b, c) > 0$.*

The proof of Lemma 4.3 follows almost identically to that as done in [1, Lemma 5]. However, we reproduce the proof here to extend the result for generalized Ω and to fill in omitted details. Before proving Lemma 4.3, it will be worth while to prove the following result:

Proposition 4.4. *Let $Q \in \mathcal{H}^\Omega_\infty$ with $\widetilde{Q} = Q - Q_\infty \in \mathcal{H}^\Omega$. Then*

$$\left(-aQ - b\left(Q^2 - \frac{1}{3}|Q|^2 I\right) + c|Q|^2 Q\right) \cdot \widetilde{Q} \sim c|\widetilde{Q}|^4$$

as $|\widetilde{Q}| \to \infty$.

Proof of Proposition 4.4. By linearity of the inner product,

$$\left(-aQ - b\left(Q^2 - \frac{1}{3}|Q|^2 I\right) + c|Q|^2 Q\right) \cdot \widetilde{Q} = -aQ \cdot \widetilde{Q} - bQ^2 \cdot \widetilde{Q} + \frac{b}{3}|Q|^2 I \cdot \widetilde{Q} + c|Q|^2 Q \cdot \widetilde{Q}.$$

Let us now analyze the following terms individually

(a) $\quad - aQ \cdot \widetilde{Q}$

(b) $\quad - bQ^2 \cdot \widetilde{Q}$

(c) $\quad \frac{b}{3} |Q|^2 I \cdot \widetilde{Q}$

(d) $\quad c |Q|^2 Q \cdot \widetilde{Q}$

and then comment on their asymptotic behaviour.

(a)

Rewriting,

$$\begin{aligned} Q \cdot \widetilde{Q} &= \left(Q_\infty + \widetilde{Q}\right) \cdot \widetilde{Q} \\ &= \operatorname{tr}\left(\widetilde{Q}\left(Q_\infty + \widetilde{Q}\right)\right) \\ &= \operatorname{tr}\left(\widetilde{Q}Q_\infty\right) + |\widetilde{Q}|^2 \\ &= -\frac{s_*}{3}\left(\widetilde{Q}_{11} + \widetilde{Q}_{22}\right) + \frac{2s_*}{3}\widetilde{Q}_{33} + |\widetilde{Q}|^2 \\ &= -\frac{s_*}{3}\left(-\widetilde{Q}_{33}\right) + \frac{2s_*}{3}\widetilde{Q}_{33} + |\widetilde{Q}|^2 \qquad (\text{since } \widetilde{Q} \in \mathcal{S}_0) \\ &= s_*\widetilde{Q}_{33} + |\widetilde{Q}|^2. \end{aligned}$$

Of course, since $|\widetilde{Q}|^2 = \sum_{ij} \widetilde{Q}_{ij}^2 \geq s_*\widetilde{Q}_{33}$ for $|\widetilde{Q}|$ large enough, we have that $-aQ \cdot \widetilde{Q} \sim -a|\widetilde{Q}|^2$ as $|\widetilde{Q}| \to \infty$.

(b)

In this step, we will not comment on asymptotic behaviour, but will recognize useful upper bounds needed later.

$$Q^2 \cdot \widetilde{Q} = \operatorname{tr}\left(\widetilde{Q}\left(Q_\infty + \widetilde{Q}\right)^2\right) = \operatorname{tr}\left(\widetilde{Q}Q_\infty^2\right) + 2\operatorname{tr}\left(\widetilde{Q}^2Q_\infty\right) + \operatorname{tr}\left(\widetilde{Q}^3\right).$$

Calculating the first two terms, we have

$$\begin{aligned}\operatorname{tr}\left(\widetilde{Q}Q_\infty^2\right) &= \frac{s_*^2}{9}\left(\widetilde{Q}_{11}+\widetilde{Q}_{22}\right)+\frac{4s_*^2}{9}\widetilde{Q}_{33}\\ &= \frac{s_*^2}{9}\left(-\widetilde{Q}_{33}\right)+\frac{4s_*^2}{9}\widetilde{Q}_{33}\\ &= \frac{s_*^2}{3}\widetilde{Q}_{33}\end{aligned}$$

and

$$\begin{aligned}2\operatorname{tr}\left(\widetilde{Q}^2Q_\infty\right) &= -\frac{2s_*}{3}\left(\widetilde{Q}_{11}^2+\widetilde{Q}_{12}^2+\widetilde{Q}_{13}^2\right)-\frac{2s_*}{3}\left(\widetilde{Q}_{12}^2+\widetilde{Q}_{22}^2+\widetilde{Q}_{23}^2\right)+\frac{4s_*}{3}\left(\widetilde{Q}_{13}^2+\widetilde{Q}_{23}^2+\widetilde{Q}_{33}^2\right)\\ &\le 0+0+4s_*\left(2\widetilde{Q}_{13}^2+2\widetilde{Q}_{23}^2+\widetilde{Q}_{33}^2\right)\\ &\le 4s_*|\widetilde{Q}|^2\end{aligned}$$

Furthermore, from [10, Lemma 13]

$$\operatorname{tr}\left(\widetilde{Q}^3\right)\le\frac{|\widetilde{Q}|^3}{\sqrt{6}}.$$

Comparing all terms, it is obvious that for $|\widetilde{Q}|$ sufficiently large, $Q^2\cdot\widetilde{Q}\le|\widetilde{Q}|^3$. Therefore, we expect the asymptotic behaviour of $bQ^2\cdot\widetilde{Q}$ to be no larger than $b|\widetilde{Q}|^3$.

(c)

It is easy to see that

$$\frac{b}{3}\left|Q\right|^2 I\cdot\widetilde{Q}=\frac{b}{3}\left|Q\right|^2\operatorname{tr}\left(\widetilde{Q}I\right)=0$$

since $\widetilde{Q}\in\mathcal{S}_0$.

(d)

Finally,

$$\begin{aligned}c\left|Q\right|^2 Q\cdot\widetilde{Q} &= c\left|Q_\infty+\widetilde{Q}\right|^2\operatorname{tr}\left(\widetilde{Q}\left(Q_\infty+\widetilde{Q}\right)\right)\\ &= c\left|Q_\infty+\widetilde{Q}\right|^2\left(\operatorname{tr}\left(\widetilde{Q}Q_\infty\right)+|\widetilde{Q}|^2\right)\\ &= c\left|Q_\infty+\widetilde{Q}\right|^2\left(s_*\widetilde{Q}_{33}+|\widetilde{Q}|^2\right).\end{aligned}$$

Also,

$$\left|Q_\infty + \widetilde{Q}\right|^2 = \frac{2s_*^2}{3} + 2s_*\widetilde{Q}_{33} + |\widetilde{Q}|^2$$

and thus

$$c\,|Q|^2\,Q\cdot\widetilde{Q} = c\left(\frac{2s_*^2}{3} + 2s_*\widetilde{Q}_{33} + |\widetilde{Q}|^2\right)\left(s_*\widetilde{Q}_{33} + |\widetilde{Q}|^2\right) \sim c|\widetilde{Q}|^4.$$

Comparing parts (a) through (d), we gather that the term $c\,|Q|^2\,Q\cdot\widetilde{Q}$ from part (d) dominates for large $|\widetilde{Q}|$. Therefore,

$$\left(-aQ - b\left(Q^2 - \frac{1}{3}\,|Q|^2\,I\right) + c\,|Q|^2\,Q\right)\cdot\widetilde{Q} \sim c|\widetilde{Q}|^4$$

as $|\widetilde{Q}| \to \infty$. $\square$

We may now proceed with the proof of Lemma 4.3. For the sake of space and notation, we label the righthand side of (18)

$$\nabla f_B(Q) = -aQ - b\left(Q^2 - \frac{1}{3}|Q|^2 I\right) + c|Q|^2 Q$$

as done in [1].

Proof of Lemma 4.3. By definition of $\mathcal{H}_\infty^\Omega$, the matrix Q has the form $Q = Q_\infty + \widetilde{Q}$ where $\widetilde{Q} \in \mathcal{H}^\Omega$. Since Q_∞ is a constant matrix, $\Delta Q = \Delta(Q_\infty + \widetilde{Q}) = \Delta\widetilde{Q}$ and so the Euler-Lagrange equations can be written as

$$L\Delta\widetilde{Q} = \nabla f_B(Q_\infty + \widetilde{Q}). \tag{24}$$

Consider a function $\Psi \in \mathcal{H}^\Omega$ of the form $\Psi = V\widetilde{Q}$ where $V \in C_0^\infty(\overline{\Omega})$ with $V \geq 0$. Multiplying equation (24) by Ψ and integrating by parts gives

$$L\int_\Omega \nabla\widetilde{Q}\cdot\nabla\Psi\;dx = -\int_\Omega V\nabla f_B(Q_\infty + \widetilde{Q})\cdot\widetilde{Q}\;dx + \int_{\partial\Omega} V\widetilde{Q}\cdot\frac{\partial\widetilde{Q}}{\partial\nu}\;ds. \tag{25}$$

Appealing to Proposition 4.4, we know that the quantity $\nabla f_B(Q_\infty + \widetilde{Q})\cdot\widetilde{Q} \sim c|\widetilde{Q}|^4$ as $|\widetilde{Q}| \to \infty$. Therefore, we can find some $c_1 = c_1(a,b,c) > 0$ for which $\nabla f_B(Q_\infty + \widetilde{Q})\cdot\widetilde{Q} \geq 0$ for $|\widetilde{Q}| \geq c_1$. Since Q_s is smooth, we also have that the difference $|Q_s - Q_\infty|$ attains is maximum $c_2 = c_2(Q_s) \geq 0$ on the compact set $\partial\Omega$. Thus, for $\tilde{\gamma} := \max\{c_1, c_2\}$,

$$\nabla f_B(Q_\infty + \widetilde{Q}) \cdot \widetilde{Q} \geq 0 \quad \text{for } |\widetilde{Q}| \geq \tilde{\gamma} \qquad \text{and} \qquad |Q_s - Q_\infty| \leq \tilde{\gamma}. \tag{26}$$

Define

$$(|\widetilde{Q}|^2 - \tilde{\gamma}^2)_+ := \begin{cases} |\widetilde{Q}|^2 - \tilde{\gamma}^2 & \text{if } |\widetilde{Q}| - \tilde{\gamma} > 0 \\ 0 & \text{otherwise} \end{cases}$$

and let $U := \min\{(|\widetilde{Q}|^2 - \tilde{\gamma}^2)_+, M\}$ where M is some arbitrary positive constant. Take V to be of the form $V = U\varphi$ with $0 \leq \varphi \in C_0^\infty(\overline{\Omega})$ and note that due to the definition of U, V is compactly supported on the set $\{|\widetilde{Q}| \geq \tilde{\gamma}\}$ and is non-negative.

We claim that

$$L \int_\Omega \nabla\widetilde{Q} \cdot \nabla\Psi \; dx \leq 0. \tag{27}$$

To see this, first note that by our definition of V and observations above, $V\nabla f_B(Q_\infty + \widetilde{Q}) \cdot \widetilde{Q} \geq 0$ which directly gives

$$-\int_\Omega V\nabla f_B(Q_\infty + \widetilde{Q}) \cdot \widetilde{Q} \; dx \leq 0.$$

In the case of strong anchoring, $\partial\tilde{Q}/\partial\nu = 0$ and thus immediately forces the last integral in (25) to be zero. For weak anchoring we can write

$$\begin{aligned} \frac{\partial\widetilde{Q}}{\partial\nu} = \frac{W}{L}\left(Q_s - \widetilde{Q} - Q_\infty\right) \implies \widetilde{Q} \cdot \frac{\partial\widetilde{Q}}{\partial\nu} &= \frac{W}{L}\widetilde{Q} \cdot \left(Q_s - \widetilde{Q} - Q_\infty\right) \\ &= \frac{W}{L}\left(-|\widetilde{Q}|^2 + \widetilde{Q} \cdot (Q_s - Q_\infty)\right). \end{aligned}$$

By the Cauchy-Schwarz inequality and (26),

$$\widetilde{Q} \cdot (Q_s - Q_\infty) \leq |\widetilde{Q}||Q_s - Q_\infty| \leq |\widetilde{Q}|\tilde{\gamma}$$

and so

$$\widetilde{Q} \cdot \frac{\partial\widetilde{Q}}{\partial\nu} \leq \frac{W}{L}\left(-|\widetilde{Q}|^2 + |\widetilde{Q}|\tilde{\gamma}\right) = \frac{W}{L}|\widetilde{Q}|\left(-|\widetilde{Q}| + \tilde{\gamma}\right).$$

Applying (26) once more, we obtain

$$\widetilde{Q} \cdot \frac{\partial \widetilde{Q}}{\partial \nu} \leq \frac{W}{L} |\widetilde{Q}| \left(-\tilde{\gamma} + \tilde{\gamma}\right) = 0$$

which gives (27). Using $\Psi = U\varphi\widetilde{Q}$,

$$\begin{aligned} L \int_\Omega \nabla\widetilde{Q} \cdot \nabla\Psi \; dx &= L \int_\Omega \nabla\widetilde{Q} \cdot \nabla \left(U\varphi\widetilde{Q}\right) dx \\ &= L \int_\Omega \nabla\widetilde{Q} \cdot \left((\varphi\nabla U + U\nabla\varphi) \cdot \widetilde{Q} + U\varphi\nabla\widetilde{Q} \right) dx \\ &= L \int_\Omega \varphi \left(U|\nabla\widetilde{Q}|^2 + \nabla\widetilde{Q} \cdot \widetilde{Q} \cdot \nabla U \right) dx + L \int_\Omega U\nabla\widetilde{Q} \cdot \nabla\varphi \cdot \widetilde{Q} \; dx. \end{aligned}$$

Next, we claim

$$\nabla\widetilde{Q} \cdot \widetilde{Q} \cdot \nabla U = \frac{1}{2} |\nabla U|^2. \tag{28}$$

In the cases where either $|\widetilde{Q}| \leq \tilde{\gamma}$ or $U = M$, we obviously have $\nabla U = 0$ and thus (28) holds. If $M > |\widetilde{Q}|^2 - \tilde{\gamma}^2 > 0$, then

$$\begin{aligned} \nabla U &= \nabla \left(|\widetilde{Q}|^2 - \tilde{\gamma}^2 \right) \\ &= 2 \sum_{i,j=1}^{3} \left(\widetilde{Q}_{ij} \frac{\partial \widetilde{Q}_{ij}}{\partial x_1}, \widetilde{Q}_{ij} \frac{\partial \widetilde{Q}_{ij}}{\partial x_2}, \widetilde{Q}_{ij} \frac{\partial \widetilde{Q}_{ij}}{\partial x_3} \right) \\ &= 2\widetilde{Q} \cdot \nabla\widetilde{Q}. \end{aligned}$$

Therefore

$$\nabla\widetilde{Q} \cdot \widetilde{Q} \cdot \nabla U = \frac{1}{2} \nabla U \cdot \nabla U = \frac{1}{2} |\nabla U|^2$$

so we may write

$$L \int_\Omega \nabla\widetilde{Q} \cdot \nabla\Psi \; dx = L \int_\Omega \varphi \left(U|\nabla\widetilde{Q}|^2 + \frac{1}{2}|\nabla U|^2 \right) dx + L \int_\Omega U\nabla\widetilde{Q} \cdot \nabla\varphi \cdot \widetilde{Q} \; dx$$

and applying observation (27) leaves us with

$$\int_\Omega \varphi \left(U|\nabla\widetilde{Q}|^2 + \frac{1}{2}|\nabla U|^2 \right) dx \leq - \int_\Omega U\nabla\widetilde{Q} \cdot \nabla\varphi \cdot \widetilde{Q} \; dx.$$

Take $\varphi = \varphi_R$,

$$\varphi_R(x) := \begin{cases} 1 & \text{for } |x| \leq R \\ 0 & \text{for } |x| \geq 2R \end{cases} \qquad \text{with} \quad |\nabla \varphi_R| \leq \frac{C}{|x|}$$

for some constant $C > 0$ independent of R. Then, since $\nabla \varphi_R = 0$ for $|x| \leq R$

$$\begin{aligned} -\int_\Omega U \nabla \widetilde{Q} \cdot \nabla \varphi_R \cdot \widetilde{Q}\, dx &\leq \int_{|x|\geq R} \left| U \nabla \widetilde{Q} \cdot \nabla \varphi_R \cdot \widetilde{Q} \right| dx \\ &\leq MC \int_{|x|\geq R} |\nabla \widetilde{Q}| \frac{|\widetilde{Q}|}{|x|} dx \\ &\leq MC \|\nabla \widetilde{Q}\|_{L^2(|x|\geq R)} \|\widetilde{Q}/|x|\|_{L^2(|x|\geq R)} \qquad \text{(by Hölder's inequality).} \end{aligned}$$

Since $\widetilde{Q} \in \mathcal{H}^\Omega$, both $\|\nabla \widetilde{Q}\|_{L^2(|x|\geq R)} \to 0$ and $\|\widetilde{Q}/|x|\|_{L^2(|x|\geq R)} \to 0$ as $R \to \infty$. Thus,

$$\int_\Omega \left(U|\nabla \widetilde{Q}|^2 + \frac{1}{2}|\nabla U|^2 \right) dx = 0$$

and therefore $U = \min\{(|\widetilde{Q}|^2 - \tilde{\gamma}^2)_+, M\} = 0$ almost everywhere. Since $M > 0$, it must be that $|\widetilde{Q}| \leq \tilde{\gamma}$ almost everywhere. By the triangle inequality,

$$|Q| = |\widetilde{Q} + Q_\infty| \leq |\widetilde{Q}| + |Q_\infty| \leq \tilde{\gamma} + s_* \sqrt{\frac{2}{3}}$$

and so

$$|Q_{ij}(x)| \leq \tilde{\gamma} + s_* \sqrt{\frac{2}{3}}$$

almost everywhere for each $1 \leq i, j \leq 3$. In particular,

$$\|Q\|_{L^\infty(\Omega)} \leq \sum_{i,j=1}^{3} \left(\tilde{\gamma} + s_* \sqrt{\frac{2}{3}} \right) = 9 \left(\tilde{\gamma} + s_* \sqrt{\frac{2}{3}} \right).$$

Defining $\gamma := 9(\tilde{\gamma} + s_* \sqrt{2/3})$, we obtain $\|Q\|_{L^\infty(\Omega)} \leq \gamma$ for $\gamma > 0$. □

This result can now be used to prove that minimizers of $\mathcal{F}_\Omega$ satisfy the pointwise condition (11).

Corollary 4.5. *If $\Omega \in \mathcal{ED}$ and $Q \in \mathcal{H}^\Omega_\infty$ minimizes $\mathcal{F}_\Omega$, then Q is uniformly continuous and*

$$\lim_{|x|\to\infty} Q(x) = Q_\infty.$$

Proof of Corollary 4.5. By Lemma 4.3, $Q \in L^\infty(\Omega; \mathcal{S}_0)$. Observing the Euler–Lagrange equations

$$L\Delta Q = -aQ - b\left(Q^2 - \frac{1}{3}|Q|^2 I\right) + c|Q|^2 Q,$$

the righthand side is purely in terms of Q which immediately gives $\Delta Q \in L^\infty(\Omega; \mathcal{S}_0)$. Applying results from [1, Lemma 5] and the Sobolev inequality, Q is uniformly continuous and

$$\lim_{|x|\to\infty} |\widetilde{Q}(x)| = \lim_{|x|\to\infty} |Q(x) - Q_\infty| = 0 \implies \lim_{|x|\to\infty} Q(x) = Q_\infty$$

as desired. □

In view again of Lemma 4.3, a similar result can be said of the norm on $\mathcal{H}^\Omega$ and is found in the proof of [1, Theorem 1]. The following corollary is an extension of this for generalized $\Omega \in \mathcal{ED}$ and Q_s. The proof still follows closely to that shown in [1, Theorem 1] and omitted details are filled.

Corollary 4.6. *Suppose $\Omega \in \mathcal{ED}$ and $Q_{L,W} \in \mathcal{H}^\Omega_\infty$ is a minimizer of $\mathcal{F}_\Omega$. Then $\widetilde{Q}_{L,W} = Q_{L,W} - Q_\infty$ is uniformly bounded in the norm on $\mathcal{H}^\Omega$ with respect to $L \geq 1$ and $W > 0$.*

Proof of Corollary 4.6. Let φ be a smooth function on $\overline{\Omega}$ such that $\varphi(x) = 1$ on $\partial\Omega$ and $\varphi(x) \equiv 0$ outside the open ball $B_R(0)$ where $R = \operatorname{diam}(\Omega^c) + 1$. Define the 'energy competitor'

$$P(x) = \varphi(x)Q_s + (1 - \varphi(x))Q_\infty.$$

Obviously, $P \in \mathcal{H}^\Omega_\infty$ and $\mathcal{F}_\Omega[P] < \infty$. Furthermore, P is independent of L and W. Since $Q_{L,W}$ is a minimizer of $\mathcal{F}_\Omega$, we can write

$$\mathcal{F}_\Omega[Q_{L,W}] \leq \mathcal{F}_\Omega[P] = \int_\Omega \left(\frac{L}{2}|\nabla P|^2 + f_B(P)\right) dx + \frac{W}{2}\int_{\partial\Omega} |Q_s - P|^2 \, dA < \infty.$$

Using the fact $F_E[Q_{L,W}] \leq \mathcal{F}_\Omega[Q_{L,W}]$ and $P = Q_s$ on $\partial\Omega$,

$$\frac{L}{2}\int_\Omega |\nabla Q_{L,W}|^2 \, dx \leq \mathcal{F}_\Omega[Q_{L,W}] \leq \frac{L}{2}\int_\Omega |\nabla P|^2 \, dx + \int_\Omega f_B(P) \, dx < \infty.$$

Multiplying through by $4/L$,

$$\begin{aligned} 2\int_\Omega |\nabla Q_{L,W}|^2 \, dx &\leq 2\int_\Omega |\nabla P|^2 \, dx + \frac{4}{L}\int_\Omega f_B(P) \, dx \\ &\leq 2\int_\Omega |\nabla P|^2 \, dx + 4\int_\Omega f_B(P) \, dx \qquad \text{(since } L \geq 1\text{)}. \end{aligned}$$

Now, $\nabla Q_{L,W} = \nabla(\widetilde{Q}_{L,W} + Q_\infty) = \nabla\widetilde{Q}_{L,W}$ and by Hardy's inequality,

$$2\int_\Omega |\nabla\widetilde{Q}_{L,W}|^2\ dx \geq \int_\Omega |\nabla\widetilde{Q}_{L,W}|^2\ dx + C\int_\Omega \frac{|\widetilde{Q}_{L,W}|^2}{|x|^2}\ dx$$

where C is a constant independent of L and W. If $C \geq 1$, then

$$\|\widetilde{Q}_{L,W}\|^2_{\mathcal{H}^\Omega} \leq 2\int_\Omega |\nabla P|^2\ dx + 4\int_\Omega f_B(P)\ dx < \infty.$$

If $C < 1$, then

$$C\|\widetilde{Q}_{L,W}\|^2_{\mathcal{H}^\Omega} \leq 2\int_\Omega |\nabla P|^2\ dx + 4\int_\Omega f_B(P)\ dx < \infty.$$

In either case, $\widetilde{Q}_{L,W}$ is uniformly bounded in $\mathcal{H}^\Omega$ with respect to $L \geq 1$ and $W > 0$. $\square$

5 The Small Particle Limit

Recall from section 3.3 that the functional $\mathcal{F}_\Omega$ had been nondimensionalized via some natural length scale μ which characterizes the relative size of the colloid particle given by Ω^c. As a result we saw that prior to relabeling, the nondimensionalized coefficients $\hat{L}$ and $\hat{W}$ were of the form

$$\hat{L} = \frac{L}{\mu^2 a}, \qquad \hat{W} = \frac{W\mu a}{L}$$

where a is the reference energy and both incorporate the relative colloid particle size μ. Thus, in a sense, varying the relative particle size can be seen through an appropriate change in $\hat{L}$ and $\hat{W}$. The benefit in this setup allows us to consider solutions $Q_{L,W} \in \mathcal{H}^\Omega_\infty$ to the minimization problem (17) and interpret their limits (with respect to (L, W)) in the sense of relative particle size. In this section, we study a particular limiting regime called the *small particle limit*. This is done by considering

$$(L, W) \to (\infty, w), \quad \frac{L}{W} \to \frac{1}{w}.$$

Here, we allow $w \in (0, +\infty]$ so that both the Robin and Dirichlet boundary conditions can be investigated. To analyze this limit rigorously, we resort to the Euler–Lagrange equations.

5.1 Revisiting the Euler–Lagrange Equations

Suppose $L \geq 1$ and $Q_{L,W}$ is a solution to the minimization problem (17). In the weak formulation of (18), $Q_{L,W}$ satisfies

$$\begin{aligned}\int_\Omega Q_{L,W} \cdot \Delta\Phi \, dx &= \frac{1}{L}\int_\Omega \left(-aQ_{L,W} - b\left(Q_{L,W}^2 - \frac{1}{3}|Q_{L,W}|^2 I\right) + c|Q_{L,W}|^2 Q_{L,W}\right) \cdot \Phi \, dx \\ &= \frac{1}{L}\int_\Omega \nabla f_B(Q_{L,W}) \cdot \Phi \, dx\end{aligned}$$

for all smooth, compactly supported $\mathcal{S}_0$-valued functions Φ. By Corollary 4.6, the $\mathcal{H}^\Omega$-component $\widetilde{Q}_{L,W} = Q_{L,W} - Q_\infty \in \mathcal{H}^\Omega$ is uniformly bounded in the $\mathcal{H}^\Omega$-norm with respect to L and W. Therefore, there exists a subsequence that converges to some $\widetilde{Q}_0 \in \mathcal{H}^\Omega$ weakly in $\mathcal{H}^\Omega$ in the small particle limit $(L, W) \to (\infty, w)$. Furthermore, Lemma 4.3 directly gives $\|\nabla f_B(Q_{L,W})\|_{L^\infty(\Omega)} \leq \gamma$ for some $\gamma > 0$ independent of L and W. Using these facts and defining $Q_0 := \widetilde{Q}_0 + Q_\infty$, we pass to the limit in the weak formulation and obtain

$$\int_\Omega Q_0 \cdot \Delta\Phi \; dx = 0$$

for all smooth, compactly supported $\mathcal{S}_0$-valued functions Φ. In the same way, the limiting condition $L/W \to 1/w$ implies Q_0 weakly satisfies the boundary condition

$$\frac{1}{w}\frac{\partial Q_0}{\partial \nu} = Q_s - Q_0.$$

Therefore, the small particle limit is a Q-tensor $Q_0 \in \mathcal{H}_\infty^\Omega$ weakly satisfying

$$\begin{cases} \Delta Q_0 = 0 & \text{in } \Omega \\ \frac{1}{w}\frac{\partial Q_0}{\partial \nu} = Q_s - Q_0 & \text{on } \partial\Omega \end{cases}. \tag{29}$$

Moreover, Q_0 is the unique $\mathcal{H}_\infty^\Omega$ solution to (29) and this fact is proven in [1, Theorem 1].

Also done in [1], the authors prove that in the case of a spherical colloid, the small particle solution Q_0 admits a 'Saturn ring' defect about the particle when homeotropic (normal) boundary conditions are enforced. Specifically, it was shown that there exists a circle about the particle for which the principal eigenvector of $Q_0(x)$ is discontinuous. This defect is physically interpreted as the liquid crystal being uniaxial along the circle and biaxial everywhere else. Thus, the defect occurs when two eigenvalues of Q_0 become equal, which happens exactly along a circle about the particle and presents itself as a discontinuity in the approximate director.

For the remainder of this paper, our focus will be to study alignment configurations of the small particle limit Q_0 in two specific cases. Namely, the cases where the colloid particles are taken to be a prolate spheroid and an oblate spheroid with 'almost homeotropic' strong anchoring. Since the prolate and oblate spheroids we are choosing will closely resemble that of the spherical colloid, it is hypothesized that the small particle limits in these cases will also admit Saturn ring defects.

Indeed, over the next two sections we will derive closed-form axially-symmetric solutions to (29) for both prolate and oblate spheroidal colloid particles with strong anchoring. Once these solution have been obtained, we observe (qualitatively) the existence of a Saturn ring defect around the particles.

5.2 A Prolate Spheroidal Colloid With Strong Anchoring

We derive a closed-form solution to the small particle limit problem (29)

$$\begin{cases} \Delta Q_0 = 0 & \text{in } \Omega \\ Q_0 = Q_s & \text{on } \partial\Omega \end{cases}$$

where $\Omega \in \mathcal{ED}$ is taken to be the complement of the set

$$K = \left\{ x \in \mathbb{R}^3 : \frac{x_1^2 + x_2^2}{A^2} + \frac{x_3^2}{B^2} \leq 1 \right\}$$

for $A = \sinh(1)$ and $B = \cosh(1)$. The choice of constants A and B is a natural one, as it allows us to view Ω easily under the *prolate spheroidal coordinate system* defined by

$$x_1 = \sinh(\eta)\cos(\theta)\sin(\phi), \quad x_2 = \sinh(\eta)\sin(\theta)\sin(\phi), \quad x_3 = \cosh(\eta)\cos(\phi) \tag{30}$$

where $0 \leq \eta < \infty$, $0 \leq \theta < 2\pi$ and $0 \leq \phi \leq \pi$. Indeed, Ω recast under (30) takes the form $\Omega = \{x(\eta,\theta,\phi) \in \mathbb{R}^3 : \eta > 1\}$ with $\partial\Omega = \{x(\eta,\theta,\phi) \in \mathbb{R}^3 : \eta = 1\}$. Please see [11] for more details on this coordinate system.

Boundary Conditions on $\partial\Omega$

In order to obtain a closed-form solution, we construct a specific boundary condition Q_s on $\partial\Omega$. Consider first the function

$$F(x_1, x_2, x_3) := \frac{x_1^2 + x_2^2}{A} + \frac{x_3^2}{B}$$

and define the vector field

$$n(x_1, x_2, x_3) := \frac{\nabla F}{|\nabla F|} = \frac{1}{|v|}\left(\frac{x_1}{A}, \frac{x_2}{A}, \frac{x_3}{B}\right)$$

where $v = \left(\frac{x_1}{A}, \frac{x_2}{A}, \frac{x_3}{B}\right)$. The matrix $Q_s(x)$ defined by

$$Q_s(x) := s_*\left(n \otimes n - \frac{1}{3}I\right) = s_* \begin{pmatrix} \frac{x_1^2}{A^2|v|} - \frac{1}{3} & \frac{x_1x_2}{A^2|v|} & \frac{x_1x_3}{AB|v|} \\ \frac{x_1x_2}{A^2|v|} & \frac{x_2^2}{A^2|v|} - \frac{1}{3} & \frac{x_2x_3}{AB|v|} \\ \frac{x_1x_3}{AB|v|} & \frac{x_2x_3}{AB|v|} & \frac{x_3^2}{B^2|v|} - \frac{1}{3} \end{pmatrix}$$

will act as our boundary condition.

In doing this, we are imposing that n be the director of Q_0 along the boundary. Observing a cross section of the colloid particle, alignment configuration along the boundary given by $n(x)$ appears as in Figure 6.

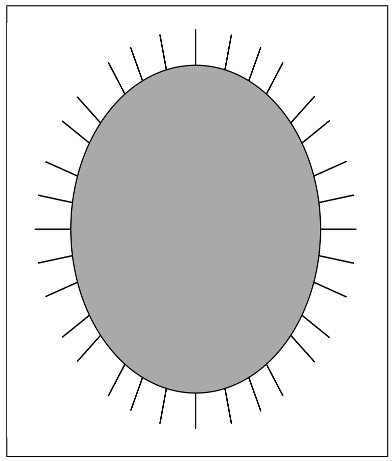

Figure 6: Molecule alignment profile along colloid boundary.

Note that the boundary conditions are incredibly close to being homeotropic. Although they are not exactly, this 'almost homeotropic' setting allows us to make reasonable comparisons between [1] and our work.

Converting to prolate spheroidal coordinates and evaluating at $\eta = 1$, Q_s on $\partial\Omega$ takes the form

$$Q_s =$$

$$s_* \begin{pmatrix} \cos^2(\theta) - \frac{1}{3} - \cos^2(\theta)\cos^2(\phi) & \sin^2(\phi)\cos(\theta)\sin(\theta) & \cos(\phi)\sin(\phi)\cos(\theta) \\ \sin^2(\phi)\cos(\theta)\sin(\theta) & \frac{2}{3} - \cos^2(\phi) - \cos^2(\theta) + \cos^2(\theta)\cos^2(\phi) & \cos(\phi)\sin(\phi)\sin(\theta) \\ \cos(\phi)\sin(\phi)\cos(\theta) & \cos(\phi)\sin(\phi)\sin(\theta) & \cos^2(\phi) - \frac{1}{3} \end{pmatrix}.$$

Due to the e_z-axial symmetry of our problem, it will be convenient to write Q_s in the cylindrical basis described in section 2.2. We have

$$Q_s = \sum_{j=1}^{5} p_j(\phi) E_j(\theta)$$

where

$$p_1(\phi) = Q_s \cdot E_1 = \frac{s_*}{\sqrt{6}}(3\cos^2(\phi) - 1), \quad p_2(\phi) = Q_s \cdot E_2 = \frac{s_*}{\sqrt{2}}\sin^2(\phi),$$
$$p_3(\phi) = Q_s \cdot E_3 = s_*\sqrt{2}\sin(\phi)\cos(\phi), \quad p_4(\phi) = Q_s \cdot E_4 = 0, \qquad .$$
$$p_5(\phi) = Q_s \cdot E_5 = 0$$

Condition at ∞

Recall that since we are seeking $Q_0 \in \mathcal{H}^{\Omega}_{\infty}$, we also would like our solution to satisfy

$$\lim_{|x|\to\infty} Q_0(x) = Q_\infty = s_* \begin{pmatrix} -\frac{1}{3} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & \frac{2}{3} \end{pmatrix}.$$

Using the same cylindrical basis, we have

$$Q_\infty = \sum_{j=1}^{5} u_j E_j(\theta)$$

where

$$u_1 = Q_\infty \cdot E_1 = s_*\sqrt{\frac{2}{3}}, \quad u_j = Q_\infty \cdot E_j = 0 \ \text{ for } \ 2 \le j \le 5.$$

Again, due to the symmetry of our problem, we will attempt to seek an e_z-axially symmetric solution to (29). As given in [1], these solutions will be Q-tensors exactly of the form

$$Q_0(\rho, \phi, \theta) = \sum_{j=1}^{5} q_j(\rho, \phi) E_j(\theta)$$

where ρ, ϕ and θ still correspond to the cylindrical coordinates described in section 2.2. Converting this into prolate spheroidal coordinates, we let $\rho = \sinh(\eta)$ which gives Q_0 the new form

$$Q_0(\eta, \phi, \theta) = \sum_{j=1}^{5} q_j(\eta, \phi) E_j(\theta).$$

At $\eta = 1$, we require $q_j(1, \phi) = p_j(\phi)$, $(j = 1, \ldots, 5)$ and for the condition at ∞,

$$\lim_{\eta\to\infty} q_j(\eta, \phi) = u_j, \quad j = 1, \ldots, 5.$$

Since $p_4(\phi) = p_5(\phi) = u_4 = u_5 = 0$, this suggests that we may attempt to find Q_0 of the form

$$Q_0(\eta, \phi, \theta) = \sum_{j=1}^{3} q_j(\eta, \phi) E_j(\theta).$$

Before we continue, it is worth while to note that in this form, it is an easy calculation to obtain the eigenvalues of Q_0. They are given by

$$\begin{aligned} \lambda_1 &= -\frac{q_1}{\sqrt{6}} - \frac{q_2}{\sqrt{2}} \\ \lambda_2 &= \frac{q_1}{2\sqrt{6}} + \frac{q_2}{2\sqrt{2}} + \frac{1}{4}\sqrt{6q_1^2 - 4\sqrt{3}q_1 q_2 + 2q_2^2 + 8q_3^2} \\ \lambda_3 &= \frac{q_1}{2\sqrt{6}} + \frac{q_2}{2\sqrt{2}} - \frac{1}{4}\sqrt{6q_1^2 - 4\sqrt{3}q_1 q_2 + 2q_2^2 + 8q_3^2} \end{aligned} \tag{31}$$

and note also that they are *independent* of θ.

To find $q_1(\eta, \phi)$, $q_2(\eta, \phi)$ and $q_3(\eta, \phi)$, we observe that the entries of Q_0

$$Q_{033} = \sqrt{\frac{2}{3}} q_1(\eta, \phi), \qquad Q_{012} = \sqrt{2}\cos(\theta)\sin(\theta) q_2(\eta, \phi), \qquad Q_{013} = \frac{1}{\sqrt{2}}\cos(\theta) q_3(\eta, \phi)$$

are such that each q_j is isolated. Therefore, we may approach the problem by calculating

$$\Delta Q_{033} = \Delta Q_{012} = \Delta Q_{013} = 0.$$

The Laplace operator in prolate spheroidal coordinates is

$$\Delta = h_1(\eta, \phi)\left[\frac{\partial^2}{\partial \eta^2} + \coth(\eta)\frac{\partial}{\partial \eta} + \frac{\partial^2}{\partial \phi^2} + \cot(\phi)\frac{\partial}{\partial \phi}\right] + h_2(\eta, \phi)\frac{\partial^2}{\partial \theta^2}$$

where

$$h_1(\eta, \phi) = \frac{1}{\sinh^2(\eta) + \sin^2(\phi)} \quad \text{and} \quad h_2(\eta, \phi) = \frac{1}{\sinh^2(\eta)\sin^2(\phi)}.$$

Using separation of variables, we have that $\Delta Q_{033} = 0$ implies $q_1(\eta, \phi) = N_1(\eta) T_1(\phi)$ solves

$$\begin{cases} N_1'' = \sigma_1 N_1 - \coth(\eta) N_1' \\ T_1'' = -\sigma_1 T_1 - \cot(\phi) T_1' \end{cases} \tag{32}$$

for σ_1 a constant.

Similarly, $\Delta Q_{012} = 0$ implies $q_2(\eta, \phi) = N_2(\eta)T_2(\phi)$ solves

$$\begin{cases} N_2'' = \sigma_2 N_2 - \coth(\eta) N_2' + \dfrac{4N_2}{\sinh^2(\eta)} \\ T_2'' = -\sigma_2 T_2 - \cot(\phi) T_2' + \dfrac{4T_2}{\sin^2(\phi)} \end{cases}$$

and $\Delta Q_{013} = 0$ implies $q_3(\eta, \phi) = N_3(\eta)T_3(\phi)$ solves

$$\begin{cases} N_3'' = \sigma_3 N_3 - \coth(\eta) N_3' + \dfrac{N_3}{\sinh^2(\eta)} \\ T_3'' = -\sigma_3 T_3 - \cot(\phi) T_3' + \dfrac{T_3}{\sin^2(\phi)} \end{cases}.$$

If $\sigma_j = 6$ for $j = 1, 2, 3$ then we find that for appropriate constants,

$$T_1(\phi) = \frac{s_*}{\sqrt{6}}(3\cos^2(\phi) - 1), \quad T_2(\phi) = \frac{s_*}{\sqrt{2}}\sin^2(\phi), \quad T_3(\phi) = s_*\sqrt{2}\cos(\phi)\sin(\phi)$$

solve their corresponding ODEs and $T_j(\phi) = p_j(\phi)$ for each $j = 1, 2, 3$.

Using $\sigma_j = 6$ for the remaining equations for $N_j(\eta)$, we have

$$N_1(\eta) = C_1 \cosh^2(\eta)\left((\tanh^2(\eta) + 2)\ln(\coth(\eta) + \operatorname{csch}(\eta)) - 3\operatorname{sech}(\eta)\right)$$

$$N_2(\eta) = C_2\left(\cosh(\eta)(2\coth^2(\eta) - 5) + 3\sinh^2(\eta)\ln\left(\coth(\eta) + \operatorname{csch}(\eta)\right)\right)$$

$$N_3(\eta) = C_3 \sinh(\eta)\left(\coth^2(\eta) - 3\cosh(\eta)\ln(\coth(\eta) + \operatorname{csch}(\eta)) + 2\right)$$

where it can be checked that

$$\lim_{\eta\to\infty} N_j(\eta) = 0$$

for each $j = 1, 2, 3$. For $q_j(\eta, \phi)$ to satisfy their boundary conditions at $\eta = 1$, we take

$$C_1 = \frac{1}{\cosh^2(1)\left((\tanh^2(1) + 2)\ln(\coth(1) + \operatorname{csch}(1)) - 3\operatorname{sech}(1)\right)}$$

$$C_2 = \frac{1}{\left(\cosh(1)(2\coth^2(1) - 5) + 3\sinh^2(1)\ln\left(\coth(1) + \operatorname{csch}(1)\right)\right)}$$

$$C_3 = \frac{1}{\sinh(1)\left(\coth^2(1) - 3\cosh(1)\ln(\coth(1) + \operatorname{csch}(1)) + 2\right)}$$

so that $N_j(1) = 1$.

Lastly, we solve for another solution to (32) but with

$$\lim_{\eta\to\infty} N_1(\eta) = u_1 = s_*\sqrt{\frac{2}{3}}$$

and $N_1(1) = 0$ so that all boundary conditions and limits for Q_0 are satisfied.

To do this, take $\sigma_1 = 0$ and solving for $N_1(\eta)$ gives a solution

$$N_1(\eta) = c_1\left(\ln\left(\sinh\left(\frac{\eta}{2}\right)\right) - \ln\left(\cosh\left(\frac{\eta}{2}\right)\right)\right) + c_2$$

where

$$\lim_{\eta\to\infty} N_1(\eta) = c_2.$$

Therefore, if we choose

$$c_1 = -\frac{s_*\sqrt{\frac{2}{3}}}{\ln\left(\sinh\left(\frac{1}{2}\right)\right) - \ln\left(\cosh\left(\frac{1}{2}\right)\right)},$$
$$c_2 = s_*\sqrt{\frac{2}{3}}$$

then the limit condition is satisfied along with $N_1(1) = 0$.

Adding together both solutions from (32), we obtain $\Delta Q_{033} = 0$ for

$$q_1(\eta,\phi) = \frac{s_*\cosh^2(\eta)\left((\tanh^2(\eta)+2)\ln(\coth(\eta)+\operatorname{csch}(\eta)) - 3\operatorname{sech}(\eta)\right)(3\cos^2(\phi)-1)}{\sqrt{6}\cosh^2(1)\left((\tanh^2(1)+2)\ln(\coth(1)+\operatorname{csch}(1)) - 3\operatorname{sech}(1)\right)} + s_*\sqrt{\frac{2}{3}}\left(1 - \frac{\ln\left(\sinh\left(\frac{\eta}{2}\right)\right) - \ln\left(\cosh\left(\frac{\eta}{2}\right)\right)}{\ln\left(\sinh\left(\frac{1}{2}\right)\right) - \ln\left(\cosh\left(\frac{1}{2}\right)\right)}\right)$$

such that $q_1(1,\phi) = p_1(\phi)$ and $\lim_{\eta\to\infty} q_1(\eta,\phi) = u_1$. Similarly,

$$q_2(\eta,\phi) = \frac{s_*\left(\cosh(\eta)(2\coth^2(\eta)-5) + 3\sinh^2(\eta)\ln\left(\coth(\eta)+\operatorname{csch}(\eta)\right)\right)\sin^2(\phi)}{\sqrt{2}\left(\cosh(1)(2\coth^2(1)-5) + 3\sinh^2(1)\ln\left(\coth(1)+\operatorname{csch}(1)\right)\right)}$$

and

$$q_3(\eta,\phi) = \frac{s_*\sqrt{2}\sinh(\eta)\left(\coth^2(\eta) - 3\cosh(\eta)\ln(\coth(\eta)+\operatorname{csch}(\eta)) + 2\right)\cos(\phi)\sin(\phi)}{\sinh(1)\left(\coth^2(1) - 3\cosh(1)\ln(\coth(1)+\operatorname{csch}(1)) + 2\right)}$$

solve $\Delta Q_{012} = 0$ and $\Delta Q_{013} = 0$ respectively with desired boundary conditions.

Therefore, the small particle solution Q_0 is given by

$$Q_0(\eta, \theta, \phi) = \sum_{j=1}^{3} q_j(\eta, \phi) E_j(\theta)$$

for $q_j(\eta, \phi)$, $j = 1, 2, 3$ as above. Refering to the theory discussed prior to this section, Q_0 is in fact the unique $\mathcal{H}_\infty^\Omega$ solution to (29).

To obtain an explicit formula for the Saturn ring defect as in [1] for the spherical colloid case, an expression for the approximate director is needed. Given the complicated form of our solution, we will restrict ourselves to observing the existence of the Saturn ring defect in a qualitative manner. In the spherical case, the ring defect occurs in the plane $x_3 = 0$ (or equivalently, $\phi = \pi/2$). Due to the geometry of our problem, we expect the same for the prolate spheroid.

Using the calculated eigenvalues (31) of Q_0, we plot $\lambda_1(\eta, \pi/2)$, $\lambda_2(\eta, \pi/2)$ and $\lambda_3(\eta, \pi/2)$ in Figure 7 below:

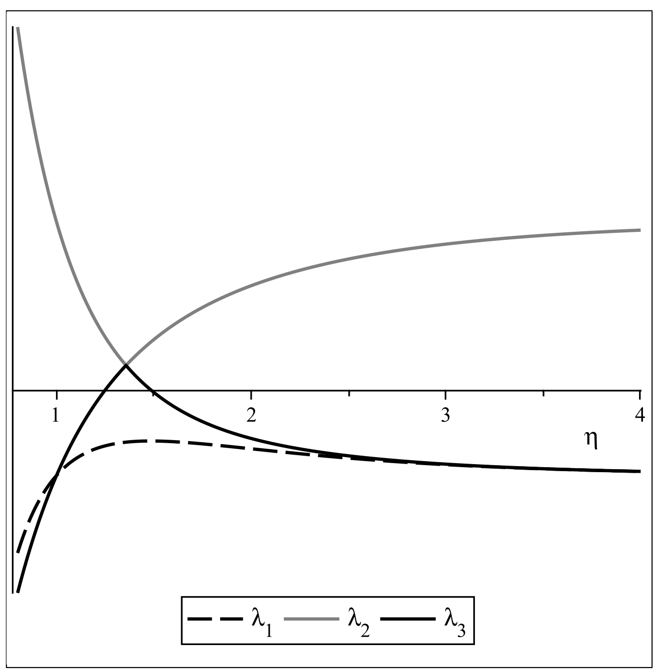

Figure 7: Eigenvalues of Q_0 at $\phi = \dfrac{\pi}{2}$ (prolate spheroidal colloid).

As constructed, we observe that Q_0 is uniaxial on the boundary $\eta = 1$ which is highlighted by the eigenvalue crossing $\lambda_1(1, \pi/2) = \lambda_3(1, \pi/2)$. Also, we observe that for some $5/4 < \eta_0 < 3/2$, there is another eigenvalue crossing $\lambda_2(\eta_0, \pi/2) = \lambda_3(\eta_0, \pi/2)$. Since the eigenvalues (31) are independent of θ, we must have then, that Q_0 is uniaxial at all points $(\eta_0, \pi/2, \theta)$, $\theta \in [0, 2\pi)$. Geometrically, this traces a circle in the $x_3 = 0$ plane about the prolate spheroid. Hence, the prolate spheroid does admit a Saturn ring defect with our chosen boundary conditions.

The Saturn ring defect can also be seen through a numerical scheme which we've performed in MATLAB. Due to the symmetry of the domain, the integral curves of the approximate director field can be plotted in any one quadrant and then reflected in the rest. Figure 8 below represents any cross section of these curves containing the x_3-axis (taken to be the vertical).

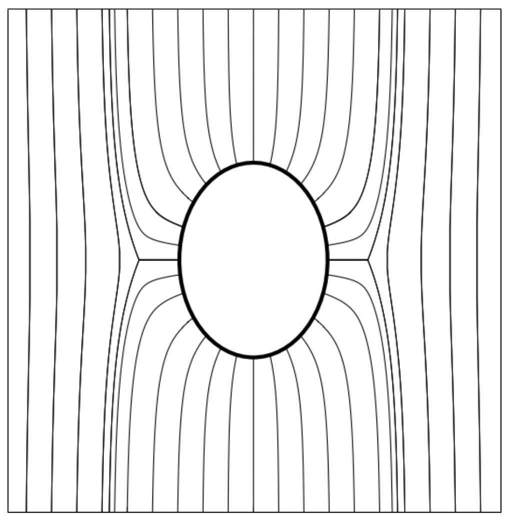

Figure 8: Integral curves of approximate director field (prolate spheroidal colloid).

5.3 An Oblate Spheroidal Colloid With Strong Anchoring

Next, we derive a closed-form solution to the small particle limit problem (29)

$$\begin{cases} \Delta Q_0 = 0 & \text{in } \Omega \\ Q_0 = Q_s & \text{on } \partial\Omega \end{cases}$$

where $\Omega \in \mathcal{ED}$ is taken to be the complement of the set

$$K = \left\{ x \in \mathbb{R}^3 : \frac{x_1^2 + x_2^2}{A^2} + \frac{x_3^2}{B^2} \leq 1 \right\}$$

but now for $A = \cosh(1)$ and $B = \sinh(1)$. Similar to the prolate case, the choice of constants A and B allows us to view Ω easily under the *oblate spheroidal coordinate system*.

This is given by

$$x_1 = \cosh(\eta)\cos(\theta)\sin(\phi), \quad x_2 = \cosh(\eta)\sin(\theta)\sin(\phi), \quad x_3 = \sinh(\eta)\cos(\phi)$$

where $0 \leq \eta < \infty$, $0 \leq \theta < 2\pi$ and $0 \leq \phi \leq \pi$. Just as before, Ω recast under these coordinates takes the form $\Omega = \{x(\eta,\theta,\phi) \in \mathbb{R}^3 : \eta > 1\}$ with $\partial\Omega = \{x(\eta,\theta,\phi) \in \mathbb{R}^3 : \eta = 1\}$. The same reference [11] can be used for further details on this coordinate system.

Using the same methods as before, we construct Q_s by considering the function

$$G(x_1, x_2, x_3) := \frac{x_1^2 + x_2^2}{A} + \frac{x_3^2}{B}$$

and defining the vector field

$$n(x_1, x_2, x_3) := \frac{\nabla G}{|\nabla G|} = \frac{1}{|v|}\left(\frac{x_1}{A}, \frac{x_2}{A}, \frac{x_3}{B}\right)$$

where $v = \left(\frac{x_1}{A}, \frac{x_2}{A}, \frac{x_3}{B}\right)$. We set

$$Q_s = s_*\left(n \otimes n - \frac{1}{3}I\right)$$

and find that Q_s under the oblate spheroidal coordinates is identical to that calculated in the prolate case. As before, the boundary conditions are observed to be 'almost homeotropic'.

We proceed using the same process from the prolate case. The only difference now is that the Laplace operator must be changed to the oblate spheroidal coordinate system. The Laplace operator in oblate spheroidal coordinates is of the form

$$\Delta = g_1(\eta,\phi)\left[\frac{\partial^2}{\partial\eta^2} + \tanh(\eta)\frac{\partial}{\partial\eta} + \frac{\partial^2}{\partial\phi^2} + \cot(\phi)\frac{\partial}{\partial\phi}\right] + g_2(\eta,\phi)\frac{\partial^2}{\partial\theta^2}$$

where

$$g_1(\eta,\phi) = \frac{1}{\cosh^2(\eta) - \sin^2(\phi)} \quad \text{and} \quad g_2(\eta,\phi) = \frac{1}{\cosh^2(\eta)\sin^2(\phi)}.$$

Solving the same equations

$$\Delta Q_{033} = \Delta Q_{012} = \Delta Q_{013} = 0$$

using the boundary conditions Q_s and conditions at ∞, we obtain the unique $\mathcal{H}_\infty^\Omega$ solution

$$Q_0(\eta,\theta,\phi) = \sum_{j=1}^{3} q_j(\eta,\phi) E_j(\theta)$$

where

$$q_1(\eta,\phi) = \frac{s_* \cosh^2(\eta)\left(\left(2\tanh^2(\eta)+1\right)\ln\left(\tanh(\eta)+i\,\mathrm{sech}(\eta)\right) - 3i\tanh(\eta)\,\mathrm{sech}(\eta)\right)\left(3\cos^2(\phi)-1\right)}{\sqrt{6}\cosh^2(1)\left(\left(2\tanh^2(1)+1\right)\ln\left(\tanh(1)+i\,\mathrm{sech}(1)\right) - 3i\tanh(1)\,\mathrm{sech}(1)\right)}$$
$$+ s_*\sqrt{\frac{2}{3}}\left(\frac{\tan^{-1}\left(\tanh\left(\frac{\eta}{2}\right)\right)}{\frac{\pi}{4}-\tan^{-1}\left(\tanh\left(\frac{1}{2}\right)\right)} - \frac{\tan^{-1}\left(\tanh\left(\frac{1}{2}\right)\right)}{\frac{\pi}{4}-\tan^{-1}\left(\tanh\left(\frac{1}{2}\right)\right)}\right)$$

$$q_2(\eta,\phi) = \frac{s_*\left(3i\left(\cosh^2(\eta)+\frac{2}{3}\right)\tanh(\eta)\,\mathrm{sech}(\eta) - 3\cosh^2(\eta)\left(\ln(\mathrm{sech}(\eta)) + \ln(\sinh(\eta)+i)\right)\right)\sin^2(\phi)}{\sqrt{2}\left(3i\left(\cosh^2(1)+\frac{2}{3}\right)\tanh(1)\,\mathrm{sech}(1) - 3\cosh^2(1)\left(\ln(\mathrm{sech}(1)) + \ln(\sinh(1)+i)\right)\right)}$$

$$q_3(\eta,\phi) = \frac{s_*\sqrt{2}\left(i\,\mathrm{sech}(\eta) + 3\cosh(\eta)\left(\sinh(\eta)\left(\ln(\mathrm{sech}(\eta)) + \ln(\sinh(\eta)+i)\right) - i\right)\right)\cos(\phi)\sin(\phi)}{i\,\mathrm{sech}(1) + 3\cosh(1)\left(\sinh(1)\left(\ln(\mathrm{sech}(1)) + \ln(\sinh(1)+i)\right) - i\right)}.$$

Since Q_0 is of the same form in the prolate case, the eigenvalues are still given by equations (31). Plotting all eigenvalues for $\phi = \pi/2$, we again see an eigenvalue crossing, giving the Saturn ring defect about the colloid.

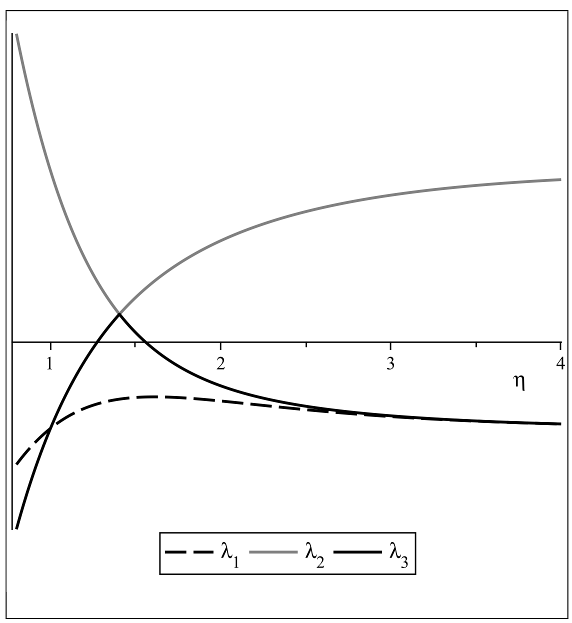

Figure 9: Eigenvalues of Q_0 at $\phi = \frac{\pi}{2}$ (oblate spheroidal colloid).

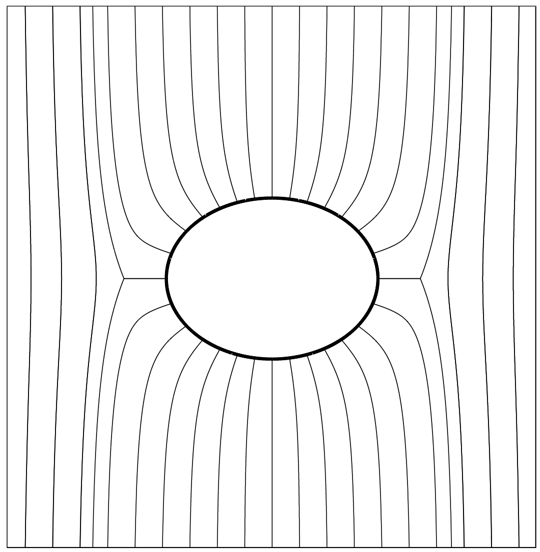

Figure 10: Integral curves of approximate director field (oblate spheroidal colloid).

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