PLANAR ANCHORING FOR A COLLOID IN NEMATIC LIQUID CRYSTAL WITH A MAGNETIC FIELD

PLANAR ANCHORING FOR A COLLOID IN NEMATIC LIQUID CRYSTAL WITH A MAGNETIC FIELD

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Abstract

We study minimizers of the Landau-de Gennes energy in the exterior region around a smooth 2-manifold in $\mathbb{R}^3$ with a constant external magnetic field present. Uniaxial boundary data and a strong tangential anchoring are imposed on the surface of the manifold and we consider the large particle limit in a regime where the magnetic field is relatively weak. Before studying the general manifold, we analyze a more simple case in which the manifold is spherical. After deriving a lower bound for the energy in this limiting regime, we prove that a director field on the boundary which maximizes its vertical component yields a minimal lower bound. We then construct a recovery sequence to show that this lower bound is in fact the optimal energy bound. These steps are later repeated in more generality for a larger class of smooth manifolds.

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Contents

1 Introduction

Liquid crystals are a type of matter which possesses properties of both a crystalline solid and an isotropic fluid. That is, depending on the phase of the liquid crystal it can have varying degrees of ordering within its fluid-like composition. Typically, liquid crystal is a collection of rod-like molecules occupying some space and so we describe its physical properties in terms of the orientations and positions of such molecules. Depending on this structure at a molecular level, we can classify the phase of the liquid crystal into three categories: nematic, smectic, and cholesteric [4]. In this paper, we are concerned with the nematic phase, in which the molecules are free to flow, similar to a liquid, but still have a preferred direction of alignment on small regions.

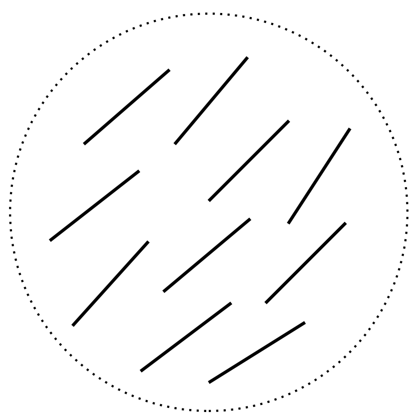

Figure 1: Sample of uniaxial nematic liquid crystal.

Although there are several models which can be used to study nematic liquid crystals, we focus on the Landau-de Gennes model in which the liquid crystal is described by a symmetric, traceless, 3×3 matrix, called a $Q-$tensor. Since the head and tail of the rod-like molecules that comprise the nematic liquid crystal are often indistinguishable, this model is preferred as $Q-$tensors allow us to describe the orientation of such molecules with respect to $\mathbb{R}P^2$, rather than $\mathbb{S}^2$. Another benefit of using the Landau-de Gennes model is that it allows for a finer description of defect cores, due to their structures having finite energy [5]. For a nematic liquid crystal, there are two main orientation states that occur: *uniaxial* and *biaxial*. In a uniaxial state the molecules align locally about one axis, while in a biaxial state there is no axis of rotational symmetry for the molecular alignment, but three mutually orthogonal axes of reflective symmetry. Although the Landau-de Gennes framework can be more challenging than other models of nematic liquid crystals, it has the ability to characterize these two different states using $Q-$tensors, which is a very desirable property for a liquid crystal model.

In this paper, we consider the case of liquid crystal outside of a colloid, which we describe by the 3-dimensional exterior region of a smooth 2-manifold $\mathcal{M}$. We are interested in the energy of this system when we impose a planar anchoring of the molecules at the surface of the manifold, i.e. we impose a Dirichlet boundary condition in which the boundary data is uniaxial and the principal eigenvector of the $Q-$tensor matrix is tangent to the surface of the manifold. More specifically, we are interested in the observable effects that occur when a magnetic field is introduced. We will study the energy of this system in what is called the *large particle limit*, using a method similar to $\Gamma-$convergence, but not quite as strong as we will only consider sequences of minimizers.

Previous results in the case of normal anchoring were obtained in [1–3]. This work is inspired by their approaches, although significant modifications have been made and new ideas introduced.

We will first study a much simpler case where the manifold $\mathcal{M}$ is the sphere $\mathbb{S}^2$. This will give us a sense of the steps needed for the more general case and some ideas will carry over quite nicely. We will then move on to the case of the general manifold, where some strategies used in the spherical case will break down since we can no longer make use of the symmetries of the sphere and the simple structure of its defect locations. Therefore, we must introduce new methods to get around these difficulties. However, before we can do this, we will introduce the notations and definitions to be used throughout this thesis as well as a more rigorous framework and description of our problem.

2 Preliminaries

2.1 Points, Sets, and Coordinate Systems

We will be working with regions in $\mathbb{R}^3 = \mathbb{R} \times \mathbb{R} \times \mathbb{R}$, where points $x \in \mathbb{R}^3$ are written as $x = (x_1, x_2, x_3)$. We will denote the standard basis vectors of $\mathbb{R}^3$ by e_1, e_2, and e_3. This space is equipped with the standard Euclidean norm

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

Let $U \subset \mathbb{R}^3$, then we denote the closure and the boundary of U by $\overline{U}$ and ∂U respectively. We will also work with smooth, compact, oriented 2-manifolds, $\mathcal{M}$, equipped with the distance function, $\mathrm{dist}_{\mathcal{M}} : \mathcal{M} \times \mathcal{M} \to [0, \infty)$, which gives the geodesic distance between any two points on $\mathcal{M}$. We denote the unit normal vector field on $\mathcal{M}$ which points into Ω by $\nu : \mathcal{M} \to \mathbb{S}^2$. Let κ_1 and κ_2 denote the principal curvatures of $\mathcal{M}$, then we define $\kappa = \max\{|\kappa_1|, |\kappa_2|\}$. This gives the inequalities

$$\left|\frac{\partial \nu}{\partial \omega_i}\right| \leq \kappa \quad \text{and} \quad |\nabla_\omega \nu| = \sqrt{\left|\frac{\partial \nu}{\partial \omega_1}\right|^2 + \left|\frac{\partial \nu}{\partial \omega_2}\right|^2} \leq \sqrt{2}\kappa\,,$$

for $i = 1, 2$ and where ω_1, ω_2 denote the two parameters of the local coordinate system on $\mathcal{M}$ and ∇_ω denotes the gradient with respect to that coordinate system. Let $B(x, r)$ be the open ball around the point $x \in \mathbb{R}^3$ of radius $r > 0$,

$$B(x, r) := \{y \in \mathbb{R}^3 : |x - y| < r\}\,.$$

For convenience, we will use the same notation for an open ball in $\mathcal{M}$, but it will be made clear by context. We denote the open ball in $\mathcal{M}$ around $\omega \in \mathcal{M}$ of radius $r > 0$ by

$$B(\omega, r) = \{p \in \omega : \mathrm{dist}_{\mathcal{M}}(p, \omega) < r\}\,.$$

Let $\mathbb{S}^2$ be the unit sphere $\mathbb{S}^2 = \{x \in \mathbb{R}^3 : |x| = 1\}$, then we define the upper and lower half spheres by

$$\mathbb{S}^2_+ := \{x \in \mathbb{S}^2 : x_3 > 0\} \quad \text{and} \quad \mathbb{S}^2_- := \{x \in \mathbb{S}^2 : x_3 < 0\}\,.$$

Let $U \subset \mathcal{M}$ be a measurable subset, then we define the cone of length ρ by

$$\mathcal{C}_\rho(U) := \{\omega + r\nu(\omega) : \omega \in U \text{ and } r \in (0,\rho)\}. \tag{2.1}$$

We often find it convenient to use spherical coordinates, (r,θ,ϕ), where r denotes the distance from x to the origin, θ denotes the angle in the counterclockwise direction from the positive x_1 axis to the projection of x onto the $\{x_3 = 0\}$ plane, and ϕ denotes the angle between x and e_3. We take the standard basis vectors for spherical coordinates:

$$e_r = (\cos\theta\sin\phi, \sin\theta\sin\phi, \cos\phi), \quad e_\theta = (-\sin\theta, \cos\theta, 0),$$
$$\text{and} \quad e_\phi = (\cos\theta\cos\phi, \sin\theta\cos\phi, -\sin\phi).$$

In the spherical case we will often simplify 3 dimensional problems to 2 dimensional problems, where we consider sets of the form $K \subset \{(r,\phi) : 1 < r < \infty,\ 0 \le \phi \le \pi\}$. To return to the 3 dimensional framework, we define K' as follows,

$$K' := \{(r,\theta,\phi) : (r,\phi) \in K, 0 \le \theta < 2\pi\}. \tag{2.2}$$

In the case of a general manifold $\mathcal{M}$ we will use the coordinate system (r,ω) to parameterize the exterior region of $\mathcal{M}$ up to some distance r_0. For a general manifold, we will choose

$$r_0 = \frac{1}{2\kappa}\,, \tag{2.3}$$

to guarantee that this parameterization is well defined, but this is not necessary when the domain inside of $\mathcal{M}$ is convex, like in the spherical case. For any point x in this exterior region $\mathcal{C}_{r_0}(\mathcal{M})$, we choose ω to be the closest point on $\mathcal{M}$ to x and we choose r to be the distance from x to ω.
For any set $U \subset \mathbb{R}^3$, we will denote the Lebesgue measure of the set by $|U|$ and it will also be understood that if $V \subset \mathcal{M}$, then $|V|$ is the measure of V with respect to the surface measure on $\mathcal{M}$. Finally, dx will denote integration with respect to the Lebesgue measure on $\mathbb{R}^3$ and $d\omega$ will denote integration with respect to the surface measure of $\mathcal{M}$.

2.2 $Q-$Tensors Valued Functions

The Landau-de Gennes model uses $Q-$tensors to describe the liquid crystal, so we must first develop the notation and structure on this class of matrices. Let $M_3(\mathbb{R})$ be the space of 3×3 matrices, then we define the trace and transpose operations respectively by

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

for any matrix $Q \in M_3(\mathbb{R})$. We then define the inner product for any two matrices $Q_1, Q_2 \in M_3(\mathbb{R})$,

$$\langle Q_1, Q_2 \rangle = \operatorname{tr}(Q_1^T Q_2)\,,$$

and this induces the norm

$$|Q| = (\langle Q, Q\rangle)^{1/2}, \quad Q \in M_3(\mathbb{R})\,.$$

We will be focused on the class of symmetric, traceless 3×3 matrices, which we denote by

$$\mathrm{Sym}_0 := \{Q \in M_3(\mathbb{R}) : \; Q = Q^T, \; \operatorname{tr}(Q) = 0\}\,.$$

On this class of matrices, the norm reduces to

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

and $(\mathrm{Sym}_0, |\cdot|)$ defines a Banach space.

Let $C^k(U; \mathrm{Sym}_0)$ denote the set of $k-$times continuously differentiable functions from $U \subset \mathbb{R}^3$ to Sym_0, for $k \geq 0$. A $Q-$tensor valued function $Q(x)$ is $k-$times continuously differentiable if each of its component functions $Q_{ij}(x)$ are themselves $k-$times continuously differentiable in all variables. If $Q : U \to \mathrm{Sym}_0$ is differentiable, then the gradient is defined as $\nabla Q = (\nabla Q_{ij})$ and the norm of ∇Q is given by

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

In spherical coordinates, $|\nabla Q|^2$ evaluates to

$$|\nabla Q|^2 = \left|\frac{\partial Q}{\partial r}\right|^2 + \frac{1}{r^2}\left|\frac{\partial Q}{\partial \phi}\right|^2 + \frac{1}{r^2 \sin^2 \phi}\left|\frac{\partial Q}{\partial \theta}\right|^2 . \tag{2.4}$$

While for a general manifold, using the local coordinate system (ω_1, ω_2) we have

$$|\nabla Q|^2 = \left|\frac{\partial Q}{\partial r}\right|^2 + \frac{1}{(1+r|\kappa_1|)^2}\left|\frac{\partial Q}{\partial \omega_1}\right|^2 + \frac{1}{(1+r|\kappa_2|)^2}\left|\frac{\partial Q}{\partial \omega_2}\right|^2 . \tag{2.5}$$

The usual definitions for L^p spaces extend to the class of $Q-$tensor valued functions in that for $1 \leq p \leq \infty$, $Q \in L^p(U; \mathrm{Sym}_0)$ if each $Q_{ij} \in L^p(U; \mathbb{R})$ for $i, j = 1, 2, 3$. It then follows that the Sobolev spaces are defined by

$$W^{k,p}(U; \mathrm{Sym}_0) := \{Q \in L^p(U; \mathrm{Sym}_0) : D^\alpha Q_{ij} \in L^p(U; \mathbb{R}) \ \forall \ i, j = 1, 2, 3, \text{ and } \forall \ |\alpha| \leq k\}$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ is a multi-index such that $|\alpha| = \alpha_1 + \alpha_2 + \alpha_3$ and $D^\alpha Q_{ij}$ is a the derivative of Q_{ij} in the weak sense. We will mainly focus on $H^1(U; \mathrm{Sym}_0) = W^{1,2}(U; \mathrm{Sym}_0)$ and in this space, the H^1 norm is given by,

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

This is a very special space as it is also a Hilbert space with the inner product

$$\langle Q_1, Q_2 \rangle_{H^1} = \int_U Q_1 \cdot Q_2 + \nabla Q_1 \cdot \nabla Q_2 \, dx \, .$$

2.3 Landau-de Gennes Theory

Let $\Omega_\mu \subset \mathbb{R}^3$ denote the exterior region of a colloidal particle of size $\mu > 0$, then the Landau-de Gennes model with a magnetic field on Ω_μ is described by the following energy functional:

$$E(Q) = \int_{\Omega_\mu} \frac{L}{2}|\nabla Q|^2 + f(Q) + h^2 g(Q)\, dx \, ,$$

where $L > 0$ is a material-dependent elastic constant and h is the magnetic field strength. After non-dimensionalization, this becomes

$$E_{\xi,\eta}(Q) = \int_\Omega \frac{1}{2}|\nabla Q|^2 + \frac{1}{\xi^2}f(Q) + \frac{1}{\eta^2}g(Q)\,dx\,,$$

for two coupled parameters $\xi, \eta > 0$, as done in [3]. Through this non-dimensionalization, we have the relations

$$\xi \sim \mu^{-1} \quad \text{and} \quad \eta \sim \frac{\xi}{h}\,, \tag{2.6}$$

where μ is some natural length-scale of Ω_μ and now Ω is the re-scaled domain with natural length scale 1. Let $U \subset \Omega$, then we define the energy on U by

$$E_{\xi,\eta}(Q;U) = \int_U \frac{1}{2}|\nabla Q|^2 + \frac{1}{\xi^2}f(Q) + \frac{1}{\eta^2}g(Q)\,dx\,.$$

The functions f and g in the energy functional are defined as

$$f(Q) = -\frac{a}{2}|Q|^2 - \frac{b}{3}\mathrm{tr}(Q^3) + \frac{c}{4}|Q|^4 + C \quad \text{and} \quad g(Q) = \sqrt{\frac{2}{3}} - \frac{Q_{33}}{|Q|}\,, \tag{2.7}$$

where we choose $a = 1$, $b = 3$, $c = 3$ and $C = \frac{2}{9}$. This choice of constants ensures that $f(Q) \geq 0$ for all $Q \in \mathrm{Sym}_0$ and $f(Q) = 0$ exactly when $Q = n \otimes n - \frac{1}{3}I$. We define the set of uniaxial $Q-$tensors such that it is precisely the set where f achieves its minimum, i.e.

$$\mathcal{N} := \left\{ Q \in \mathrm{Sym}_0 : Q = n \otimes n - \frac{1}{3}I \text{ for some } n \in \mathbb{S}^2 \right\}.$$

The bulk energy of the system is given by

$$\int_\Omega \frac{1}{\xi^2}f(Q)\,dx\,,$$

and this term penalizes biaxiality in the sense that $f(Q) \geq C(\mathrm{dist}(Q,\mathcal{N}))^2$ for all $Q \in \mathrm{Sym}_0$ and for some constant $C > 0$. The term

$$\int_\Omega \frac{1}{\eta^2}g(Q)\,dx$$

is the symmetry breaking term, in that rotations $R \in SO(3)$ which satisfy $g(R^TQR) = g(Q)$ must have e_3 as an eigenvector, whereas $f(R^TQR) = f(Q)$ for all $R \in SO(3)$. We also note that $g(Q) = 0$ exactly when $Q = sQ_\infty$, for any $s \in (0, \infty)$ and

$$Q_\infty := e_3 \otimes e_3 - \frac{1}{3}I \, .$$

This is because $g(Q)$ is scale invariant and favours alignment with the vertical magnetic field. We note that $f(Q) + g(Q) = 0$ if and only if $Q = Q_\infty$. It will often be useful to obtain upper bounds on f and g when estimating the energy of the system and we can easily see that,

$$f(Q) \leq \frac{1}{2}|Q|^2 + |Q|^3 + \frac{3}{4}|Q|^4 + \frac{2}{9}$$

since $|\mathrm{tr}(Q^3)| = |\langle Q^2, Q\rangle| \leq |Q|^3$. Therefore if $|Q|$ is bounded on some set, then so is $f(Q)$. It also holds that

$$g(Q) \leq \sqrt{\frac{2}{3}} + 1 \, ,$$

for any $Q \in \mathrm{Sym}_0$. We also note that if $Q \in \mathcal{N}$, then $g(Q)$ simplifies to

$$g(Q) = \sqrt{\frac{3}{2}}(1 - n_3^2),$$

where $Q = n \otimes n - \frac{1}{3}I$. When Q is uniaxial, we will frequently use the notation $g(n)$ to denote $g(Q)$. For any $Q \in \mathrm{Sym}_0$, we can decompose it into the form

$$Q = s\left(n \otimes n - \frac{1}{3}I + t\left(m \otimes m - \frac{1}{3}I\right)\right) \, ,$$

where $n \perp m$, $s \in [0, \infty)$ and $t \in [0, 1]$. The choice of s and t come from the eigenvalues of Q in that $\lambda_1 = s$ and $\lambda_2 = st$ are the two leading eigenvalues of Q. Provided that $t \neq 1$ and $Q \neq 0$, we can choose n and m uniquely up to their sign since

$$n \otimes n = (-n) \otimes (-n) \, . \tag{2.8}$$

We define the set where the decomposition is not unique by

$$\mathcal{B} := \{Q \in \mathrm{Sym}_0 : Q = 0 \text{ or } \lambda_1(Q) = \lambda_2(Q)\}\,. \tag{2.9}$$

Away from $\mathcal{B}$, we can define the function $n : \mathrm{Sym}_0 \setminus \mathcal{B} \to \mathbb{R}P^2$ by taking $n(Q) = [n]$ for n from the decomposition and $[n] = \{n, -n\}$ being the equivalence class for n in $\mathbb{S}^2$. We then use this to define the projection of $Q \in \mathrm{Sym}_0 \setminus \mathcal{B}$ onto $\mathcal{N}$. Let $P : \mathrm{Sym}_0 \setminus \mathcal{B} \to \mathcal{N}$ be

$$P(Q) = n(Q) \otimes n(Q) - \frac{1}{3}I\,, \tag{2.10}$$

where we note that this is well defined by (2.8).

3 Mathematical Framework

We consider the non-dimensionalized Landau-de Gennes framework with a colloid described by a smooth, compact, oriented 2-manifold $\mathcal{M}$ and we define Ω to be the region of $\mathbb{R}^3$ exterior to $\mathcal{M}$. Let

$$\mathcal{M}_d = \{\omega \in \mathcal{M} : \nu(\omega) = \pm e_3\}\,, \tag{3.1}$$

then we also impose that $\mathcal{M}_d$ consist of finitely many isolated points and finitely many smooth curves of finite length. This assumption greatly simplifies the construction in Section 6 as it excludes very badly behaved sets and sets of positive measure. For any $Q \in Q_\infty + H^1(\Omega; \mathrm{Sym}_0)$, the energy in Ω is given by

$$E_{\xi,\eta}(Q) = \int_\Omega \frac{1}{2}|\nabla Q|^2 + \frac{1}{\xi^2} f(Q) + \frac{1}{\eta^2} g(Q)\, dx\,,$$

so we want to consider minimizers of this energy which have a tangential boundary constraint on $\mathcal{M}$. We define the class of admissible boundary conditions

$$\mathcal{A}_b = \{Q_b : \mathcal{M} \to \mathcal{N} \text{ where } Q_b \text{ is } C^1 \text{ except at finitely many points and } n(Q_b)\cdot\nu = 0 \text{ a.e.}\}\,,$$

then we search for minimizers $Q_{\xi,\eta}$ of $E_{\xi,\eta}$ subject to a fixed boundary condition $Q_{\xi,\eta} = Q_b \in \mathcal{A}_b$ on $\mathcal{M}$. The full potential, $f(Q) + h^2 g(Q)$ is minimized exactly when $Q = Q_\infty$ and the potential can be estimated from below by

$$f(Q) + h^2 g(Q) \geq C_h |Q - Q_\infty|^2\,,$$

for some constant $C_h > 0$ which depends only on h. The coercivity of this estimate guarantees the existence of a minimizer in the affine space $Q_\infty + H^1(\Omega; \mathrm{Sym}_0)$.

We are interested in the large particle limit, which corresponds to very small values of $\xi > 0$ as $\xi \sim \mu^{-1}$ from (2.6). More specifically, we are interested in the regime where we take both $\xi, \eta \to 0$ in such a way that,

$$\frac{\eta}{\xi} \to \infty.$$

We have that $f(Q_b) = 0$ for $Q_b \in \mathcal{A}_b$, but $g(Q_b) \neq 0$ unless $Q_b = Q_\infty$. Because of this, a transition takes place in a boundary layer around $\mathcal{M}$ and this transition turns out to be governed by the one-dimensional energy

$$F_\lambda(Q) = \int_0^\infty \frac{1}{2}\left|\frac{dQ}{dr}\right|^2 + \lambda^2 f(Q) + g(Q)\ dr, \tag{3.2}$$

defined for $Q \in Q_\infty + H^1((0,\infty), \mathrm{Sym}_0)$. However, we are mostly interested in the case where $\lambda = \infty$ when

$$F_\infty(Q) = \begin{cases} \displaystyle\int_0^\infty \frac{1}{2}\left|\frac{dQ}{dr}\right|^2 + g(Q)\ dr, & Q \text{ is uniaxial a.e.,} \\ +\infty, & \text{otherwise.} \end{cases} \tag{3.3}$$

We can subsequently define the minimal value of F_λ for a given boundary condition, $Q_0 \in \mathrm{Sym}_0$ by

$$D_\lambda(Q_0) = \inf\{F_\lambda(Q) : Q \in Q_\infty + H^1((0,\infty), \mathrm{Sym}_0) \text{ and } Q(0) = Q_0\}. \tag{3.4}$$

This minimal energy will be very important in characterizing the energy around $\mathcal{M}$ in the large particle limit.

4 Model Case: The Sphere

Disclaimer: *The following work comes from [7] where some minor modification have been made to better fit the notation and style of this thesis.*

We begin with a much simpler case where the manifold $\mathcal{M}$ is the unit sphere, $\mathbb{S}^2$. Many of the ideas that will be used for the general manifold will carry over from this easier case. This section will be split into three parts, in which we will prove the following theorems.

Theorem 4.1 (Lower bound). *Let $Q_{\xi,\eta}$ minimize $E_{\xi,\eta}$ with $Q_{\xi,\eta} = Q_b \in \mathcal{A}_b$ on $\mathbb{S}^2$. If*

$$\frac{\eta}{\xi} \to \infty \quad as \quad \xi, \eta \to 0,$$

then for any measurable set $U \subset \mathbb{S}^2$,

$$\liminf_{\xi,\eta\to 0} \, \eta E_{\xi,\eta}(Q_{\xi,\eta}; \mathcal{C}_\infty(U)) \;\geq\; \int_U D_\infty(Q_b(\omega)) \, d\omega.$$

The lower bound in Theorem 4.1 follows from an elementary rescaling and the properties of $\lambda \mapsto D_\lambda$ as in [1] with only minor modifications. Note that this lower bound is valid for any admissible Q_b. So a natural question is for which choice of Q_b does the energy density $D_\infty(Q_b(\omega))$ attain its minimum. It is in Section 4.2 that we will show $Q_b^* = e_\phi \otimes e_\phi - \frac{1}{3}I$ is the boundary condition which yields the minimal energy of D_∞. Next, using this definition of Q_b^*, we can construct an upper bound that matches the lower bound in Theorem 4.1.

Theorem 4.2 (Recovery sequence). *If*

$$\frac{\eta}{\xi} \to \infty \quad as \quad \xi, \eta \to 0\,,$$

then there exists $Q_{\xi,\eta}$ with $Q_{\xi,\eta}|_{\mathbb{S}^2} \in \mathcal{A}_b$ such that

$$\limsup_{\xi,\eta\to 0} \, \eta E_{\xi,\eta}(Q_{\xi,\eta}) \;\leq\; \int_U D_\infty(Q_b^*(\omega)) \, d\omega.$$

We note that although this result is analogue to [1], the construction necessary to obtain Theorem 4.2 is very different. The main difference is that the singular structure appearing for $Q_b = Q_b^*$ is no longer a line defect (with isotropic or biaxial core), but two half-point defects (so called *boojums*). Those defects are located at opposite poles and can be constructed to be uniaxial everywhere. To realize this recovery sequence, it is necessary that all constructions be done within the uniaxial manifold. In particular, the interpolations between point defects and the optimal profile achieving the minimal energy density $D_\infty(Q_b^*)$ have to take place in the *phase* rather than a direct linear interpolation of the $Q-$tensor components.

4.1 Lower Bound for $\mathbb{S}^2$

In this section we prove Theorem 4.1. The proof is very similar to [1] where the case $Q_b = e_r \otimes e_r - \frac{1}{3}I$ was considered. For the convenience of the reader we recall the main steps here:
we first change to spherical coordinates by $x = r\omega$, $(r,\omega) \in (1,\infty) \times \mathbb{S}^2$, then define

$$\widetilde{Q}(\tilde{r},\omega) := Q_{\xi,\eta}(1+\eta\tilde{r},\omega),$$

where $r = 1+\eta\tilde{r}$. Applying this change of variables, we have

$$\begin{aligned} \eta E_{\xi,\eta}(Q_{\xi,\eta};\mathcal{C}_\infty(U)) &= \eta \int_U \int_1^\infty \left[\frac{1}{2}\left|\nabla Q_{\xi,\eta}\right|^2 + \frac{1}{\xi^2} f(Q_{\xi,\eta}) + \frac{1}{\eta^2} g(Q_{\xi,\eta})\right] r^2\, dr\, d\omega \\ &\geq \int_U \int_0^\infty \left[\frac{1}{2}\left|\frac{\partial \widetilde{Q}}{\partial \tilde{r}}\right|^2 + \frac{\eta^2}{\xi^2} f(\widetilde{Q}) + g(\widetilde{Q})\right] d\tilde{r}\, d\omega\,. \end{aligned} \tag{4.1}$$

Then using the definitions (3.3) and (3.4), we see that

$$\eta E_{\xi,\eta}(Q_{\xi,\eta};\mathcal{C}_\infty(U)) \geq \int_U F_{\frac{\eta}{\xi}}(\widetilde{Q}(\cdot,\omega))\, d\omega \geq \int_U D_{\frac{\eta}{\xi}}(Q_b(\omega))\, d\omega\,.$$

We now use Lemma 2.2 from [1] which states that for any $Q_0 \in \mathrm{Sym}_0$ and $\lambda \in (0,\infty]$,

$$D_\lambda(Q_0) = \lim_{\mu\to\lambda} D_\mu(Q_0).$$

This result along with Fatou's lemma gives the desired lower bound

$$\liminf_{\xi,\eta\to 0}\ \eta E_{\xi,\eta}(Q_{\xi,\eta};\mathcal{C}_\infty(U)) \geq \int_U D_\infty(Q_b(\omega))\, d\omega\,.$$

4.2 Optimal Boundary Condition

The goal of this section is to prove that $D_\infty(Q_b)$ is minimized when we choose $Q_b = e_\phi \otimes e_\phi - \frac{1}{3}I$. Intuitively this is expected as $(\mp)e_\phi$ is the unit tangent vector closest to $(\pm)e_3$ at each point on $\mathbb{S}^2 \setminus \{\pm e_3\}$.

Proposition 4.3. *Let $\omega \in \mathbb{S}^2$ be fixed, define $Q_\phi = e_\phi \otimes e_\phi - \frac{1}{3}I$ and $Q_v = v \otimes v - \frac{1}{3}I$, where $v \in \mathbb{S}^2$ with $v \cdot \omega = 0$, then*

$$D_\infty(Q_\phi) \leq D_\infty(Q_v)$$

with equality if and only if $v = \pm e_\phi$.

Due to the symmetry of the problem, it will suffice to prove this for $\omega \in \mathbb{S}^2$ with $0 \leq \omega_3 < 1$, although the case where $\omega_3 = 0$ is trivial as $Q_\phi = Q_\infty$, so $D_\infty(Q_\phi)$ is attained by the constant map. It will also make sense to only consider vectors $v \in \mathbb{S}^2$ such that $v_1 < 0$, $v_2 = 0$ and $0 \leq v_3 < 1$. This will be explained further in the proof of Proposition 4.3, but for now we consider the following related lemma which deals with the quantity G_∞ defined to be,

$$G_\infty(n) \ := \int_0^\infty \left|\frac{\partial n}{\partial t}\right|^2 + g(n)\ dt\,,$$

recalling that $g(n) = \sqrt{\frac{3}{2}}(1 - n_3^2) = g(Q)$ for $Q = n \otimes n - \frac{1}{3}I$.
This lemma is a reformulation of [1, Lemma 3.4] and provides an explicit description of the minimizers of G_∞ among functions $n \in H^1((0,\infty);\mathbb{R}^3) + e_3$ with $|n| = 1$ and a given initial condition.

Lemma 4.4. *Let $v \in \mathbb{S}^2$ with $v_1 < 0$, $v_2 = 0$ and $0 \leq v_3 < 1$, then if n^* minimizes G_∞ with $n^*(0,\varphi) = v$, n^* is of the form, $n^* = (-\sqrt{1-(n_3^*)^2}, 0, n_3^*)$, where*

$$n_3^*(t,\varphi) = \frac{A(\varphi) - e^{-\sqrt[4]{24}t}}{A(\varphi) + e^{-\sqrt[4]{24}t}}, \quad \textit{and} \quad A(\varphi) = \frac{1+\cos\varphi}{1-\cos\varphi}, \tag{4.2}$$

with φ being the angle between v and e_3. Further, there exists a constant $C > 0$ independent of φ such that

$$\left|\frac{\partial n^*}{\partial t}\right|^2, \left|\frac{\partial n^*}{\partial \varphi}\right|^2, |n_1^*|^2 \leq C e^{-\sqrt[4]{24}t}. \tag{4.3}$$

Using this Lemma, we can now proceed with the proof of Proposition 4.3.

Proof of Proposition 4.3. We begin by treating the case $\omega = \pm e_3$, in which case the rotational symmetry of the problem implies that all unit tangent vectors v have equal energy $D_\infty(Q_v)$. Next, we consider $\omega \in \mathbb{S}^2$ with $\omega_3 = 0$, then $Q_\phi = Q_\infty$, so

$$D_\infty(Q_\phi) = 0 \leq D_\infty(Q_v).$$

We then use the symmetry of the setup to reduce the problem to the case where $0 < \omega_3 < 1$, $v_1 < 0$, $v_2 = 0$ and $0 \leq v_3 < 1$. First, since $Q_v = Q_{-v}$ for any $v \in \mathbb{S}^2$, it holds $D_\infty(Q_v) = D_\infty(Q_{-v})$. If $D_\infty(Q_\phi) \leq D_\infty(Q_v)$ at ω, the same holds at $-\omega$, so we can impose without loss of generality that $v_3 \geq 0$. Now let $v = (v_1, v_2, v_3)$. Then there exists θ_0 and a rotation about the x_3-axis R_{θ_0} such that for $u = R_{\theta_0} v$, we have $u_1 < 0$ and $u_2 = 0$. If n minimizes G_∞ subject to $n(0) = u$, then $\tilde{n} = R_{-\theta_0} n$ minimizes G_∞ subject to $\tilde{n}(0) = v$ and

$$D_\infty(Q_v) = G_\infty(\tilde{n}) = G_\infty(n).$$

In this setup, $D_\infty(Q_v) = G_\infty(n^*(\cdot, \varphi))$ where n^* is as defined in Lemma 4.4, so we can compute $D_\infty(Q_v)$ explicitly.

$$D_\infty(Q_v) = \int_0^\infty \left|\frac{\partial n^*}{\partial t}\right|^2 + g(n^*)\ dt = \int_0^\infty 2\left|\frac{\partial n^*}{\partial t}\right| \sqrt{g(n^*)}\ dt\,,$$

where n^* was chosen specifically to satisfy this equality. By a direct computation, we get that

$$D_\infty(Q_v) \;=\; \sqrt[4]{24}\int_0^\infty \left|\frac{\partial n_3^*}{\partial t}\right|\ dt = \sqrt[4]{24}(1 - v_3)\,.$$

We note that if $v \cdot \omega = 0$, then v_3 is maximized for $v = -e_\phi$, and thus $D_\infty(Q_v)$ is minimized by Q_ϕ. □

Using Lemma 4.4, we define $Q_b^* = Q_\phi$ on $\mathbb{S}^2 \setminus \{\pm e_3\}$. This gives the following corollary.

Corollary 4.5. *Let $Q_{\xi,\eta}$ minimize $E_{\xi,\eta}$ with $Q_{\xi,\eta} = Q_b \in \mathcal{A}_b$ on $\mathbb{S}^2$. If*

$$\frac{\eta}{\xi} \to \infty \quad as \quad \xi, \eta \to 0\,,$$

then for any measurable set $U \subset \mathbb{S}^2$*,*

$$\liminf_{\xi,\eta\to 0} \ \eta E_{\xi,\eta}(Q_{\xi,\eta};\mathcal{C}_\infty(U)) \geq \int_U D_\infty(Q_b^*(\omega))\, d\omega\,.$$

4.3 Upper Bound for $\mathbb{S}^2$

In this section we prove the upper bound in Theorem 4.2 by constructing a sequence of competitors. Theorem 4.2 thus follows immediately from Proposition 4.6.

Proposition 4.6. *If* $Q_{\xi,\eta}$ *minimizes* $E_{\xi,\eta}$ *with boundary condition* $Q_{\xi,\eta} = Q_b^*$ *on* $\mathbb{S}^2$ *and*

$$\frac{\eta}{\xi} \to \infty \quad as \quad \xi,\eta \to 0,$$

then,

$$\limsup_{\xi,\eta\to 0} \ \eta E_{\xi,\eta}(Q_{\xi,\eta}) \leq \int_{\mathbb{S}^2} D_\infty(Q_b^*(\omega)) \ d\omega.$$

To do this, we will construct a sequence of maps which are uniaxial a.e., equivariant and symmetric with respect to $\{x_3 = 0\}$.

Proof of Proposition 4.6. To simplify the construction, we will construct the recovery sequence on $\Omega_0^+ := \{(r,\phi) : 1 < r < \infty,\ 0 < \phi < \frac{\pi}{2}\}$ and then extend it to Ω via a rotation and a subsequent reflection, yielding an equivariant map. For the construction we partition Ω_0^+ into smaller regions Ω_k, $k = 1, ..., 4$ (see Figure 2). Since the recovery sequence will consist of uniaxial maps, it is enough to define a continuous and piecewise smooth map $\widehat{n} : \Omega_0^+ \to \mathbb{S}^2$ and then take

$$\widehat{Q}_\xi(r,\phi) = \begin{cases} \widehat{n}(r,\phi) \otimes \widehat{n}(r,\phi) - \frac{1}{3}I, & 0 < \phi < \frac{\pi}{2}, \\ (T \circ \widehat{n}(r,\pi-\phi)) \otimes (T \circ \widehat{n}(r,\pi-\phi)) - \frac{1}{3}I, & \frac{\pi}{2} < \phi < \pi, \end{cases}$$

where $T : \mathbb{S}^2 \to \mathbb{S}^2$ is the reflection $T(x_1,x_2,x_3) = (x_1,x_2,-x_3)$. The competitor sequence is then $\overline{Q_{\xi,\eta}}(r,\theta,\phi) = R_\theta^T \widehat{Q}_\xi(r,\phi) R_\theta$. Note that we will use the notation, $\Omega_k' := \{(r,\theta,\phi) : (r,\phi) \in \Omega_k,\ 0 \leq \theta < 2\pi\}$, for $k = 1,\ldots,4$ to allow us to define the maps on Ω_0^+, but consider the energy on the entire upper space Ω^+.

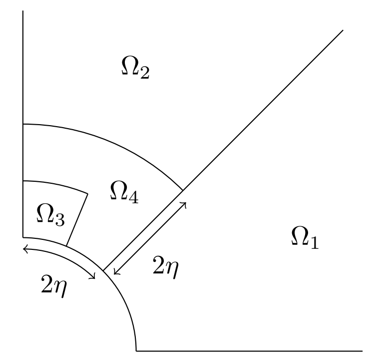

Figure 2: Subdivision of Ω_0^+ for the proof of Proposition 4.6

<u>*Energy in* Ω_1</u>: We begin by defining

$$\Omega_1 := \left\{(r,\phi) : 1 < r < \infty,\ 2\eta < \phi < \frac{\pi}{2}\right\},$$

and take $\widehat{n}(r,\phi) = n^*\left(\frac{r-1}{\eta}, \frac{\pi}{2} - \phi\right)$ where n^* is given as in Lemma 4.4. Note that the use of $\frac{\pi}{2} - \phi$ is due to the fact that ϕ is representing the point on the sphere instead of the angle between the tangent vector and e_3. Expressing the energy in spherical coordinates (r, θ, ϕ) and using equivariance for the $\theta-$derivative

$$\eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}}; \Omega_1') = 2\pi\eta \int_{2\eta}^{\frac{\pi}{2}} \int_1^\infty r^2 \sin\phi \left|\frac{\partial \widehat{n}}{\partial r}\right|^2 + \sin\phi \left|\frac{\partial \widehat{n}}{\partial \phi}\right|^2 + \frac{|\widehat{n}_1|^2}{\sin\phi} + \frac{r^2 \sin\phi}{\eta^2} g(\widehat{n})\ drd\phi\,.$$

Then by the change of variables $r = 1 + \eta t$, we obtain:

$$\eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}}; \Omega_1') = 2\pi \int_{2\eta}^{\frac{\pi}{2}} \int_0^\infty (1+\eta t)^2 \sin\phi \left|\frac{\partial n}{\partial t}\right|^2 + \eta^2 \sin\phi \left|\frac{\partial n}{\partial \phi}\right|^2 + \frac{\eta^2 |n_1|^2}{\sin\phi} + (1+\eta t)^2 \sin\phi\ g(n)\ dtd\phi.$$

We divide this integral into two parts:

$$\eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}}; \Omega_1') = 2\pi \int_{2\eta}^{\frac{\pi}{2}} \left(\int_0^\infty \left[\left|\frac{\partial n}{\partial t}\right|^2 + g(n)\right]\ dt\right) \sin\phi\ d\phi + \mathcal{A}_\xi \tag{4.4}$$

where,

$$\mathcal{A}_\xi = 2\pi \int_{2\eta}^{\frac{\pi}{2}} \int_0^\infty \Bigg[(2\eta t + \eta^2 t^2) \sin\phi \left| \frac{\partial n}{\partial t} \right|^2 + \eta^2 \sin\phi \left| \frac{\partial n}{\partial \phi} \right|^2 + \frac{\eta^2 |n_1|^2}{\sin\phi} \\ + (2\eta t + \eta^2 t^2) \sin\phi \; g(n) \Bigg] \, dt d\phi.$$

We identify the first term in (4.4) as D_∞, while we will show that the second term $\mathcal{A}_\xi$ vanishes in the limit. For this second part, we note that since $2\eta < \phi < \frac{\pi}{2}$, we still have $0 < \frac{\pi}{2} - \phi < \frac{\pi}{2}$ so we can use the bounds from (4.3) to get,

$$\mathcal{A}_\xi \leq 2\pi \int_{2\eta}^{\frac{\pi}{2}} \int_0^\infty \Big[(2\eta t + \eta^2 t^2) C e^{-\sqrt[4]{24} t} + C\eta^2 e^{-\sqrt[4]{24} t} + \frac{C\eta^2 e^{-\sqrt[4]{24} t}}{\sin 2\eta} \\ + (2\eta t + \eta^2 t^2) \sqrt{\frac{3}{2}} C e^{-\sqrt[4]{24} t} \Big] \, dt d\phi.$$

Then by straightforward computations, we get,

$$\mathcal{A}_\xi \leq 2\pi \left(\frac{\pi}{2} - 2\eta \right) \left(C\eta + C\eta^2 + \frac{C\eta^2}{\sin 2\eta} \right)$$

for some constants $C > 0$, which tends to 0 as $\eta \to 0$. Now from (4.4) and using Lemma 4.4,

$$\eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}}; \Omega_1') = 2\pi \int_{2\eta}^{\frac{\pi}{2}} D_\infty(Q_b^*(0,\phi)) \sin\phi \; d\phi + \mathcal{A}_\xi \leq \int_{\mathbb{S}^2_+} D_\infty(Q_b^*(\omega)) \; d\omega + \mathcal{A}_\xi,$$

therefore when taking $\xi, \eta \to 0$, we are left with

$$\limsup_{\xi,\eta \to 0} \; \eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}}; \Omega_1') \leq \int_{\mathbb{S}^2_+} D_\infty(Q_b^*(\omega)) \; d\omega.$$

Energy in Ω_2: Next consider the region Ω_2 (see also Figure 2) defined to be

$$\Omega_2 := \{(r, \phi) : 1 + 2\eta < r < \infty, \; 0 < \phi < 2\eta\}.$$

Because of equivariance, we want to take $\widehat{n} = e_3$ on the x_3-axis. Furthermore, at $\phi = 2\eta$ we need $\widehat{n}$ to be consistent with the construction from the previous region Ω_1. Let Φ denote the angle between

e_3 and our construction $\widehat{n}$ on Ω_2, then we define Φ as follows,

$$\Phi(r,\phi) = \frac{\phi}{2\eta}\cos^{-1}(\widehat{n}_3(r,2\eta)),$$

where $\widehat{n}_3(r,2\eta)$ is defined by continuous extension onto $\partial\Omega_1$. To preserve uniaxiality, we define $\widehat{n}$ by an interpolation of its angle with e_3, taking $\widehat{n} = (-\sin\Phi, 0, \cos\Phi)$ on Ω_2. We note that

$$\left|\frac{\partial \widehat{n}}{\partial r}\right|^2 = \left|\frac{\partial \Phi}{\partial r}\right|^2 \quad \text{and} \quad \left|\frac{\partial \widehat{n}}{\partial \phi}\right|^2 = \left|\frac{\partial \Phi}{\partial \phi}\right|^2,$$

so we can write the energy in this region as

$$\eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}};\Omega_2') = 2\pi\eta\int_0^{2\eta}\int_{1+2\eta}^{\infty} r^2\sin\phi\left|\frac{\partial\Phi}{\partial r}\right|^2 + \sin\phi\left|\frac{\partial\Phi}{\partial\phi}\right|^2 + \frac{\sin^2\Phi}{\sin\phi} + \frac{r^2\sin\phi}{\eta^2}\sin^2\Phi\; dr d\phi.$$

By the change of variables, $r = 1+\eta t$, and by letting $\widehat{\Phi}(t,\phi) = \Phi(1+\eta t,\phi)$, we have

$$\eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}};\Omega_2') \le 2\pi\int_0^{2\eta}\int_2^{\infty}(1+\eta t)^2\left|\frac{\partial\widehat{\Phi}}{\partial t}\right|^2 + \eta^2\left|\frac{\partial\widehat{\Phi}}{\partial\phi}\right|^2 + \frac{\eta^2\widehat{\Phi}^2}{\sin\phi} + (1+\eta t)^2\widehat{\Phi}^2\sin\phi\; dt d\phi.$$

We note that the $t-$derivative term is bounded by $Ce^{-\sqrt[4]{24}t}$ since,

$$\left|\frac{\partial\widehat{\Phi}}{\partial t}\right|^2 \le \left|\frac{\partial}{\partial t}\widehat{\Phi}(t,2\eta)\right|^2 = \left|\frac{\partial n}{\partial t}(t,2\eta)\right|^2 \le Ce^{-\sqrt[4]{24}t}.$$

by (4.3) of Lemma 4.4. We get a similar bound on the $\phi-$derivative,

$$\left|\frac{\partial\widehat{\Phi}}{\partial\phi}\right|^2 = \frac{1}{4\eta^2}\left|\cos^{-1}(n_3(t,2\eta))\right|^2 = \frac{1}{4\eta^2}\left|\widehat{\Phi}(t,2\eta)\right|^2$$

and using that $\alpha \le 2\sin\alpha$ for $0<\alpha<\frac{\pi}{2}$ we get,

$$\left|\frac{\partial\widehat{\Phi}}{\partial\phi}\right|^2 \le \frac{1}{4\eta^2}\left|2\sin(\widehat{\Phi}(t,2\eta))\right|^2 = \frac{1}{\eta^2}|n_1(t,2\eta)|^2 \le \frac{Ce^{-\sqrt[4]{24}t}}{\eta^2}. \tag{4.5}$$

Using

$$\frac{\eta^2(\widehat{\Phi}(t,\phi))^2}{\sin\phi} = \frac{\phi^2(\cos^{-1}(n_3(t,2\eta))^2}{4\sin\phi} \le \frac{\phi\left(\widehat{\Phi}(t,2\eta)\right)^2}{4} \le C|n_1(t,2\eta)|^2,$$

we have the following bound on the energy,

$$\begin{aligned}\eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}};\Omega_2') &\leq 2\pi\int_0^{2\eta}\int_2^\infty Ce^{-\sqrt[4]{24}t}((1+\eta t)^2+1)+C|n_1(t,2\eta)|^2+(1+\eta t^2)|n_1(t,2\eta)|^2\ dtd\phi\\ &\leq 2\pi\int_0^{2\eta}\int_2^\infty Ce^{-\sqrt[4]{24}t}((1+\eta t)^2+1)\ dtd\phi\ \leq\ 4\pi\eta C,\end{aligned}$$

for some constant $C > 0$. Therefore the energy contribution from Ω_2 is negligible in the limit $\xi, \eta \to 0$.

<u>*Energy in* Ω_3</u>: In this region, we must define $\overline{Q_{\xi,\eta}}$ to have a point singularity at the pole of the sphere, due to the discontinuity in the boundary condition at this point, however the energy will still be bounded since point singularities in 3D have finite energy. With the additional $\eta-$prefactor in our energy, the energy contribution from Ω_3 will therefore be negligible as well. Let

$$\Omega_3 := \{(r,\phi) : 1 < r < 1+\eta,\ 0 < \phi < \eta\}.$$

On a flat domain, it would be possible to define $\widehat{n}$ to be the "standard" point singularity at $(0,0)$,

$$m(s,\tau) := \left(\frac{-\tau}{\sqrt{\tau^2+s^2}}, 0, \frac{s}{\sqrt{\tau^2+s^2}}\right). \tag{4.6}$$

Because our domain is curved, we have to slightly adapt this profile in order to match the boundary conditions. Thus,

$$\widehat{n}(r,\phi) = R_\phi m\left(\frac{r-1}{\eta}, \frac{\phi}{\eta}\right), \quad \text{where} \quad R_\phi = \begin{pmatrix}\cos\phi & 0 & \sin\phi\\ 0 & 1 & 0\\ -\sin\phi & 0 & \cos\phi\end{pmatrix}. \tag{4.7}$$

so we have $r = 1+\eta s$ and $\phi = \eta\tau$, thus if $(r,\phi)\in\Omega_3$, then $(s,\tau)\in(0,1)\times(0,1)$. We first consider the $r-$derivative term,

$$\left|\frac{\partial\widehat{n}}{\partial r}\right|^2 = \frac{1}{\eta^2}\left|\frac{\partial m}{\partial s}\right|^2 = \frac{1}{\eta^2}\left(\frac{\tau^2}{|(s,\tau)|^4}\right) \tag{4.8}$$

by a direct computation. Here $|(s,\tau)|$ denotes the standard Euclidean 2-norm. The derivative in ϕ is more complicated, due to the rotation in the definition of $\widehat{n}$. But again by a direct computation we can show that,

$$\left|\frac{\partial \widehat{n}}{\partial \phi}\right|^2 = |m|^2 + \frac{1}{\eta^2}\left|\frac{\partial m}{\partial \tau}\right| + \frac{2}{\eta}\left(m_3\frac{\partial m_1}{\partial \tau} - m_1\frac{\partial m_3}{\partial \tau}\right) \leq 1 + \frac{1}{\eta^2}\left|\frac{\partial m}{\partial \tau}\right|^2.$$

After computing the $\tau-$derivative explicitly, we have

$$\left|\frac{\partial \widehat{n}}{\partial \phi}\right|^2 \leq 1 + \frac{1}{\eta^2}\left(\frac{s^2}{|(s,\tau)|^4}\right). \tag{4.9}$$

Next we have $\widehat{n}_1 = m_1 \cos\phi + m_3 \sin\phi$ and we notice that since $|m| = 1$, it follows that $|\widehat{n}_1|^2$ and $g(\overline{Q_{\xi,\eta}})$ are bounded by a constant. However in order to get the required estimate for the $\theta-$derivative, we need a more exact bound on $|\widehat{n}_1|$. By definition of $\widehat{n}_1$ and since $\frac{1}{2}\phi \leq \sin\phi$,

$$\frac{|\widehat{n}_1|^2}{\sin\phi} \leq \frac{2(m_1\cos\phi + m_3\sin\phi)^2}{\phi} = \frac{2(m_1^2\cos^2\phi + 2m_1m_3\sin\phi\cos\phi + m_3^2\sin^2\phi)}{\phi}.$$

Then using $\sin\phi \leq \phi$ and substituting $\phi = \eta\tau$, it holds,

$$\frac{|\widehat{n}_1|^2}{\sin\phi} \leq \frac{2m_1^2}{\eta\tau} + 6 = \frac{C}{\eta}\left(\frac{\tau}{|(s,\tau)|^2}\right) + 6.$$

for some constant $C > 0$. Now we are ready to compute the energy in this region. Altogether, we observe that the energy in Ω_3' is estimated as follows.

$$\begin{aligned}
\eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}};\Omega_3') &= 2\pi\eta\int_0^\eta\int_1^{1+\eta} r^2\sin\phi\left|\frac{\partial \widehat{n}}{\partial r}\right|^2 + \sin\phi\left|\frac{\partial \widehat{n}}{\partial \phi}\right|^2 + \frac{|\widehat{n}_1|^2}{\sin\phi} + \frac{r^2\sin\phi}{\eta^2}g(\overline{Q_{\xi,\eta}})\ drd\phi \\
&\leq 2\pi\eta\int_0^1\int_0^1 C\sin(\eta\tau)\left(\frac{\tau^2}{|(s,\tau)|^4} + \frac{s^2}{|(s,\tau)|^4}\right) + \eta^2 + \frac{C\eta\tau}{|(s,\tau)|^2} + C\eta\ dsd\tau \\
&\leq 2\pi\eta\int_0^1\int_0^1 C\eta\left(\frac{\tau^3}{|(s,\tau)|^4} + \frac{s^2\tau}{|(s,\tau)|^4} + \frac{\tau}{|(s,\tau)|^2}\right) + C\eta\ dsd\tau \\
&\leq 2\pi C\eta^2.
\end{aligned} \tag{4.10}$$

Taking the limit $\xi,\eta \to 0$, the energy contribution of Ω_3' vanishes.

Energy in Ω_4: Finally we consider Ω_4 where we will define $\widehat{n}$ by a Lipschitz extension. Let

$$\Omega_4 := \{(r,\phi) : 1 < r < 1+2\eta,\ 0 < \phi < 2\eta\} \setminus \overline{\Omega_3},$$

then we will first define a function Φ on Ω_4 and then let $\widehat{n} = (\sin\Phi, 0, \cos\Phi)$. The boundary $\partial\Omega_4$ can be split into 6 pieces as shown in Figure 3.

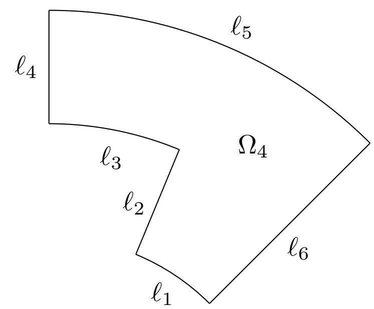

Figure 3: Boundary components of Ω_4 for Proposition 4.6

On ℓ_1 we choose Φ so that $\widehat{n} = e_\phi$ as required by the boundary condition, then on ℓ_2 and ℓ_3, we define $\widehat{n}$ so that it is consistent with the construction on Ω_3. On ℓ_4 we let $\Phi = 0$ so that $\widehat{n} = e_3$ and on ℓ_5 and ℓ_6 we define $\widehat{n}$ to be consistent with Ω_2 and Ω_1 respectively. We will then show that Φ, being the angle between $\widehat{n}$ and e_3, is Lipschitz on $\partial\Omega_4$ with Lipschitz constant proportional to η^{-1} so we can extend Φ to all of Ω_4 with the same Lipschitz constant using the Kirszbraun Theorem, see Theorem 2.10.43 from [9]. To show Φ has this Lipschitz constant, we consider the derivatives along each component of the boundary.

First on ℓ_1, Q_b^* is Lipschitz with constant 2, so Φ is also Lipschitz with a constant that has no dependence on η. Next on ℓ_2 and ℓ_3, we consider the derivatives,

$$\left|\frac{\partial\widehat{n}}{\partial r}\right|^2 = \frac{C}{\eta^2}\left(\frac{\tau^2}{|(s,\tau)|^4}\right) \leq \frac{C}{\eta^2} \quad \text{and} \quad \left|\frac{\partial\widehat{n}}{\partial\phi}\right|^2 = 1 + \frac{1}{\eta^2}\left(\frac{s^2}{|(s,\tau)|^4}\right) \leq \frac{C}{\eta^2}$$

using (4.8) and (4.9) since $\tau = 1$ and $s = 1$ on ℓ_2 and ℓ_3 respectively. On ℓ_4, Φ is constant, so it has Lipschitz constant 0. For ℓ_5, we have

$$\left|\frac{\partial\widehat{n}}{\partial\phi}\right|^2 \leq \frac{Ce^{-\sqrt[4]{24}t}}{\eta^2} \leq \frac{C}{\eta^2}$$

by (4.5) and using that $t = 2$ here. Finally, on ℓ_6,

$$\left|\frac{\partial\widehat{n}}{\partial r}\right|^2 = \frac{1}{\eta^2}\left|\frac{\partial n}{\partial t}\right|^2 \leq \frac{Ce^{-\sqrt[4]{24}t}}{\eta^2} \leq \frac{C}{\eta^2}$$

since $0 < t < 2$ on this region. So Φ is Lipschitz with constant $C\eta^{-1}$ on $\partial\Omega_4$ and evoking Kirszbraun Theorem there exists a Lipschitz extension Φ to all of Ω_4 with the same Lipschitz constant. Thus each derivative of Φ on Ω_4 is bounded by $C\eta^{-1}$. Using the Lipschitz constant, we get that $|\Phi(\phi) - \Phi(0)| \leq C\eta^{-1}|\phi|$ and therefore,

$$\begin{aligned}
\eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}}; \Omega_4') &\leq 2\pi\eta \int_0^{2\eta} \int_\gamma^{1+2\eta} \frac{Cr^2 \sin\phi}{\eta^2} + \frac{C\sin\phi}{\eta^2} + \frac{2\phi}{\eta^2} + \sqrt{\frac{3}{2}} \frac{r^2\phi^3}{\eta^2} \; drd\phi \\
&\leq 2\pi\eta \int_0^{2\eta} \int_\gamma^{1+2\eta} \frac{C(1+2\eta)^2}{\eta} + \frac{C}{\eta} + \frac{4}{\eta} + C(1+2\eta)^2\eta \; drd\phi \\
&\leq 2\pi\eta(4\eta^2) \left[\frac{C(1+2\eta)^2}{\eta} + \frac{C}{\eta} + \frac{4}{\eta} + C(1+2\eta)^2\eta \right].
\end{aligned}$$

Thus when we take $\xi, \eta \to 0$, the whole energy will vanish on this region.

<u>*Conclusion*</u>: Now that we have analyzed the energy on each region, we are ready to put the regions together and get a bound on the energy in all of Ω. We have that

$$\eta E_{\xi,\eta}(Q_{\xi,\eta}) \leq \eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}}) = 2\eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}}; \Omega_+) = 2\sum_{k=1}^{4} \eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}}; \Omega_k')$$

by symmetry of the construction. So applying our results from each region, we can see that

$$\begin{aligned}
\limsup_{\xi,\eta\to 0} \eta E_{\xi,\eta}(Q_{\xi,\eta}) &\leq 2\sum_{k=1}^{4} \limsup_{\xi,\eta\to 0} \eta E_{\xi,\eta}(\overline{Q_{\xi,\eta}}; \Omega_k') \\
&\leq 2\int_{\mathbb{S}^2{}_+} D_\infty(Q_b(\omega)) \; d\omega = \int_{\mathbb{S}^2} D_\infty(Q_b(\omega)) \; d\omega.
\end{aligned}$$

□

5 Lower Bound for $\mathcal{M}$

We now move on to the more general case where we consider a smooth, compact, oriented 2-manifold without boundary, denoted by $\mathcal{M}$. Note that $\mathcal{M}_d$ as defined in (3.1) does not consist of just points anymore but can also contain lines. This will make the construction of the upper bound much more delicate. In this section, we prove the corresponding lower bound for such a manifold.

Theorem 5.1. *Let $Q_{\xi,\eta}$ minimize $E_{\xi,\eta}$ with $Q_{\xi,\eta} = Q_b \in \mathcal{A}_b$ on $\mathcal{M}$. If,*

$$\frac{\eta}{\xi} \to \infty \quad as \quad \xi, \eta \to 0\,,$$

then for any measurable set $U \subset \mathcal{M}$,

$$\liminf_{\xi,\eta\to 0} \eta E_{\xi,\eta}(Q_{\xi,\eta}; \mathcal{C}_{r_0}(U)) \geq \int_U D_\infty(Q_b(\omega))\, d\omega\,.$$

Although this theorem is very similar to Theorem 4.1, the proof strategy is very different. This is due to the fact that we are now on a finite length scale of r_0 as opposed to the infinite length of the cone from a sphere. We are unable to define the cone of infinite length everywhere on $\mathcal{M}$ as the region enclosed by the manifold, need not be convex.

5.1 Regularity of Minimizers

In order to obtain the lower bound from Theorem 5.1, we first need some regularity for the minimizers $Q_{\xi,\eta}$. This can be done by using the Euler-Lagrange equations which minimizers must satisfy. However, the Euler-Lagrange equations will have terms involving g, but since g is not smooth at $Q = 0$, we will not be able to obtain very good regularity estimates on the minimizers. Therefore we modify the energy slightly so that we are able to apply standard elliptic estimates. Since the only singularity of g occurs at $Q = 0$, we want to "cut" out this point. So fix a number $0 < q_0 < \sqrt{\frac{2}{3}}$ and take a smooth scalar cut-off function $\varphi : \mathrm{Sym}_0 \to [0,1]$ with $\varphi(Q) = 1$ for $|Q| \geq q_0$ and $\varphi(Q) = 0$ for $|Q| < \frac{q_0}{2}$. Then we define the modified energy $\widetilde{E}_{\xi,\eta}$ to be

$$\widetilde{E}_{\xi,\eta}(Q) = \int_\Omega \frac{1}{2}|\nabla Q|^2 + \frac{1}{\xi^2} f(Q) + \frac{1}{\eta^2}\varphi(Q) g(Q)\, dx\,.$$

For the remainder of this section we focus on results for the modified energy $\widetilde{E}_{\xi,\eta}$. Note that it is sufficient to show the lower bound from Theorem 5.1 for $\widetilde{E}_{\xi,\eta}$ replacing $E_{\xi,\eta}$ as $E_{\xi,\eta}(Q) \geq \widetilde{E}_{\xi,\eta}(Q)$ since $\varphi \leq 1$ and $g(Q) \geq 0$. We begin by proving a Lipschitz bound for the minimizers of $\widetilde{E}_{\xi,\eta}$. Let $\mathcal{M}_b$ denote the set of points on $\mathcal{M}$ where the boundary condition Q_b is discontinuous and let $\widetilde{Q}_{\xi,\eta}$ minimize $\widetilde{E}_{\xi,\eta}$, then we want to find a Lipschitz bound for $\widetilde{Q}_{\xi,\eta}$ away from $\mathcal{M}_b$. We define the $\delta-$neighbourhood around $\mathcal{M}_b$,

$$\mathcal{M}_b^\delta := \{\omega \in \mathcal{M} : \operatorname{dist}_{\mathcal{M}}(\omega, \mathcal{M}_b) < \delta\},$$

and then recall the definition of the cone,

$$\mathcal{C}_{r_0}(\mathcal{M} \setminus \mathcal{M}_b^\delta) := \{\omega + r\nu(\omega) : \omega \in \mathcal{M} \setminus \mathcal{M}_b^\delta \text{ and } r \in (0, r_0)\}.$$

On this region, we are able to show that $|\nabla \widetilde{Q}_{\xi,\eta}|$ is bounded as follows.

Lemma 5.2. *Let $\widetilde{Q}_{\xi,\eta}$ minimize $\widetilde{E}_{\xi,\eta}$ with $\widetilde{Q}_{\xi,\eta} = Q_b$ on $\mathcal{M}$, then for $\delta > 0$ sufficiently small,*

$$|\nabla \widetilde{Q}_{\xi,\eta}(x)| \leq \frac{C_\delta}{\xi} \quad \textit{for all} \quad x \in \mathcal{C}_{r_0}(\mathcal{M} \setminus \mathcal{M}_b^\delta),$$

for some constant $C_\delta > 0$.

Proof. From the minimality of $\widetilde{Q}_{\xi,\eta}$, we obtain the Euler-Lagrange equation

$$\begin{cases} -\Delta \widetilde{Q}_{\xi,\eta} = \mathcal{F}_\xi(\widetilde{Q}_{\xi,\eta}), & \text{on } \Omega, \\ \widetilde{Q}_{\xi,\eta} = Q_b, & \text{on } \mathcal{M}, \end{cases} \tag{5.1}$$

where we define

$$\mathcal{F}_\xi(Q) := -\frac{1}{\xi^2} Df(Q) - \frac{1}{\eta^2} D(\varphi g)(Q) - \frac{1}{\xi^2}|Q|^2 I - \frac{1}{3\eta^2}\operatorname{tr}(D(\varphi g)(Q)) I.$$

We note that thanks to the introduction of φ to the energy, $\mathcal{F}_\xi$ is a sum of smooth functions and therefore is itself smooth. Since $\mathcal{M}$ is also smooth, $\widetilde{Q}_{\xi,\eta}$ is smooth on Ω, however $|\nabla \widetilde{Q}_{\xi,\eta}|$ will blow up as we approach points in $\mathcal{M}_b$. To get around this issue we define $\overline{Q}_b$ to be the harmonic extension of Q_b which vanishes at infinity, i.e.

$$\begin{cases} -\Delta \overline{Q}_b = 0\,, & \text{on } \Omega\,, \\ \overline{Q}_b = Q_b\,, & \text{on } \mathcal{M}\,, \end{cases}$$

so that we also have,

$$\begin{cases} -\Delta(\widetilde{Q}_{\xi,\eta} - \overline{Q}_b) = \mathcal{F}_\xi(\widetilde{Q}_{\xi,\eta})\,, & \text{on } \Omega\,, \\ \widetilde{Q}_{\xi,\eta} - \overline{Q}_b = 0\,, & \text{on } \mathcal{M}\,. \end{cases}$$

Now we want to apply Lemma A.2. from [6] and we remark that although the result is stated for smooth bounded regions, it still applies more generally to smooth regions with compact boundary. Using this lemma we get the bound,

$$||\nabla(\widetilde{Q}_{\xi,\eta} - \overline{Q}_b)||^2_{L^\infty(\Omega)} \leq C||\mathcal{F}_\xi(\widetilde{Q}_{\xi,\eta})||_{L^\infty(\Omega)}||\widetilde{Q}_{\xi,\eta} - \overline{Q}_b||_{L^\infty(\Omega)}\,, \tag{5.2}$$

and we bound each norm separately. We note that $|\widetilde{Q}_{\xi,\eta}|^2 \leq \frac{2}{3}$ and define $B := \{Q \in \mathrm{Sym}_0 : |Q|^2 \leq \frac{2}{3}\}$, so that

$$||\mathcal{F}_\xi(\widetilde{Q}_{\xi,\eta})||_{L^\infty(\Omega)} \leq \frac{1}{\xi^2}\Big(||Df||_{L^\infty(B)} + 2\Big) + \frac{2}{\eta^2}||D(\varphi g)||_{L^\infty(B)} + \leq C\Big(\frac{1}{\xi^2} + \frac{1}{\eta^2}\Big)\,.$$

Now since $\xi \to 0$ faster than $\eta \to 0$, we can see that for sufficiently small ξ, we get the bound $||\mathcal{F}_\xi(\widetilde{Q}_{\xi,\eta})||_{L^\infty(\Omega)} \leq C\xi^{-2}$. Furthermore, since $\overline{Q}_b$ is harmonic and vanishes at infinity, it is bounded on Ω, so $||\widetilde{Q}_{\xi,\eta} - \overline{Q}_b||_{L^\infty(\Omega)} \leq C$ and therefore,

$$||\nabla(\widetilde{Q}_{\xi,\eta} - \overline{Q}_b)||_{L^\infty(\Omega)} \leq \frac{C}{\xi}\,.$$

Now using that $\mathcal{C}_{r_0}(\mathcal{M} \setminus \mathcal{M}_b^\delta) \subset \Omega$, we can see that

$$\begin{aligned} ||\nabla\widetilde{Q}_{\xi,\eta}||_{L^\infty(\mathcal{C}_{r_0}(\mathcal{M}\setminus\mathcal{M}_b^\delta))} &\leq ||\nabla(\widetilde{Q}_{\xi,\eta} - \overline{Q}_b)||_{L^\infty(\Omega)} + ||\nabla\overline{Q}_b||_{L^\infty(\mathcal{C}_{r_0}(\mathcal{M}\setminus\mathcal{M}_b^\delta))} \\ &\leq \frac{C}{\xi} + ||\nabla\overline{Q}_b||_{L^\infty(\mathcal{C}_{r_0}(\mathcal{M}\setminus\mathcal{M}_b^\delta))}\,, \end{aligned}$$

so it remains to bound $|\nabla\overline{Q}_b|$. However, the region $\overline{\mathcal{C}_{r_0}(\mathcal{M} \setminus \mathcal{M}_b^\delta)}$ is compact and $\overline{Q}_b$ is C^1 on this region, therefore $||\nabla\overline{Q}_b||_{L^\infty(\mathcal{C}_{r_0}(\mathcal{M}\setminus\mathcal{M}_b^\delta))} \le C_\delta$, for some $C_\delta > 0$. So for sufficiently small ξ, we have

$$||\nabla\widetilde{Q}_{\xi,\eta}||_{L^\infty(\mathcal{C}_{r_0}(\mathcal{M}\setminus\mathcal{M}_b^\delta))} \le \frac{C}{\xi} + C_\delta \le \frac{C_\delta}{\xi}\,.$$

□

Now that we have an estimate on the regularity away from the defects, we wish to find the regions where minimizers are far from being uniaxial. That is, we want to better understand the set

$$K_\varepsilon := \{x \in \Omega : \operatorname{dist}(\widetilde{Q}_{\xi,\eta}(x), \mathcal{N}) \ge \varepsilon\}$$

for some $\varepsilon > 0$. More precisely we will show that $K_\varepsilon \cap \mathcal{C}_{r_0/2}(\mathcal{M}\setminus\mathcal{M}_b^\delta)$ is negligible in the limit $\xi, \eta \to 0$. To do this, we first show that we can cover this set by a union of small balls. The necessary number of balls cannot be bounded uniformly in ξ, but we can control the speed at which the number goes to infinity as in [2, Lemma 4.6].

Lemma 5.3. *For $\varepsilon > 0$ sufficiently small, there exists a number $I \in \mathbb{N}$ and finitely many points $x_i \in K_\varepsilon \cap \mathcal{C}_{r_0/2}(\mathcal{M}\setminus\mathcal{M}_b^\delta)$ for $i = 1, \ldots, I$ such that*

$$K_\varepsilon \cap \mathcal{C}_{r_0/2}(\mathcal{M}\setminus\mathcal{M}_b^\delta) \subset \bigcup_{i=1}^{I} B\Big(x_i, \frac{\varepsilon\xi}{L}\Big) \subset K_{\varepsilon/2} \cap \mathcal{C}_{r_0}(\mathcal{M}\setminus\mathcal{M}_b^{\delta/2})\,,$$

where $L = 2C_{\delta/2}$ for $C_{\delta/2}$ from Lemma 5.2. Moreover,

$$I \;\le\; \frac{C_{\delta/2}^3}{C\varepsilon^3\eta\xi f_{\min}^{\varepsilon/2}}\,,$$

for some constant $C > 0$ and for $f_{\min}^{\varepsilon/2} = \min\{f(Q) : \operatorname{dist}(Q, \mathcal{N}) \ge \varepsilon/2\}$.

Proof. We begin by choosing any $x_0 \in K_\varepsilon \cap \mathcal{C}_{r_0/2}(\mathcal{M}\setminus\mathcal{M}_b^\delta)$ and we claim that

$$B\Big(x_0, \frac{\varepsilon\xi}{L}\Big) \subset K_{\varepsilon/2} \cap \mathcal{C}_{r_0}(\mathcal{M}\setminus\mathcal{M}_b^{\delta/2})\,.$$

For $x \in B(x_0, \frac{\varepsilon\xi}{L})$ it holds that

$$\begin{aligned}\operatorname{dist}(\widetilde{Q}_{\xi,\eta}(x),\mathcal{N}) &\geq \operatorname{dist}(\widetilde{Q}_{\xi,\eta}(x_0),\mathcal{N}) - \operatorname{dist}(\widetilde{Q}_{\xi,\eta}(x),\widetilde{Q}_{\xi,\eta}(x_0)) \\ &\geq \varepsilon - \operatorname{dist}(x,x_0)||\nabla\widetilde{Q}_{\xi,\eta}||_{L^\infty(\mathcal{C}_{r_0}(\mathcal{M}\setminus\mathcal{M}_b^{\delta/2}))} \geq \varepsilon - \left(\frac{\varepsilon\xi}{2C_{\delta/2}}\right)\frac{C_{\delta/2}}{\xi} = \frac{\varepsilon}{2},\end{aligned}$$

thus $x \in K_{\varepsilon/2}$. Now since Q_b is uniaxial on $\mathcal{M}$, but $\widetilde{Q}_{\xi,\eta}(x)$ is bounded away from being uniaxial, it must be that x_0 is sufficiently far from $\mathcal{M}$ that $B(x_0, \frac{\varepsilon\xi}{L})$ does not intersect $\mathcal{M}$. Using this fact, we can choose ξ sufficiently small such that $B(x_0, \frac{\varepsilon\xi}{L}) \subset \mathcal{C}_{r_0}(\mathcal{M}\setminus\mathcal{M}_b^{\delta/2})$. Clearly we can take the radius of these balls to be a factor $\frac{1}{3}$ smaller and maintain the same inclusions. Now using that $K_\varepsilon \cap \mathcal{C}_{r_0/2}(\mathcal{M}\setminus\mathcal{M}_b^\delta)$ is totally bounded, we can choose finitely many points $x_i \in K_\varepsilon \cap \mathcal{C}_{r_0/2}(\mathcal{M}\setminus\mathcal{M}_b^\delta)$ for $i = 1, \ldots, N$ such that

$$K_\varepsilon \cap \mathcal{C}_{r_0/2}(\mathcal{M}\setminus\mathcal{M}_b^\delta) \subset \bigcup_{i=1}^N B\Big(x_i, \frac{\varepsilon\xi}{3L}\Big) \subset K_{\varepsilon/2} \cap \mathcal{C}_{r_0}(\mathcal{M}\setminus\mathcal{M}_b^{\delta/2}).$$

However we do not have any control on the size of N as $\xi,\eta \to 0$. Using Vitali's finite covering lemma, there exists $I \leq N$ such that for $k = 1, ..., I$, we can choose $x_{i_k} \in \{x_1, \ldots, x_N\}$ such that $B(x_{i_k}, \frac{\varepsilon\xi}{3L}) \cap B(x_{i_j}, \frac{\varepsilon\xi}{3L}) = \emptyset$ for all $k \neq j$ and

$$K_\varepsilon \cap \mathcal{C}_{r_0/2}(\mathcal{M}\setminus\mathcal{M}_b^\delta) \subset \bigcup_{k=1}^I B\Big(x_{i_k}, \frac{\varepsilon\xi}{L}\Big) \subset K_{\varepsilon/2} \cap \mathcal{C}_{r_0}(\mathcal{M}\setminus\mathcal{M}_b^{\delta/2}).$$

It remains to prove the bound on I. First recall that $f(Q) \geq C(\operatorname{dist}(Q,\mathcal{N}))^2$, so $f_{\min^{\varepsilon/2}} \geq C\varepsilon^2$. Next we have that

$$\begin{aligned}C &\geq \eta\widetilde{E}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}) \geq \frac{\eta}{\xi^2}\int_{K_{\varepsilon/2}\cap\mathcal{C}_{r_0}(\mathcal{M}\setminus\mathcal{M}_b^{\delta/2})} f(Q)\,dx \geq \frac{\eta f_{\min}^{\varepsilon/2}}{\xi^2}|K_{\varepsilon/2}\cap\mathcal{C}_{r_0}(\mathcal{M}\setminus\mathcal{M}_b^{\delta/2})| \\ &\geq \frac{\eta f_{\min}^{\varepsilon/2}}{\xi^2}\Big|B\Big(x_{i_k}, \frac{\varepsilon\xi}{3L}\Big)\Big|\, I.\end{aligned}$$

This implies that

$$I \leq \frac{C_{\delta/2}^3}{C\varepsilon^3\eta\xi f_{\min}^{\varepsilon/2}}.$$

□

Finally we want to be able to exclude any points $\omega \in \mathcal{M} \setminus \mathcal{M}_b^\delta$ such that the set $\{\omega + r\nu(\omega) : r \in (0, r_0/2)\}$ intersects K_ε. We will show that we are able to exclude such ω because in the limit $\xi, \eta \to 0$, this collection of points is of measure zero. To do this, we first define the projection of a subset $U \subset \mathcal{C}_{r_0}(\mathcal{M})$ onto $\mathcal{M}$ by

$$\operatorname{proj}(U) := \{\omega \in \mathcal{M} : \omega + r\nu(\omega) \in U \text{ for some } r \in (0, r_0)\},$$

then we consider the following proposition.

Proposition 5.4. *Let $\varepsilon, \delta > 0$, with K_ε and $\mathcal{C}_{r_0/2}(\mathcal{M} \setminus \mathcal{M}_b^\delta)$ defined as above. Then*

$$\limsup_{\xi,\eta \to 0} |\operatorname{proj}(K_\varepsilon \cap \mathcal{C}_{r_0/2}(\mathcal{M} \setminus \mathcal{M}_b^\delta))| \ = \ 0 .$$

Proof. Using Lemma 5.3, we choose I many points $x_i \in K_\varepsilon \cap \mathcal{C}_{r_0}(\mathcal{M} \setminus \mathcal{M}_b^\delta)$ such that the union of the balls of radius $\frac{\varepsilon\xi}{L}$ centred at these points, cover the set $K_\varepsilon \cap \mathcal{C}_{r_0/2}(\mathcal{M} \setminus \mathcal{M}_b^\delta)$. Therefore,

$$\operatorname{proj}(K_\varepsilon \cap \mathcal{C}_{r_0/2}(\mathcal{M} \setminus \mathcal{M}_b^\delta)) \subset \operatorname{proj}\Big(\bigcup_{i=1}^{I} B\Big(x_i, \frac{\varepsilon\xi}{L}\Big)\Big),$$

so it suffices to prove the area of the projection of the cover goes to zero in the limit. We note that for each x_i using the same reasoning as in the proof of Lemma 5.3, $B(x_i, \frac{3\varepsilon\xi}{2L}) \subset K_{\varepsilon/4} \cap \mathcal{C}_{r_0}(\mathcal{M} \setminus \mathcal{M}_b^\delta)$, so the projection onto $\mathcal{M}$ is well-defined for balls of this radius. We now consider the volume integral

$$\Big|B\Big(x_i, \frac{3\varepsilon\xi}{2L}\Big)\Big| = \int_{B(x_i, \frac{3\varepsilon\xi}{2L})} 1 \, dx = \int_{\operatorname{proj}(B(x_i, \frac{3\varepsilon\xi}{2L})} \int_{h_1(\omega)}^{h_2(\omega)} (1 + r\kappa_1)(1 + r\kappa_2) \, dr d\omega$$

where,

$$h_1(\omega) = \inf\Big\{r : \omega + r\nu(\omega) \in B\Big(x_i, \frac{3\varepsilon\xi}{2L}\Big)\Big\}$$

and

$$h_2(\omega) = \sup\Big\{r : \omega + r\nu(\omega) \in B\Big(x_i, \frac{3\varepsilon\xi}{2L}\Big)\Big\}.$$

So if $\omega \in \operatorname{proj}(B(x_i, \frac{\varepsilon\xi}{L}))$, then $h_2(\omega) - h_1(\omega) \geq \frac{\varepsilon\xi}{L}$. Therefore,

$$\Big|B\Big(x_i, \frac{3\varepsilon\xi}{2L}\Big)\Big| \geq \int_{\operatorname{proj}(B(x_i, \frac{\varepsilon\xi}{L}))} \int_{h_1(\omega)}^{h_2(\omega)} (1 - r_0\kappa)^2 \, dr d\omega \geq \frac{1}{4}\Big|\operatorname{proj}\Big(B\Big(x_i, \frac{\varepsilon\xi}{L}\Big)\Big)\Big|\Big(\frac{\varepsilon\xi}{L}\Big).$$

We can bound the area of the projection as follows,

$$\Big|\mathrm{proj}\Big(B\Big(x_i, \frac{\varepsilon\xi}{L}\Big)\Big)\Big| \le \frac{C\varepsilon^2\xi^2}{C_{\delta/2}^2}\,.$$

Finally, using Lemma 5.3 we have that,

$$\Big|\mathrm{proj}\Big(\bigcup_{i=1}^{I} B\Big(x_i, \frac{\varepsilon\xi}{L}\Big)\Big)\Big| \le I\cdot\Big|\mathrm{proj}\Big(B\Big(x_i, \frac{\varepsilon\xi}{L}\Big)\Big)\Big| \le \frac{C_{\delta/2}}{C\varepsilon f_{\min}^{\varepsilon/2}}\Big(\frac{\xi}{\eta}\Big) \to 0$$

since $\frac{\xi}{\eta} \to 0$ as $\xi, \eta \to 0$, by assumption. □

We define $\mathcal{M}_b^{\delta,\varepsilon} := \mathrm{proj}(K_\varepsilon \cap \mathcal{C}_{r_0/2}(\mathcal{M}\setminus\mathcal{M}_b^\delta)) \cup \mathcal{M}_b^\delta$ so that from now on we can consider the energy in the region $\mathcal{C}_{r_0/2}(\mathcal{M}\setminus\mathcal{M}_b^{\delta,\varepsilon})$. If $x \in \mathcal{C}_{r_0/2}(\mathcal{M}\setminus\mathcal{M}_b^{\delta,\varepsilon})$ then we have shown that $\mathrm{dist}(\widetilde{Q}_{\xi,\eta}(x), \mathcal{N}) < \varepsilon$ and $|\nabla\widetilde{Q}_{\xi,\eta}(x)| \le C_\delta\xi^{-1}$.

5.2 Computing the Lower Bound

This section is dedicated to proving Theorem 5.1, but as previously stated, it suffices to prove the lower bound for $\widetilde{E}_{\xi,\eta}$. We would like to follow a similar approach as in the spherical case, where we considered the energy along a ray of infinite length. However, since $\mathcal{M}$ need not be convex, we must adapt the method to work on rays of finite length. To do this, we first define the energy along a *half-ray* from $\omega \in \mathcal{M}$ as,

$$\widetilde{\mathcal{E}}_{\xi,\eta}(Q,\omega) = \int_0^{r_0/2}\Big(\frac{1}{2}\Big|\frac{\partial Q}{\partial r}\Big|^2 + \frac{1}{\xi^2}f(Q) + \frac{1}{\eta^2}(\varphi g)(Q)\Big)(1+r\kappa_1(\omega))(1+r\kappa_2(\omega))\,dr\,. \tag{5.3}$$

where the term half-ray denotes a length of $r_0/2$ as opposed to r_0. We note that,

$$|\nabla\widetilde{Q}_{\xi,\eta}|^2 = \left|\frac{\partial\widetilde{Q}_{\xi,\eta}}{\partial r}\right|^2 + \frac{1}{(1+r|\kappa_1|)^2}\left|\frac{\partial\widetilde{Q}_{\xi,\eta}}{\partial\omega_1}\right|^2 + \frac{1}{(1+r|\kappa_2|)^2}\left|\frac{\partial\widetilde{Q}_{\xi,\eta}}{\partial\omega_2}\right|^2 \ge \left|\frac{\partial\widetilde{Q}_{\xi,\eta}}{\partial r}\right|^2\,,$$

so this combined with (5.3) gives the inequality,

$$\eta\widetilde{E}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta};\mathcal{C}(U)) \ge \int_U \eta\widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega),\omega)\,d\omega\,.$$

For each $\omega \in U$ there are two possibilities. It could be that $\eta\widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega),\omega) \ge D_\infty(Q_b(\omega))$, for all $\eta, \xi > 0$ sufficiently small, in which case there is nothing left to prove. The other possibility is that there always exist $\eta, \xi > 0$ very small such that $\eta\widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega),\omega) < D_\infty(Q_b(\omega))$. As preparation for the estimates in this case, we provide some useful definitions. Define L_g to be

$$L_g \ := \ \sup\left\{ \frac{|g(Q_1) - g(Q_2)|}{|Q_1 - Q_2|} \ : \ Q_j \in \mathrm{Sym}_0 \text{ with } q_0 \le |Q_j| \le 1\,, j = 1,2\} \right\}, \tag{5.4}$$

i.e. L_g is the Lipschitz constant of g on the set $\{Q \in \mathrm{Sym}_0 : q_0 \le |Q| \le 1\}$. In particular, small neighbourhoods of $\mathcal{N}$ are contained in this set and $\varphi g = g$ there as well. We then choose $\alpha := \sqrt{\frac{8}{3}}(1 + L_g) + 4$ and for $\varepsilon > 0$ we define the sets

$$A^\varepsilon := \{Q \in \mathrm{Sym}_0 : |Q - Q_\infty|^2 < \alpha\varepsilon,\ \mathrm{dist}(Q, \mathcal{N}) < \varepsilon\}\,,$$

and

$$B^\varepsilon := \{Q \in \mathrm{Sym}_0 : |Q - Q_\infty|^2 \ge \alpha\varepsilon,\ \mathrm{dist}(Q, \mathcal{N}) < \varepsilon\}\,.$$

The definition of these sets and the inspiration for the following lemma come from [2, Lemma 5.3].

Lemma 5.5. *Let $\varepsilon, \delta > 0$ be sufficiently small, let $\omega \in \mathcal{M} \setminus \mathcal{M}_b^{\delta,\varepsilon}$ and $\xi, \eta > 0$. Assume that*

$$\eta\,\widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega),\omega) \ < \ D_\infty(Q_b(\omega))\,.$$

Then, for $I^\varepsilon := \{r \in (0, r_0/2) : |\widetilde{Q}_{\xi,\eta}(r,\omega) - Q_\infty|^2 < \alpha\varepsilon\}$ it holds

$$|I^\varepsilon| \ge \frac{r_0}{2} - c\frac{\eta}{\varepsilon}$$

for some constant $c > 0$.

Proof. We begin by recognizing that since $\omega \in \mathcal{M}\setminus\mathcal{M}_b^{\delta,\varepsilon}$, we have that $\mathrm{dist}(\widetilde{Q}_{\xi,\eta}(r,\omega), \mathcal{N}) < \varepsilon$ for all $r \in (0, r_0/2)$, so this ensures that $\widetilde{Q}_{\xi,\eta}(r,\omega) \in A^\varepsilon \cup B^\varepsilon$ and that I^ε is exactly the set of $r \in (0, r_0/2)$ where $\widetilde{Q}_{\xi,\eta}(r,\omega) \in A^\varepsilon$. If we define $J^\varepsilon := \{r \in (0, r_0/2) : \widetilde{Q}_{\xi,\eta}(r,\omega) \in B^\varepsilon\}$, then,

$$|I^\varepsilon| = \frac{r_0}{2} - |J^\varepsilon|\,,$$

so we require an upper bound on $|J^\varepsilon|$. We can see that

$$D_\infty(Q_b(\omega)) \;\geq\; \eta\, \widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega)) \;\geq\; \frac{1}{\eta}\int_{J^\varepsilon} g(\widetilde{Q}_{\xi,\eta})(1-r_0\kappa)^2\, dr \;\geq\; \frac{1}{4\eta}|J^\varepsilon| g^\varepsilon_{\min}\,,$$

where $g^\varepsilon_{\min} = \min\{g(Q) : Q \in B^\varepsilon\}$. This implies that

$$|J^\varepsilon| \leq \frac{4\eta D_\infty(Q_b(\omega))}{g^\varepsilon_{\min}}\,.$$

It remains to show that $g^\varepsilon_{\min}$ is bounded below independent of ξ or η. Note that for ε sufficiently small, B^ε is contained in $\{Q \in \mathrm{Sym}_0 : q_0 \leq |Q| \leq 1\}$, so we can use Lipschitz continuity of g with the Lipschitz constant L_g. Let $Q \in B^\varepsilon$ and recall from (2.10) that $P(Q)$ is the projection of Q onto $\mathcal{N}$. Then it holds that

$$g(P(Q)) - g(Q) \;\leq\; L_g|P(Q) - Q| \;=\; L_g \operatorname{dist}(Q,\mathcal{N}) \;<\; L_g\varepsilon\,,$$

from which

$$g(Q) \;>\; g(P(Q)) - L_g\varepsilon\,.$$

Since $P(Q)$ is uniaxial and $|P(Q) - Q_\infty|^2 = 2(1-(n_3(Q))^2)$, we can write $g(P(Q))$ as

$$\begin{aligned} g(P(Q)) \;&=\; \sqrt{\frac{3}{8}}|P(Q) - Q_\infty|^2 \;\geq\; \sqrt{\frac{3}{8}}(|Q-Q_\infty| - |P(Q)-Q|)^2 \\ &\geq\; \sqrt{\frac{3}{8}}(|Q-Q_\infty|^2 - 2|Q-Q_\infty|\operatorname{dist}(Q,\mathcal{N})) \;\geq\; \sqrt{\frac{3}{8}}(\alpha\varepsilon - 2\varepsilon|Q-Q_\infty|)\,. \end{aligned}$$

Next we have $|Q - Q_\infty| \leq \operatorname{dist}(Q,\mathcal{N}) + \operatorname{diam}(\mathcal{N}) \leq \varepsilon + 2\sqrt{\frac{2}{3}} \leq 2$, so

$$g(P(Q)) \;\geq\; \sqrt{\frac{3}{8}}(\alpha - 4)\varepsilon = (1+L_g)\varepsilon \quad \text{and} \quad g(Q) \;\geq\; (1+L_g)\varepsilon - L_g\varepsilon \;=\; \varepsilon\,.$$

Therefore $g^\varepsilon_{\min} \geq \varepsilon$, so we obtain the bounds

$$|J^\varepsilon| \;\leq\; 4\eta D_\infty(Q_b(\omega))\Big(\frac{\eta}{\varepsilon}\Big) \quad \text{and} \quad |I^\varepsilon| \;\geq\; \frac{r_0}{2} - 4\eta D_\infty(Q_b(\omega))\Big(\frac{\eta}{\varepsilon}\Big)\,.$$

□

With Lemma 5.5 in hand, we are now ready to prove the lower bound.

Proof of Theorem 5.1. We begin by restricting our attention to $\mathcal{C}_{r_0/2}(\mathcal{M} \setminus \mathcal{M}_b^{\delta,\varepsilon})$, so that

$$\begin{aligned}\eta \widetilde{E}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}) &\geq \eta \int_{\mathcal{M}\setminus\mathcal{M}_b^{\delta,\varepsilon}} \widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega),\omega)\, d\omega \\ &= \eta \left(\int_{\mathcal{M}_1^{\delta,\varepsilon}} \widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega),\omega)\, d\omega + \int_{\mathcal{M}_2^{\delta,\varepsilon}} \widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega),\omega)\, d\omega \right),\end{aligned}$$

where

$$\mathcal{M}_1^{\delta,\varepsilon} := \left\{ \omega \in \mathcal{M} \setminus \mathcal{M}_b^{\delta,\varepsilon} : \liminf_{\xi,\eta\to 0} \eta \widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega)) \geq D_\infty(Q_b(\omega)) \right\},$$

and $\mathcal{M}_2^{\delta,\varepsilon} := (\mathcal{M} \setminus \mathcal{M}_b^{\delta,\varepsilon}) \setminus \mathcal{M}_1^{\delta,\varepsilon}$. Let $\omega \in \mathcal{M}_2^{\delta,\varepsilon}$. Then, using Lemma 5.5, we can choose $r_\omega^\varepsilon \in I^\varepsilon$ such that $r_\omega^\varepsilon \leq c(\frac{\eta}{\varepsilon})$. Thus, we have that

$$\eta \widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega),\omega) \geq \int_0^{r_\omega^\varepsilon} \frac{\eta}{2}\Big|\frac{\partial \widetilde{Q}_{\xi,\eta}}{\partial r}\Big|^2 + \frac{1}{\eta} g(\widetilde{Q}_{\xi,\eta})\, dr\,.$$

Then using Lemma 17 in [8] we have the bound

$$\int_0^{r_\omega^\varepsilon} \frac{\eta}{2}\Big|\frac{\partial \widetilde{Q}_{\xi,\eta}}{\partial r}\Big|^2 dr \geq \int_0^{r_\omega^\varepsilon} \frac{\eta}{2}(\gamma(\widetilde{Q}_{\xi,\eta}))^2 \Big|\frac{\partial P(\widetilde{Q}_{\xi,\eta})}{\partial r}\Big|^2 dr\,,$$

where $\gamma : \mathrm{Sym}_0 \to \mathbb{R}$ is defined by $\gamma(Q) = \lambda_1(Q) - \lambda_2(Q)$, for λ_1, λ_2, the two leading eigenvalues of Q. Note that although in [8], the lemma is stated for $|\nabla Q|$ instead of the radial derivative, it is shown in the proof that the same inequality holds for a single derivative too, so we can apply this lemma without any difficulties. We can then use Lemma 13 from [8] which gives a Lipschitz bound for γ away from $\mathcal{B} = \{Q \in \mathrm{Sym}_0 : Q = 0 \text{ or } \lambda_1(Q) = \lambda_2(Q)\}$ defined in (2.9). So we have

$$\gamma(P(\widetilde{Q}_{\xi,\eta})) - \gamma(\widetilde{Q}_{\xi,\eta}) \leq 2|P(\widetilde{Q}_{\xi,\eta}) - \widetilde{Q}_{\xi,\eta}| = 2\mathrm{dist}(\widetilde{Q}_{\xi,\eta}, \mathcal{N}) \leq 2\varepsilon\,,$$

but since $\gamma(P(\widetilde{Q}_{\xi,\eta})) = 1$, this implies that, $\gamma(\widetilde{Q}_{\xi,\eta}) \geq 1 - 2\varepsilon$. Therefore,

$$\int_0^{r_\omega^\varepsilon} \frac{\eta}{2}\Big|\frac{\partial \widetilde{Q}_{\xi,\eta}}{\partial r}\Big|^2 dr \geq \int_0^{r_\omega^\varepsilon} \frac{\eta}{2}(1-2\varepsilon)^2 \Big|\frac{\partial P(\widetilde{Q}_{\xi,\eta})}{\partial r}\Big|^2 dr = \int_0^{r_\omega^\varepsilon} \eta(1-2\varepsilon)^2 \Big|\frac{\partial n(\widetilde{Q}_{\xi,\eta})}{\partial r}\Big|^2 dr\,.$$

Next we can see that

$$\int_0^{r_\omega^\varepsilon} \frac{1}{\eta} g(\widetilde{Q}_{\xi,\eta})\,dr \geq \int_0^{r_\omega^\varepsilon} \frac{1}{\eta} g(P(\widetilde{Q}_{\xi,\eta}))\,dr - \int_0^{r_\omega^\varepsilon} \frac{1}{\eta} |g(\widetilde{Q}_{\xi,\eta}) - g(P(\widetilde{Q}_{\xi,\eta}))|\,dr\,.$$

We then use that g is Lipschitz as well as the Cauchy Schwartz inequality to get,

$$\int_0^{r_\omega^\varepsilon} \frac{1}{\eta} |g(\widetilde{Q}_{\xi,\eta}) - g(P(\widetilde{Q}_{\xi,\eta}))|\,dr \leq \int_0^{r_\omega^\varepsilon} \frac{L_g}{\eta} \mathrm{dist}(\widetilde{Q}_{\xi,\eta}, \mathcal{N})\,dr \leq \frac{L_g}{\eta} \left(|r_\omega^\varepsilon| \int_0^{r_\omega^\varepsilon} \mathrm{dist}^2(\widetilde{Q}_{\xi,\eta}, \mathcal{N})\,dr \right)^{1/2}.$$

Note that $f(Q) \geq C\mathrm{dist}^2(Q, \mathcal{N})$ for all $Q \in \mathrm{Sym}_0$ and some constant $C > 0$, so

$$\int_0^{r_\omega^\varepsilon} \mathrm{dist}^2(\widetilde{Q}_{\xi,\eta}, \mathcal{N})\,dr \leq \frac{C\xi^2}{\eta} \int_0^{r_\omega^\varepsilon} \frac{\eta}{\xi^2} f(\widetilde{Q}_{\xi,\eta})\,dr \leq \frac{C\xi^2}{\eta} D_\infty(Q_b(\omega))\,.$$

Since furthermore $r_\omega^\varepsilon \lesssim \frac{\eta}{\varepsilon}$, we get that

$$\int_0^{r_\omega^\varepsilon} \frac{1}{\eta} |g(\widetilde{Q}_{\xi,\eta}) - g(P(\widetilde{Q}_{\xi,\eta}))|\,dr \leq \frac{C\xi}{L_g \eta \varepsilon^{1/2}} (D_\infty(Q_b(\omega))^{1/2} \to 0\,,$$

as $\xi, \eta \to 0$. So we have that

$$\begin{aligned} \eta \widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega),\omega) &\geq \int_0^{r_\omega^\varepsilon} \eta(1-2\varepsilon)^2 \Big|\frac{\partial n(\widetilde{Q}_{\xi,\eta})}{\partial r}\Big|^2 + \frac{1}{\eta} g(P(\widetilde{Q}_{\xi,\eta}))\,dr - \mathcal{O}\Big(\frac{\xi}{\eta}\Big) \\ &\geq 2(1-2\varepsilon)^2 \int_0^{r_\omega^\varepsilon} \Big|\frac{\partial n(\widetilde{Q}_{\xi,\eta})}{\partial r}\Big| \sqrt{g(P(\widetilde{Q}_{\xi,\eta}))}\,dr - \mathcal{O}\Big(\frac{\xi}{\eta}\Big)\,. \end{aligned}$$

Since $|n(\widetilde{Q}_{\xi,\eta})| = 1$ it follows that

$$\Big|\frac{\partial n(\widetilde{Q}_{\xi,\eta})}{\partial r}\Big| \;\geq\; \frac{1}{\sqrt{1-(n_3(\widetilde{Q}_{\xi,\eta}))^2}} \Big|\frac{\partial n_3(\widetilde{Q}_{\xi,\eta})}{\partial r}\Big| \quad \text{and} \quad g(P(\widetilde{Q}_{\xi,\eta})) \;=\; \sqrt{\frac{3}{2}}(1-(n_3(\widetilde{Q}_{\xi,\eta}))^2)\,.$$

Therefore,

$$\begin{aligned} \eta \widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega),\omega) &\geq 2(1-2\varepsilon)^2 \int_0^{r_\omega^\varepsilon} \sqrt[4]{\frac{3}{2}} \Big|\frac{\partial n_3(\widetilde{Q}_{\xi,\eta})}{\partial r}\Big|\,dr - \mathcal{O}\Big(\frac{\xi}{\eta}\Big) \\ &\geq \sqrt[4]{24}(1-2\varepsilon)^2 \left| \int_0^{r_\omega^\varepsilon} \frac{\partial n_3(\widetilde{Q}_{\xi,\eta})}{\partial r}\,dr \right| - \mathcal{O}\Big(\frac{\xi}{\eta}\Big) \\ &\geq \sqrt[4]{24}(1-2\varepsilon)^2 \big(|n_3(\widetilde{Q}_{\xi,\eta}(r_\omega^\varepsilon,\omega))| - |n_3(\widetilde{Q}_{\xi,\eta}(0,\omega))| \big) - \mathcal{O}\Big(\frac{\xi}{\eta}\Big)\,. \end{aligned}$$

Next we can see that

$$|Q_\infty - P(\widetilde{Q}_\xi(r_\omega^\varepsilon,\omega))| \le |Q_\infty - \widetilde{Q}_{\xi,\eta}(r_\omega^\varepsilon,\omega)| + |\widetilde{Q}_{\xi,\eta}(r_\omega^\varepsilon,\omega) - P(\widetilde{Q}_{\xi,\eta}(r_\omega^\varepsilon,\omega))| \le \sqrt{\alpha\varepsilon} + \varepsilon\,.$$

So looking only at the difference between the bottom right entries, and using that $\varepsilon \le \sqrt{\alpha\varepsilon}$ for small $\varepsilon > 0$,

$$|Q_{\infty,33} - P(\widetilde{Q}_\xi(r_\omega^\varepsilon,\omega))_{33}| \le C\sqrt{\alpha\varepsilon}\,,$$

for some $C > 0$. We can remove the absolute value, maintaining the same inequality and write the left hand side explicitly as,

$$1 - (n_3(\widetilde{Q}_{\xi,\eta}(r_\omega^\varepsilon,\omega)))^2 \le C\sqrt{\alpha\varepsilon}\,.$$

Rearranging this inequality yields

$$|n_3(\widetilde{Q}_{\xi,\eta}(r_\omega^\varepsilon,\omega))| \ge \sqrt{1 - C\sqrt{\alpha\varepsilon}}\,.$$

Thus we have,

$$\eta\widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega),\omega) \ge \sqrt[4]{24}(1-2\varepsilon)^2\Big(\sqrt{1 - C\sqrt{\alpha\varepsilon}} - |n_3(Q_b(\omega))|\Big) - \mathcal{O}\Big(\frac{\xi}{\eta}\Big).$$

In the limit $\xi, \eta \to 0$ it holds that

$$\liminf_{\xi,\eta\to 0} \int_{\mathcal{M}_2^{\delta,\varepsilon}} \eta\widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega),\omega)\,d\omega \ge \int_{M_2^\delta} \sqrt[4]{24}(1-2\varepsilon)^2\Big(\sqrt{1 - C\sqrt{\alpha\varepsilon}} - |n_3(Q_b(\omega))|\Big)\,d\omega\,.$$

Now taking $\varepsilon \to 0$ we have

$$\liminf_{\varepsilon\to 0}\left(\liminf_{\xi,\eta\to 0} \int_{\mathcal{M}_2^{\delta,\varepsilon}} \eta\widetilde{\mathcal{E}}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta}(\cdot,\omega),\omega)\,d\omega\right) \ge \int_{M_2^\delta} \sqrt[4]{24}(1-|n_3(Q_b(\omega))|)\,d\omega = \int_{\mathcal{M}_2^\delta} D_\infty(Q_b(\omega))\,d\omega\,.$$

Finally we can combine the integrals on $\mathcal{M}_1^\delta$ and $\mathcal{M}_2^\delta$ to recover,

$$\liminf_{\varepsilon\to 0}\left(\liminf_{\xi,\eta\to 0} \eta\widetilde{E}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta})\right) \ge \int_{M_d^\delta} D_\infty(Q_b(\omega))\,d\omega\,.$$

Then take $\delta \to 0$ to obtain

$$\liminf_{\delta\to 0}\left(\liminf_{\varepsilon\to 0}\left(\liminf_{\xi,\eta\to 0}\eta\widetilde{E}_{\xi,\eta}(\widetilde{Q}_{\xi,\eta})\right)\right) \geq \int_{\mathcal{M}} D_\infty(Q_b(\omega))\,d\omega\,.$$

To show this lower bound for a measurable subset $U \subset \mathcal{M}$, it is enough that $\chi_{U\cap(\mathcal{M}\setminus\mathcal{M}_b^{\delta,\varepsilon})} \to \chi_{U\cap(\mathcal{M}\setminus\mathcal{M}_d^{\delta})}$ pointwise a.e. as $\xi,\eta \to 0$ and $\chi_{U\cap(\mathcal{M}\setminus\mathcal{M}_d^{\delta})} \to \chi_U$ pointwise a.e. as $\delta \to 0$. Using this along with Fatou's lemma, we obtain the lower bound on the cone $\mathcal{C}_{r_0}(U)$. $\square$

Similarly to what was done in the spherical case, we now want to find a smaller lower bound by choosing Q_b^* to minimize D_∞ at a.e. point on $\mathcal{M}$. To do this, we generalize e_ϕ to the manifold $\mathcal{M}$ by choosing a tangent vector with the property that it maximizes the x_3-component. This can be done by projecting $(\pm)e_3$ onto the tangent space and re-normalizing it, however this method fails when $\nu = \pm e_3$. Recall from (3.1) that $\mathcal{M}_d \subset \mathcal{M}$ is the set where $\nu = \pm e_3$ and that $|\mathcal{M}_d| = 0$ by assumption, then we define

$$v^*(\omega) = \frac{e_3 - \nu_3(\omega)\nu(\omega)}{|e_3 - \nu_3(\omega)\nu(\omega)|}, \quad \text{for} \quad \omega \in \mathcal{M}\setminus\mathcal{M}_d\,.$$

Let $Q_b^* = v^*\otimes v^* - \frac{1}{3}I$, then we have the following lemma.

Proposition 5.6. *Let $\omega \in \mathcal{M}\setminus\mathcal{M}_d$ and let $u \in \mathbb{S}^2$ with $u\cdot\nu(\omega) = 0$. Define $Q_u = u\otimes u - \frac{1}{3}I$, then*

$$D_\infty(Q_u) \geq D_\infty(Q_b^*)\,.$$

Proof. In the proof of Proposition 4.3 we see that if $u_3 \geq 0$, then

$$D_\infty(Q_u) = \sqrt[4]{24}(1-u_3)\,,$$

and we also see that $D_\infty(Q_u) = D_\infty(Q_{-u})$. Therefore, for any $u \in T_\omega\mathcal{M}$ with $|u| = 1$,

$$D_\infty(Q_u) = \sqrt[4]{24}(1-|u_3|)$$

so this quantity is minimized when $|u_3|$ is maximized. Thus, among unit vectors $u \in T_\omega\mathcal{M}$, the maximum of $|u_3|$ occurs precisely when $u = v^*$. $\square$

Using the fact that $\mathcal{M}_d$ is of measure zero, we immediately get the following corollary by combining Theorem 5.1 and Proposition 5.6.

Corollary 5.7. *Let $Q_{\xi,\eta}$ minimize $E_{\xi,\eta}$ with the boundary condition that $Q_{\xi,\eta} = Q_b \in \mathcal{A}_b$ on $\mathcal{M}$. If*

$$\frac{\eta}{\xi} \to \infty \quad as \quad \xi, \eta \to 0\,,$$

then for any measurable subset $U \subset \mathcal{M}$,

$$\liminf_{\xi,\eta\to 0}\ \eta E_{\xi,\eta}(Q_{\xi,\eta}; \mathcal{C}_{r_0}(U)) \geq \int_U D_\infty(Q_b^*(\omega))\, d\omega\,.$$

6 The Upper Bound

In this section we prove the following theorem.

Theorem 6.1. *There exists a sequence of maps* $Q^\delta_{\xi,\eta} \in Q_\infty + H^1(\Omega; \mathrm{Sym}_0)$ *with* $Q^\delta_{\xi,\eta}|_{\mathcal{M}} \in \mathcal{A}_b$ *such that if*

$$\frac{\eta}{\xi} \to \infty \quad as \quad \xi, \eta \to 0\,,$$

then

$$\limsup_{\xi,\eta\to 0}\ \eta E_{\xi,\eta}(Q^\delta_{\xi,\eta}) \leq \int_{\mathcal{M}} D_\infty(Q^*_b(\omega))\, d\omega\,.$$

The proof of this theorem consists of the construction of such a sequence of maps, which in the limit $\xi, \eta \to 0$, attain the minimal lower bound from Theorem 5.1. This is more difficult for a general manifold as the construction need not be equivariant and there are many more cases for the possible defects that can occur.

Proof. We define our competitor sequence to be $Q^\delta_{\xi,\eta} = n^\delta_\xi \otimes n^\delta_\xi - \frac{1}{3}I$, where we will define n^δ_ξ on all of Ω as needed throughout the proof. However, to improve readability, for the rest of the proof we will drop the δ, ξ from n^δ_ξ. We begin by defining $Q^\delta_{\xi,\eta}$ sufficiently far from the manifold by,

$$Q^\delta_{\xi,\eta} = Q_\infty \quad \text{on} \quad \Omega \setminus \mathcal{C}_{2H\eta}(\mathcal{M})$$

for some parameter $H > 1$ independent of ξ. Now let

$$\mathcal{M}^+ = \{\omega \in \mathcal{M} : \nu_3(\omega) > 0\},\ \mathcal{M}^0 = \{\omega \in \mathcal{M} : \nu_3(\omega) = 0\},\ \text{and}\ \mathcal{M}^- = \{\omega \in \mathcal{M} : \nu_3(\omega) < 0\}\,,$$

then we also define

$$Q^\delta_{\xi,\eta} = Q_\infty \quad \text{on} \quad \mathcal{C}_{2H\eta}(\mathcal{M}^0)\,.$$

So it remains to define $Q^\delta_{\xi,\eta}$ on $\mathcal{C}_{2H\eta}(\mathcal{M}^+ \cup \mathcal{M}^-)$. We will detail how to construct $Q^\delta_{\xi,\eta}$ on $\mathcal{C}_{2H\eta}(\mathcal{M}^+)$ and note that the exact same method can be applied to $\mathcal{C}_{2H\eta}(\mathcal{M}^-)$ by simply replacing n_3 by $-n_3$ whenever necessary. However this will have no effect on the estimates for the energy. To begin the construction on $\mathcal{C}_{2H\eta}(\mathcal{M}^+)$, we first define the boundary condition $Q^\delta_b = v \otimes v - \frac{1}{3}I$ on $\mathcal{M}^+$. These boundary values depend on a parameter $\delta > 0$, but have no dependence on η or ξ. In the past we have used the notation $\mathcal{M}_d$ to denote the set of points $\omega \in \mathcal{M}$ where $\nu(\omega) = \pm e_3$, but since we are only considering $\mathcal{M}^+$, we redefine $\mathcal{M}_d$ as

$$\mathcal{M}_d := \{\omega \in \mathcal{M}^+ : \nu(\omega) = e_3\} .$$

Next we take a $\delta-$neighbourhood of $\mathcal{M}_d$, denoted by

$$\mathcal{M}_d^\delta := \{\omega \in \mathcal{M}^+ : \mathrm{dist}_{\mathcal{M}}(\omega, \mathcal{M}_d) < \delta\} .$$

Outside of $\mathcal{M}_d^\delta$, we will set $Q_b^\delta = Q_b^*$, the optimal boundary condition by taking $v = v^*$. $\mathcal{M}_d$ can be decomposed into finitely many connected sets $\mathcal{R}_i$ for $i = 1, \dots, I$ which are all disjoint from one another and by assumption, each $\mathcal{R}_i$ is either an isolated point or a curve of finite length. We can then define the $\delta-$neighbourhood of each $\mathcal{R}_i$ in the usual way, by

$$\mathcal{R}_i^\delta := \{\omega \in \mathcal{M}^+ : \mathrm{dist}_{\mathcal{M}}(\omega, \mathcal{R}_i) < \delta\} ,$$

so this gives us the decomposition of $\mathcal{M}_d^\delta$,

$$\mathcal{M}_d^\delta = \bigcup_{i=1}^{I} \mathcal{R}_i^\delta .$$

This decomposition allows us to define $Q_b^\delta = v \otimes v - \frac{1}{3} I$ on $\mathcal{M}_d^\delta$ by detailing how to choose v on a general $\mathcal{R}_i^\delta$. For $\delta > 0$ sufficiently small, $(\partial \mathcal{R}_i^\delta) \cap \mathcal{M}_d = \emptyset$, so we can define v^* on this boundary and we note that v^* is continuous on $\partial \mathcal{R}_i^\delta$. Due to the continuity of v^*, there exists $z_i \in \mathbb{Z}$ such that,

$$\deg(v^*; \partial \mathcal{R}_i^\delta) = z_i .$$

If $z_i = 0$, then we do not need to define any point defects, otherwise choose $|z_i|-$many points, p_j^i for $j = 1 \dots, |z_i|$, in $\mathcal{R}_i^\delta$. Then for fixed $\delta > 0$, there exist $q_i \in \mathbb{N}$ such that

$$\mathrm{dist}_{\mathcal{M}} \left(B\left(p_j^i, \frac{\delta}{q_i}\right), \partial \mathcal{R}_i^\delta \right) > 0 \quad \text{and} \quad \mathrm{dist}_{\mathcal{M}} \left(B\left(p_j^i, \frac{\delta}{q_i}\right), B\left(p_k^i, \frac{\delta}{q_i}\right) \right) > 0 ,$$

for all $j, k = 1, \dots, |z_i|$. Note that since there are finitely many points p_i^j the distance between each ball as well as the distance from a ball to the boundary are both bounded below by a positive constant which depends on δ.

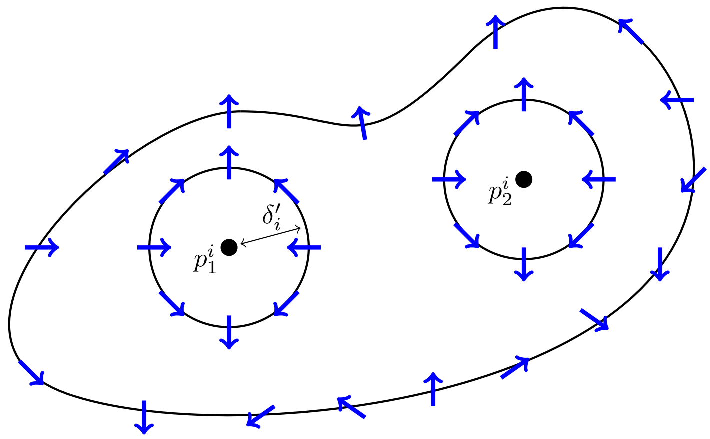

Figure 4: Top view of $\mathcal{R}_i^\delta$ with point defects for $z_i = -2$ and v on the boundary (blue).

For simplicity we let $\delta_i' = \delta/q_i$ moving forwards. On each ball $\overline{B(p_j^i, \delta_i')}$ we define a point defect of degree $\operatorname{sgn}(z_i)$ as follows. Let $\widetilde{m} : \overline{B(0,1)} \subset \mathbb{R}^2 \to \mathbb{R}^3$ be

$$\widetilde{m}(v) = (v_1, \operatorname{sgn}(z_i) v_2, 0)\,,$$

so $\widetilde{m}$ could be either a $+1$ defect or a -1 defect. We then move $\widetilde{m}$ to the manifold $\mathcal{M}$ via $\omega = \exp_{p_j^i}(\delta_i' v)$, so we can define $m : \overline{B(p_j^i, \delta_i')} \to \mathbb{R}^3$ by

$$m(\omega) = \widetilde{m}\left(\frac{1}{\delta_i'} \exp_{p_j^i}^{-1}(\omega)\right)\,.$$

We note that $m(\omega)$ is not necessarily in $T_\omega\mathcal{M}$ unless $\nu(\omega) = e_3$, so to fix this, we project m onto the tangent space and re-scale to unit length by defining $\widehat{u} : \overline{B(p_j^i, \delta_i')} \to \mathbb{S}^2$ to be

$$\widehat{u}(\omega) = \frac{m(\omega) - (m(\omega)\cdot\nu(\omega))\nu(\omega)}{|m(\omega) - (m(\omega)\cdot\nu(\omega))\nu(\omega)|}\,. \tag{6.1}$$

Now on $\overline{B(p_j^i, \delta_i')}$ we let $v = \widehat{u}$, so

$$\deg(v; B(p_j^i, \delta_i')) = \operatorname{sgn}(z_i)\,.$$

We also let $v = v^*$ on $\partial\mathcal{R}_i^\delta$ and therefore, by construction,

$$\deg\left(v; \partial\left(\mathcal{R}_i^\delta \setminus \bigcup_{j=1}^{|z_i|} B(p_j^i, \delta_i')\right)\right) = 0\,.$$

Using Theorem 1.8 from [10, p.126], there exists a continuous extension $v_0 : \overline{\mathcal{R}_i^\delta \setminus \bigcup_{j=1}^{|z_i|} B(p_j^i, \delta')} \to \mathbb{S}^2$ which agrees with v on the boundary. Let $\varepsilon > 0$ be small, then by Theorem 10.16 from [11] there exists a C^1 function $v_\varepsilon : \overline{\mathcal{R}_i^{2\delta} \setminus \bigcup_{j=1}^{|z_i|} B(p_j^i, \delta_i'/2)} \to \mathbb{R}^3$ such that

$$|v_0(\omega) - v_\varepsilon(\omega)| < \varepsilon, \quad \text{for} \quad \omega \in \mathcal{R}_i^\delta \setminus \bigcup_{j=1}^{|z_i|} B(p_j^i, \delta_i')$$

and v_ε agrees with v^* on $\overline{\mathcal{R}_i^{2\delta} \setminus \mathcal{R}_i^\delta}$ as well as $\widehat{u}$ on $\overline{\bigcup_{j=1}^{|z_i|}(B(p_j^i, \delta_i') \setminus B(p_j^i, \delta_i'/2))}$. This definition ensures that the derivative of v_ε also agrees with v^* and u on their respective boundaries, so this is in fact a C^1 extension. Since $v_\varepsilon \in \mathbb{R}^3$, and need not be tangent to $\mathcal{M}$, we again need to project into the tangent space of $\mathcal{M}$ and re-normalize the vector field, so we define

$$v(\omega) = \frac{v_\varepsilon(\omega) - (v_\varepsilon(\omega) \cdot \nu(\omega))\nu(\omega)}{|v_\varepsilon(\omega) - (v_\varepsilon(\omega) \cdot \nu(\omega))\nu(\omega)|}, \quad \text{for} \quad \omega \in \mathcal{R}_i^\delta \setminus \bigcup_{j=1}^{|z_i|} B(p_j^i, \delta')\,.$$

Now that v has been chosen on all of $\mathcal{M}^+$ we can proceed to define n and hence $Q_{\xi,\eta}^\delta$ on $\mathcal{C}_{2H\eta}(\mathcal{M}^+)$. In order to do this we define the following sub-regions:

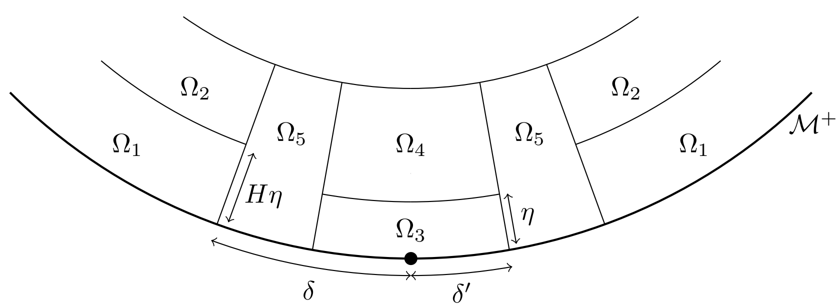

Figure 5: A cross-section of the sub-regions of $\mathcal{C}_{2H\eta}(\mathcal{M}^+)$ around a point defect of degree +1 with negative mean curvature.

Recall that $Q_{\xi,\eta}^\delta = n \otimes n - \frac{1}{3}I$ so we want to define n on $\mathcal{C}_{2H\eta}(\mathcal{M}^+)$, such that $n(0, \omega) = v(\omega)$. The first sub-region we consider is the set where we expect the energy to concentrate, i.e. a boundary layer of thickness $H\eta$, away from potential defects. In this layer we would like to take the director n to have the same energy as the optimal profile n^* from Lemma 4.4, but since the transition for n^* takes place over an infinite length, the optimal profile needs to be modified similar to [2, Proposition 6.8] to fit into a finite length while preserving the energy bound. Therefore, we introduce two layers:

$$\Omega_1 \ := \ \mathcal{C}_{H\eta}(\mathcal{M}^+ \setminus \mathcal{M}_d^\delta)\,,$$

in which we take the optimal profile, and a corresponding outer region

$$\Omega_2 \ := \ \mathcal{C}_{2H\eta}(\mathcal{M}^+ \setminus \mathcal{M}_d^\delta) \setminus \overline{\Omega_1}\,,$$

in which we interpolate to make the transition to Q_∞. This transition has asymptotically negligible energetic cost. Next, we have the sub-region where point defects occur, given by

$$\Omega_3 := \mathcal{C}_\eta\left(\bigcup_{i=1}^{I}\bigcup_{j=1}^{|z_i|} B(p_j^i, \delta_i')\right)\,.$$

In these sub-regions we define n to be defects of degree $+1$ or -1 depending on $\operatorname{sgn}(z_i)$ for each region $\mathcal{R}_i$. Next we consider

$$\Omega_4 := \mathcal{C}_{2H\eta}\left(\bigcup_{i=1}^{I}\bigcup_{j=1}^{|z_i|} B(p_j^i, \delta_i')\right) \setminus \overline{\Omega_3}\,,$$

where we again define n by an interpolation to e_3. This allows us to extend n from Ω_3 to the exterior region while having no energetic cost in the limit. Finally, we let

$$\Omega_5 := \mathcal{C}_{2H\eta}(\mathcal{M}_d^\delta) \setminus \overline{\Omega_3 \cup \Omega_4}\,.$$

Here we define n via a Lipschitz extension from the boundary of the region. Note that in the spherical case, the analogues of Ω_4 and Ω_5 were combined and we were able to do a Lipschitz extension on their union, however on the general manifold, we lose equivariance and we have more complicated geometry, so this extra region makes it much easier to control the energy. However, as in the spherical case, we will still see that the energy in all regions but Ω_1 will be negligible in the limit $\xi, \eta \to 0$.

<u>*Energy in* Ω_1</u>: Recall $\Omega_1 = \mathcal{C}_{H\eta}(\mathcal{M}^+ \setminus \mathcal{M}_d^\delta)$ on which we define

$$n(r,\omega) \;=\; R_\omega n^*\Big(\frac{r}{\eta}, \varphi(\omega)\Big)\,,$$

where $\varphi(\omega) = \cos^{-1}(v_3(\omega))$, R_ω is the rotation matrix given by

$$R_\omega \;=\; \begin{pmatrix} \frac{\nu_1}{\sqrt{1-\nu_3^2}} & \frac{-\nu_2}{\sqrt{1-\nu_3^2}} & 0 \\ \frac{\nu_2}{\sqrt{1-\nu_3^2}} & \frac{\nu_1}{\sqrt{1-\nu_3^2}} & 0 \\ 0 & 0 & 1 \end{pmatrix}\,,$$

and n^* is the minimizing energy profile from Lemma 4.4 given by

$$n^*(r,\varphi) = \Big(-\sqrt{1-(n_3^*(r,\varphi))^2}, 0, n_3^*(r,\varphi)\Big)\,.$$

Here,

$$n_3^*(r,\varphi) \;=\; \frac{A(\varphi) - e^{-\sqrt[4]{24}r}}{A(\varphi) + e^{-\sqrt[4]{24}r}} \quad \text{and} \quad A(\varphi) \;=\; \frac{1+\cos\varphi}{1-\cos\varphi}\,.$$

for φ being the angle between $v(\omega)$ and e_3. Since n^* stays in the x_1x_3-plane, we use R_ω to rotate n^* so that $Q^\delta_{\xi,\eta}(0,\omega) = Q_b^*(\omega)$ for all $\omega \in \mathcal{M}^+ \setminus \mathcal{M}_d^\delta$. In defining n this way, we ensure that

$$G_\infty(n(\cdot,\omega)) \;=\; G_\infty(n^*(\cdot,\varphi(\omega))) \;=\; D_\infty(Q_b^*(\omega))\,.$$

After defining $Q^\delta_{\xi,\eta}$ on Ω_1, we now show the required energy bounds on this region. First note that

$$\begin{aligned} \eta E_{\xi,\eta}(Q^\delta_{\xi,\eta};\Omega_1) \;&=\; \int_{\mathcal{M}^+\setminus\mathcal{M}_d^\delta}\int_0^{H\eta} \eta\left(\frac{1}{2}|\nabla Q^\delta_{\xi,\eta}|^2 + \frac{1}{\eta^2}g(Q^\delta_{\xi,\eta})\right)\prod_{i=1}^2(1+r\kappa_i)\,drd\omega \\ &=\; \int_{\mathcal{M}^+\setminus\mathcal{M}_d^\delta}\int_0^{H\eta} \eta\left(|\nabla n|^2 + \frac{1}{\eta^2}g(n)\right)\prod_{i=1}^2(1+r\kappa_i)\,drd\omega\,. \end{aligned}$$

We can estimate $|\nabla n|^2$ as

$$|\nabla n|^2 = \left|\frac{\partial n}{\partial r}\right|^2 + \frac{1}{(1+r|\kappa_1|)^2}\left|\frac{\partial n}{\partial \omega_1}\right|^2 + \frac{1}{(1+r|\kappa_2|)^2}\left|\frac{\partial n}{\partial \omega_2}\right|^2 \le \left|\frac{\partial n}{\partial r}\right|^2 + |\nabla_\omega n|^2\,.$$

So we split the energy into two parts: the first one which turns into D_∞ and a second one that contains the tangential derivatives and vanishes asymptotically. More precisely, we write

$$\eta E_{\xi,\eta}(Q^\delta_{\xi,\eta};\Omega_1) \le \int_{\mathcal{M}^+\setminus\mathcal{M}^\delta_d}\int_0^{H\eta} \eta\left(\left|\frac{\partial n}{\partial r}\right|^2 + \frac{1}{\eta^2}g(n)\right)\prod_{i=1}^2(1+r\kappa_i)\,drd\omega \\ + \int_{\mathcal{M}^+\setminus\mathcal{M}^\delta_d}\int_0^{H\eta} \eta|\nabla_\omega n|^2\prod_{i=1}^2(1+r\kappa_i)\,drd\omega\,. \tag{6.2}$$

The change of variables $\tilde{r} = \frac{r}{\eta}$ in the first integral gives

$$\int_{\mathcal{M}^+\setminus\mathcal{M}^\delta_d}\int_0^{H\eta} \eta\left(\left|\frac{\partial n}{\partial r}\right|^2 + \frac{1}{\eta^2}g(n)\right)\prod_{i=1}^2(1+r\kappa_i)\,drd\omega \\ = \int_{\mathcal{M}^+\setminus\mathcal{M}^\delta_d}\int_0^{H} \left(\left|\frac{\partial n^*}{\partial \tilde{r}}\right|^2 + g(n^*)\right)\prod_{i=1}^2(1+\eta\tilde{r}\kappa_i)\,d\tilde{r}d\omega\,.$$

Since $1+\eta\tilde{r}\kappa_i \to 1$ pointwise as $\xi,\eta\to 0$, it holds

$$\limsup_{\xi,\eta\to 0}\int_{\mathcal{M}^+\setminus\mathcal{M}^\delta_d}\int_0^{H\eta} \eta\left(\left|\frac{\partial n}{\partial r}\right|^2 + \frac{1}{\eta^2}g(n)\right)\prod_{i=1}^2(1+r\kappa_i)\,drd\omega \\ \le \int_{\mathcal{M}^+\setminus\mathcal{M}^\delta_d}\int_0^{\infty} \left(\left|\frac{\partial n^*}{\partial \tilde{r}}\right|^2 + g(n^*)\right)\,d\tilde{r}d\omega \\ = \int_{\mathcal{M}^+\setminus\mathcal{M}^\delta_d} D_\infty(Q^*_b(\omega))\,d\omega\,.$$

For the second integral from (6.2), it suffices to bound $|\nabla_\omega n|$ by a constant which is independent of η, since

$$\int_{\mathcal{M}^+\setminus\mathcal{M}^\delta_d}\int_0^{H\eta} \eta|\nabla_\omega n|^2\prod_{i=1}^2(1+r\kappa_i)\,drd\omega \;\le\; \int_{\mathcal{M}^+\setminus\mathcal{M}^\delta_d}\int_0^{H\eta} C\eta|\nabla_\omega n|^2\,drd\omega\,.$$

We have that $n(r,\omega) = R_\omega n^*(r,\varphi(\omega))$, so by product rule and chain rule

$$\frac{\partial n}{\partial \omega_i} = \Big(\frac{\partial R_\omega}{\partial \omega_i}\Big)n^* + R_\omega\Big(\frac{\partial n^*}{\partial\varphi}\Big)\Big(\frac{\partial\varphi}{\partial\omega_i}\Big)\,,$$

for $i = 1, 2$. Therefore,

$$\begin{aligned} \left|\frac{\partial n}{\partial \omega_i}\right|^2 &\le \left|\Big(\frac{\partial R_\omega}{\partial \omega_i}\Big) n^*\right|^2 + 2\left|\Big(\frac{\partial R_\omega}{\partial \omega_i}\Big) n^*\right| \left|R_\omega \Big(\frac{\partial n^*}{\partial \varphi}\Big)\Big(\frac{\partial \varphi}{\partial \omega_i}\Big)\right| + \left|R_\omega \Big(\frac{\partial n^*}{\partial \varphi}\Big)\Big(\frac{\partial \varphi}{\partial \omega_i}\Big)\right|^2 \\ &\le \left|\frac{\partial R_\omega}{\partial \omega_i}\right|^2 + 2\left|\frac{\partial R_\omega}{\partial \omega_i}\right|\left|\frac{\partial n^*}{\partial \varphi}\right|\left|\frac{\partial \varphi}{\partial \omega_i}\right| + \left|\frac{\partial n^*}{\partial \varphi}\right|^2\left|\frac{\partial \varphi}{\partial \omega_i}\right|^2 . \end{aligned}$$

Hence we can bound $|\nabla_\omega n|^2$ as follows

$$|\nabla_\omega n|^2 \;\le\; |\nabla_\omega R_\omega|^2 + 4|\nabla_\omega R_\omega|\left|\frac{\partial n^*}{\partial \varphi}\right| |\nabla_\omega \varphi| + \left|\frac{\partial n^*}{\partial \varphi}\right|^2 |\nabla_\omega \varphi|^2 .$$

From Lemma 4.4,

$$\left|\frac{\partial n^*}{\partial \varphi}\right|^2 \le C e^{-\sqrt[4]{24}\frac{r}{\eta}} \le C .$$

For the gradient of the rotation matrix we find

$$\begin{aligned} \left|\frac{\partial R_\omega}{\partial \omega_i}\right| \;\le\; & \left|\frac{\partial}{\partial \omega_i}\left(\frac{1}{\sqrt{1-\nu_3^2}}\right)\right| \left|\begin{pmatrix} \nu_1 & -\nu_2 & 0 \\ \nu_2 & \nu_1 & 0 \\ 0 & 0 & \sqrt{1-\nu_3^2} \end{pmatrix}\right| \\ & + \left(\frac{1}{\sqrt{1-\nu_3^2}}\right) \left|\frac{\partial}{\partial \omega_i}\begin{pmatrix} \nu_1 & -\nu_2 & 0 \\ \nu_2 & \nu_1 & 0 \\ 0 & 0 & \sqrt{1-\nu_3^2} \end{pmatrix}\right| , \end{aligned}$$

so by a direct computation it follows that

$$\left|\frac{\partial R_\omega}{\partial \omega_i}\right| \;\le\; \left|\frac{\partial \nu_3}{\partial \omega_i}\right| \left|\frac{\nu_3}{\sqrt{1-\nu_3^2}^3}\right| \sqrt{3(1-\nu_3^2)} + \left(\frac{1}{\sqrt{1-\nu_3^2}}\right) \frac{\sqrt{2}}{\sqrt{1-\nu_3^2}} \left|\frac{\partial \nu}{\partial \omega_i}\right| \;\le\; \left|\frac{\partial \nu}{\partial \omega_i}\right| \left(\frac{C}{1-\nu_3^2}\right) ,$$

for some constant $C > 0$. We can choose $0 < C_\delta < 1$ such that $\nu_3^2 \le C_\delta$ on $\mathcal{M} \setminus \mathcal{M}_d^\delta$, since this is a compact set and $\nu_3 \ne 1$ on that region. Thus,

$$|\nabla_\omega R_\omega|^2 \le |\nabla_\omega \nu|^2 \left(\frac{C}{(1-\nu_3^2)^2}\right) \le \frac{C\kappa^2}{(1-C_\delta)^2} .$$

Next, using the fact that $\cos(\varphi(\omega)) = v_3(\omega)$, we have

$$\frac{\partial \varphi}{\partial \omega_i} = \left(\frac{-1}{\sin\varphi}\right)\frac{\partial v_3}{\partial \omega_i} = \left(\frac{-1}{\sqrt{1-v_3^2}}\right)\frac{\partial v_3}{\partial \omega_i}\,.$$

In Lemma 3.4 of [1], it is shown that if $|n| = 1$, then

$$\frac{|\dot{n_3}|^2}{1-n_3^2} \leq |\dot{n}|^2\,, \tag{6.3}$$

so we apply this lemma to obtain the estimate

$$\left|\frac{\partial \varphi}{\partial \omega_i}\right|^2 \leq \frac{1}{1-v_3^2}\left|\frac{\partial v_3}{\partial \omega_i}\right|^2 \leq \left|\frac{\partial v}{\partial \omega_i}\right|^2\,.$$

Therefore

$$|\nabla_\omega \varphi|^2 \leq |\nabla_\omega v|^2 \leq C$$

since $v = v^*$ in this region and v^* is smooth on $\mathcal{M}^+ \setminus \mathcal{M}_d$. Finally we can bound $|\nabla_\omega n|^2$ by

$$|\nabla_\omega n|^2 \leq \frac{C\kappa^2}{(1-C_\delta)^2} + \frac{C\kappa^2}{\sqrt{1-C_\delta}^3} + \frac{C\kappa^2}{1-C_\delta} =: C_{\delta,\kappa}\,, \tag{6.4}$$

so the second integral from (6.2) has the bound

$$\begin{aligned}\int_{\mathcal{M}^+\setminus\mathcal{M}_d^\delta}\int_0^{H\eta}\eta|\nabla_\omega n|^2\prod_{i=1}^{2}(1+r\kappa_i)\,dr d\omega &\leq C\eta\int_{\mathcal{M}^+\setminus\mathcal{M}_d^\delta}\int_0^{H\eta} C_{\delta,\kappa}\,drd\omega\\ &\leq CH\eta^2|\mathcal{M}^+\setminus\mathcal{M}_d^\delta|C_{\delta,\kappa}\end{aligned}$$

which vanishes in the limit as $\xi,\eta \to 0$. Therefore we obtain the upper bound

$$\limsup_{\delta\to 0}\left(\limsup_{\xi,\eta\to 0}\eta E_{\xi,\eta}(Q^\delta_{\xi,\eta};\Omega_1)\right) \leq \int_{\mathcal{M}^+\setminus\mathcal{M}_d} D_\infty(Q_b^*(\omega))\,d\omega\,.$$

Energy in Ω_2: Next we consider the outer layer $\Omega_2 = \mathcal{C}_{2H\eta}(\mathcal{M}^+\setminus\mathcal{M}_d^\delta)\setminus\overline{\Omega_1}$ where we define n by interpolating the angle between n and e_3 from $\cos^{-1}(n_3^*(H,\varphi(\omega))$ to 0 as r goes from $H\eta$ to $2H\eta$. Let R_ω be the rotation matrix from Ω_1, then we define

$$n(r,\omega) = R_\omega(-\sin\Phi(r,\omega), 0, \cos\Phi(r,\omega))$$

where

$$\Phi(r,\omega) = \Big(2 - \frac{r}{H\eta}\Big)\Phi_0(\omega)$$

for $\Phi_0(\omega) = \cos^{-1}(n_3^*(H,\varphi(\omega)))$. By choosing Φ and Φ_0 in this way, $n(H\eta,\omega) = R_\omega n^*(H,\varphi(\omega))$ and $n(2H\eta,\omega) = e_3$, so it is a continuous extension from Ω_1 to the exterior of $\mathcal{C}_{2H\eta}(\mathcal{M})$. The energy in this region is given by

$$\eta E_{\xi,\eta}(Q^\delta_{\xi,\eta};\Omega_2) = \int_{\mathcal{M}^+\setminus\mathcal{M}^\delta_d}\int_{H\eta}^{2H\eta}\Big(\eta|\nabla n|^2 + \frac{1}{\eta}g(n)\Big)\prod_{i=1}^{2}(1+r\kappa_i)\,drd\omega\,.$$

We obtain estimates on $|\nabla n|^2$ by considering the radial and tangential derivatives separately:

$$\left|\frac{\partial n}{\partial r}\right|^2 = \left|\frac{\partial \Phi}{\partial r}\right|^2 = \frac{1}{H^2\eta^2}|\Phi_0|^2 \le \frac{C}{H^2\eta^2}\,.$$

Using product rule and chain rule, we have

$$\frac{\partial n}{\partial \omega_i} = \Big(\frac{\partial R_\omega}{\partial \omega_i}\Big)(-\sin\Phi(r,\omega),0,\cos\Phi(r,\omega)) + R_\omega\Big(\frac{\partial \Phi}{\partial\omega_i}\Big)(-\cos\Phi(r,\omega),0,-\sin\Phi(r,\omega))\,,$$

for $i = 1,2$. So,

$$\left|\frac{\partial n}{\partial \omega_i}\right| \le \left|\frac{\partial R_\omega}{\partial \omega_i}\right| + \left|\frac{\partial \Phi}{\partial \omega_i}\right|\,,$$

and

$$|\nabla_\omega n|^2 \le |\nabla_\omega R_\omega|^2 + 4|\nabla_\omega R_\omega||\nabla_\omega\Phi| + |\nabla_\omega \Phi|^2\,.$$

We already have an estimate for $|\nabla_\omega R_\omega|^2$ from Ω_1, namely $|\nabla_\omega R_\omega|^2 \le C_{\delta,\kappa}$, so it suffices to estimate $|\nabla_\omega\Phi|^2$ appropriately.

$$\left|\frac{\partial \Phi}{\partial \omega_i}\right|^2 = \Big(2 - \frac{r}{H\eta}\Big)^2\left|\frac{\partial \Phi_0}{\partial \omega_i}\right|^2 \le \left|\frac{\partial \Phi_0}{\partial \omega_i}\right|^2 = \frac{1}{1-n_3^2}\left|\frac{\partial n_3}{\partial \omega_i}(H\eta,\cdot)\right|^2\,,$$

for $i = 1,2$. Again using (6.3) and the estimates from Ω_1,

$$\left|\frac{\partial \Phi}{\partial \omega_i}\right|^2 \le \left|\frac{\partial n}{\partial \omega_i}(H\eta,\cdot)\right|^2 = \Big|\nabla_\omega\Big(R_\omega n^*(H,\varphi(\cdot))\Big)\Big|^2 \le C_{\delta,\kappa}\,,$$

therefore $|\nabla_\omega \Phi|^2 \le 2C_{\delta,\kappa}$. Using this we have, $|\nabla_\omega n|^2 \le \widetilde{C}_{\delta,\kappa}$ for some constant $\widetilde{C}_{\delta,\kappa} > 0$ which depends on δ and κ. Next,

$$g(n) = \sqrt{\frac{3}{2}}(1-n_3^2) = \sqrt{\frac{3}{2}}(1-\cos^2\Phi) = \sqrt{\frac{3}{2}}\sin^2\Phi\,.$$

But $\sin^2\Phi$ is largest when $r = H\eta$, thus $\sin^2\Phi \leq \sin^2\Phi_0$. By definition of Φ_0,

$$\sin\Phi_0(\omega) = \sqrt{1-(n_3^*(H,\omega))^2} = |n_1^*(H,\omega)|\,.$$

Then using Lemma 4.4,

$$g(n) \leq Ce^{-\sqrt[4]{24}H}\,.$$

We can combine all of these estimates to show that

$$\begin{aligned}
\eta E_{\xi,\eta}(Q_{\xi,\eta}^{\delta};\Omega_2) \leq \int_{\mathcal{M}^+\setminus\mathcal{M}_d^{\delta}}\int_{H\eta}^{2H\eta}\eta\left(\frac{C}{H^2\eta^2}+C_{\delta,\kappa}+\frac{C}{\eta^2}e^{-\sqrt[4]{24}H}\right)drd\omega \\
\leq \int_{\mathcal{M}^+\setminus\mathcal{M}_d^{\delta}}\int_{H}^{2H}\left(\frac{C}{H^2}+C_{\delta,\kappa}\eta^2+Ce^{-\sqrt[4]{24}H}\right)d\tilde{r}d\omega \\
= H|\mathcal{M}^+\setminus\mathcal{M}_d^{\delta}|\Big(\frac{C}{H^2}+C_{\delta,\kappa}\eta^2+Ce^{-\sqrt[4]{24}H}\Big)\,.
\end{aligned}$$

We then take the following limits,

$$\limsup_{\xi,\eta\to 0}\eta E_{\xi,\eta}(Q_{\xi,\eta}^{\delta};\Omega_2) \leq |\mathcal{M}^+\setminus\mathcal{M}_d^{\delta}|\Big(\frac{C}{H}+CHe^{-\sqrt[4]{24}H}\Big)\,.$$

Next, taking $\delta\to 0$, we have,

$$\limsup_{\delta\to 0}\left(\limsup_{\xi,\eta\to 0}\eta E_{\xi,\eta}(Q_{\xi,\eta}^{\delta};\Omega_2)\right) \leq |\mathcal{M}^+\setminus\mathcal{M}_d|\Big(\frac{C}{H}+CHe^{-\sqrt[4]{24}H}\Big)\,.$$

Finally we take $H\to\infty$ to see that the energy in this region vanishes.

$$\limsup_{H\to\infty}\left(\limsup_{\delta\to 0}\left(\limsup_{\xi,\eta\to 0}\eta E_{\xi,\eta}(Q_{\xi,\eta}^{\delta};\Omega_2)\right)\right) = 0\,.$$

Energy in Ω_3: Recall that Ω_3 is the region around point defects of Q_b^δ,

$$\Omega_3 := \mathcal{C}_\eta\left(\bigcup_{i=1}^{I}\bigcup_{j=1}^{|z_i|} B(p_j^i,\delta_i')\right).$$

We estimate the energy around an arbitrary point defect, $p = p_j^i$ for some $i \in \{1,\dots,I\}$ and $j \in \{1,\dots,|z_i|\}$ and we drop the indices i,j on all related quantities to improve readability. We consider the region $\mathcal{C}_\eta(B(p,\delta'))$. First define $u : B(p,\delta') \to \mathbb{R}^3$ by

$$u(\omega) = \mathrm{dist}_{\mathcal{M}}(\omega,p)\widehat{u}(\omega)\,,$$

where $\widehat{u}$ is given as in (6.1). Then we define the vector field $n : (0,\eta)\times B(p,\delta') \to \mathbb{S}^2$ by

$$n(r,\omega) = \frac{u(\omega)+r\nu(\omega)}{|u(\omega)+r\nu(\omega)|}\,.$$

Now that we have defined n, we estimate its energy

$$\eta E_{\xi,\eta}(Q_{\xi,\eta}^\delta;\mathcal{C}_\eta(B(p,\delta'))) = \int_{B(p,\delta')}\int_0^\eta \left(\eta|\nabla n|^2 + \frac{1}{\eta}g(n)\right)\prod_{i=1}^{2}(1+r\kappa_i)\,drd\omega\,.$$

We can compute the radial derivative of n to be

$$\frac{\partial n}{\partial r} = \frac{\nu|u+r\nu|^2 - (u+r\nu)[(u+r\nu)\cdot\nu)]}{|u+r\nu|^3}\,.$$

So we can estimate its norm from above by

$$\left|\frac{\partial n}{\partial r}\right| \le \frac{|u+r\nu|^2 + |u+r\nu||(u+r\nu)\cdot\nu|}{|u+r\nu|^3} \le \frac{2}{|u+r\nu|}\,.$$

Using that $u \perp \nu$, we can write $|u+r\nu| = \sqrt{|u|^2+|r\nu|^2} = \sqrt{|u|^2+r^2}$, so

$$\left|\frac{\partial n}{\partial r}\right|^2 \le \frac{C}{|u|^2+r^2} = \frac{1}{\eta^2}\left(\frac{C}{|v|^2+h^2}\right)\,, \tag{6.5}$$

since $r=\eta h$ and $|\exp_p^{-1}(\omega)| = \delta'|v|$ by definition and since $\eta<\delta'$. Next we consider the tangential derivatives of n. Let $k = 1, 2$, then

$$\frac{\partial n}{\partial \omega_k} = \frac{(\frac{\partial u}{\partial \omega_k} + r\frac{\partial \nu}{\partial \omega_k})|u + r\nu|^2 - (u + r\nu)[(u + r\nu) \cdot (\frac{\partial u}{\partial \omega_k} + r\frac{\partial \nu}{\partial \omega_k})]}{|u + r\nu|^3}$$

so we can estimate the norm by

$$\left|\frac{\partial n}{\partial \omega_k}\right| \leq \frac{C|\frac{\partial u}{\partial \omega_k} + r\frac{\partial \nu}{\partial \omega_k}|}{|u + r\nu|} \leq C\left(\frac{|\frac{\partial u}{\partial \omega_k}| + |\frac{\partial \nu}{\partial \omega_k}|}{\sqrt{(\delta')^2|v|^2 + \eta^2 h^2}}\right). \tag{6.6}$$

Since $|\nabla_\omega \nu| \leq \sqrt{2}\kappa$, it suffices to bound $|\frac{\partial u}{\partial \omega_k}|$.

$$\frac{\partial u}{\partial \omega_k} = \left(\frac{\partial}{\partial \omega_k}\mathrm{dist}_{\mathcal{M}}(\omega, p)\right)\widehat{u}(\omega) + \mathrm{dist}_{\mathcal{M}}(\omega, p)\left(\frac{\partial \widehat{u}}{\partial \omega_k}\right).$$

Therefore,

$$\left|\frac{\partial u}{\partial \omega_k}\right| \leq \left|\frac{\partial}{\partial \omega_k}\mathrm{dist}_{\mathcal{M}}(\omega, p)\right| + \delta'|v|\left|\frac{\partial \widehat{u}}{\partial \omega_k}\right| \leq C + \delta'|v|\left|\frac{\partial \widehat{u}}{\partial \omega_k}\right|$$

Next, using the definition of $\widehat{u}$ from (6.1),

$$\frac{\partial \widehat{u}}{\partial \omega_k} = \frac{\left(\frac{\partial}{\partial \omega_k}(m - (m \cdot \nu)\nu)\right)}{|m - (m \cdot \nu)\nu|} - \frac{(m - (m \cdot \nu)\nu)\Big((m - (m \cdot \nu)\nu) \cdot \big(\frac{\partial}{\partial \omega_k}(m - (m \cdot \nu)\nu)\big)\Big)}{|m - (m \cdot \nu)\nu|^2},$$

so,

$$\left|\frac{\partial \widehat{u}}{\partial \omega_k}\right| \leq \frac{2|\frac{\partial}{\partial \omega_k}(m - (m \cdot \nu)\nu)|}{|m - (m \cdot \nu)\nu|} \leq \frac{C(|\frac{\partial m}{\partial \omega_k}| + |\frac{\partial \nu}{\partial \omega_k}|)}{|m| - |m \cdot \nu|} = \frac{C(|\frac{\partial m}{\partial \omega_k}| + \sqrt{2}\kappa)}{|m|(1 - |\cos\theta|)},$$

where θ is the angle between m and ν. Since ν is close to $\pm e_3$ and $m \cdot e_3 = 0$, there exists a constant $C > 0$ such that $1 - |\cos\theta| \geq C$ for all $\omega \in B(p, \delta')$. Together with $|m| = |v|$ this implies

$$\left|\frac{\partial \widehat{u}}{\partial \omega_k}\right| \leq C|v|^{-1}\left(|\nabla_\omega m| + \sqrt{2}\kappa\right).$$

Computing $\nabla_\omega m$, we have

$$\nabla_\omega m = \nabla_v \widetilde{m} \cdot \nabla_\omega((\delta')^{-1}\exp_p^{-1}(\omega)),$$

therefore $|\nabla_\omega m| \leq C(\delta')^{-1}$ and

$$\left|\frac{\partial u}{\partial \omega_k}\right| \leq C + \delta'|v|\left(\frac{C}{\delta'|v|}\right) \leq C\,. \tag{6.7}$$

So, putting together (6.6) and (6.7), we can see that,

$$|\nabla_\omega n|^2 \leq \frac{C}{(\delta')^2|v|^2 + \eta^2 h^2} \leq \frac{C}{\eta^2}\left(\frac{1}{|v|^2 + h^2}\right)\,. \tag{6.8}$$

Finally, we note that $g(n) \leq C$ for some $C > 0$, thus the energy can be estimated by

$$\eta E_{\xi,\eta}(Q^\delta_{\xi,\eta}; \mathcal{C}_\eta(B(p,\delta'))) \leq \int_{B(0,1)}\int_0^1 \left(\frac{(\delta')^2}{(|v|^2+h^2)} + C(\delta')^2\right)|D\exp_p|\;dh\,dv\,.$$

The exponential map is C^1 near 0, so its Jacobian $|D\exp_p|$ is bounded. Thus we integrate to obtain the estimate

$$\eta E_{\xi,\eta}(Q^\delta_{\xi,\eta}; \mathcal{C}_\eta(B(p,\delta'))) \leq C(\delta')^2\,,$$

and

$$\limsup_{\delta\to 0}\left(\limsup_{\xi,\eta\to 0}\eta E_{\xi,\eta}(Q^\delta_{\xi,\eta}; \mathcal{C}_\eta(B(p,\delta')))\right) = 0\,.$$

This holds for each point p^i_j, therefore,

$$\limsup_{\delta\to 0}\left(\limsup_{\xi,\eta\to 0}\eta E_{\xi,\eta}(Q^\delta_{\xi,\eta}; \Omega_3)\right) = 0\,.$$

Energy in Ω_4: On this region, we do an interpolation of the angle between n and e_3, to continuously extend n from Ω_3 to the exterior region. First, choose any p^i_j as we did in Ω_3, then define

$$\Omega_4^{i,j} = \mathcal{C}_{2H\eta}(B(p^i_j,\delta'_i)) \setminus \overline{\mathcal{C}_\eta(B(p^i_j,\delta'_i))}$$

so that $\Omega_4 = \bigcup_{i=1}^{I}\bigcup_{j=1}^{|z_i|}\Omega_4^{i,j}$. Again we will let $p = p^i_j$ and drop the indices i, j wherever needed to improve readability. Now define $\overline{v} : B(p,\delta') \to \mathbb{S}^2$ by

$$\overline{v}(\omega) = \frac{u(\omega) + \eta\nu(\omega)}{|u(\omega) + \eta\nu(\omega)|}\,,$$

and the interpolation $\Phi : (\eta, 2H\eta) \times B(p, \delta') \to [0, \pi]$ by,

$$\Phi(r, \omega) = \left(1 - \frac{r - \eta}{2H\eta - \eta}\right) \Phi_0(\omega) \,,$$

where $\Phi_0(\omega) = \cos^{-1}(\overline{v}_3(\omega))$. Finally we let

$$n(r, \omega) = \left(\frac{\overline{v}_1(\omega) \sin \Phi(r, \omega)}{\sqrt{1 - (\overline{v}_3(\omega))^2}}, \frac{\overline{v}_2(\omega) \sin \Phi(r, \omega)}{\sqrt{1 - (\overline{v}_3(\omega))^2}}, \cos \Phi(r, \omega) \right) \,,$$

so that $n(\eta, \omega) = \overline{v}(\omega)$ and $n(2H\eta, \omega) = e_3$. The energy in $\Omega_4^{i,j}$ can be estimated by

$$\eta E_{\xi,\eta}(Q^{\delta}_{\xi,\eta}; \Omega_4^{i,j}) \leq \int_{B(p,\delta')} \int_{\eta}^{2H\eta} \left(\eta \left| \frac{\partial n}{\partial r} \right|^2 + \eta |\nabla_\omega n|^2 + \frac{1}{\eta} g(n) \right) \prod_{m=1}^{2} (1 + r\kappa_m) \, dr d\omega \,.$$

It is easy to see that,

$$\left| \frac{\partial n}{\partial r} \right|^2 = \left| \frac{\partial \Phi}{\partial r} \right|^2 = \frac{1}{(2H\eta - \eta)^2} |\Phi_0|^2 \leq \frac{C}{(2H-1)^2 \eta^2} \leq \frac{C}{\eta^2} \tag{6.9}$$

since Φ_0 is bounded and $H > 0$ is large. By a straightforward calculation, we also see that

$$\left| \frac{\partial n}{\partial \omega_k} \right|^2 = \frac{\sin^2 \Phi}{1 - \overline{v}_3^2} \left(\left| \frac{\partial \overline{v}_1}{\partial \omega_k} \right|^2 + \left| \frac{\partial \overline{v}_1}{\partial \omega_k} \right|^2 \right) + \left| \frac{\partial \Phi}{\partial \omega_k} \right|^2 - \frac{\overline{v}_3^2 \sin^2 \Phi}{(1 - \overline{v}_3^2)^2} \left| \frac{\partial \overline{v}_3}{\partial \omega_k} \right|^2 \,,$$

but using that $\sin \Phi \leq \sqrt{1 - \overline{v}_3^2}$, we can further estimate the gradient by

$$|\nabla_\omega n|^2 \leq |\nabla_\omega \overline{v}|^2 + |\nabla_\omega \Phi|^2 \,. \tag{6.10}$$

Next we consider the tangential derivatives of Φ and we see that they are bounded by the derivatives of Φ_0 as follows,

$$\left| \frac{\partial \Phi}{\partial \omega_k} \right|^2 = \left(1 - \frac{r - \eta}{2H\eta - \eta}\right)^2 \left| \frac{\partial \Phi_0}{\partial \omega_k} \right|^2 \leq \left| \frac{\partial \Phi_0}{\partial \omega_k} \right|^2 \,,$$

for $k = 1, 2$. Using the definition of Φ_0,

$$\left| \frac{\partial \Phi_0}{\partial \omega_k} \right|^2 = \frac{1}{1 - \overline{v}_3^2} \left| \frac{\partial \overline{v}_3}{\partial \omega_k} \right|^2 \leq \left| \frac{\partial \overline{v}}{\partial \omega_k} \right|^2 \,,$$

where the last inequality comes (6.3). From here it follows that $|\nabla_\omega \Phi|^2 \leq |\nabla_\omega \overline{v}|^2$, so that combining with (6.8) we obtain the estimate

$$|\nabla_\omega n|^2 \leq 2|\nabla_\omega \overline{v}|^2 \leq C\left(\frac{1}{(\delta')^2|v|^2+\eta^2}\right) \leq \frac{C}{\eta^2}\,. \tag{6.11}$$

With these estimates in hand, we bound the energy in this region by

$$\eta E_{\xi,\eta}(Q^\delta_{\xi,\eta};\Omega_4^{i,j}) \leq \int_{B(p,\delta')}\int_\eta^{2H\eta} \frac{C}{\eta}\ dr d\omega = C(2H-1)|B(p,\delta')|\,.$$

Therefore, taking $\xi,\eta \to 0$ followed by $\delta \to 0$, we can see that

$$\limsup_{\delta\to 0}\left(\limsup_{\xi,\eta\to 0}\eta E_{\xi,\eta}(Q^\delta_{\xi,\eta};\Omega_4^{i,j})\right) = 0\,.$$

<u>*Energy in* Ω_5</u>: The last region we need to consider is

$$\Omega_5 = \mathcal{C}_{2H\eta}(\mathcal{M}^\delta_d) \setminus \overline{\Omega_3 \cup \Omega_4}\,.$$

We do the construction generally for a region $\mathcal{R}^\delta_i$ for some $i = 1,\ldots,I$. Recall that $Q^\delta_b = v\otimes v - \frac{1}{3}I$ and that v as given in (6) is C^1 away from the point defects p^i_j, so there exists a constant $C_\delta > 0$ which depends only on $\delta > 0$ such that

$$|\nabla_\omega v|^2 \leq C_\delta, \quad \text{for} \quad \omega \in \mathcal{R}^\delta_i \setminus \bigcup_{j=1}^{|z_i|} B(p^i_j,\delta'_i)$$

To simplify notation, we define

$$\Omega^i_5 := \mathcal{C}_{2H\eta}\left(\mathcal{R}^\delta_i \setminus \bigcup_{j=1}^{|z_i|} B(p^i_j,\delta'_i),\right) \quad \text{so that} \quad \Omega_5 = \bigcup_{i=1}^{I}\Omega^i_5\,.$$

On Ω^i_5, we want to do a Lipschitz extension of $Q^\delta_{\xi,\eta}$ based on a Lipschitz extension of the angle $\widehat{\Phi}$ between n and e_3. To define $\widehat{\Phi}$ on $\partial\Omega^i_5$, we note that there exists a continuous extension of n from each of the neighbouring regions Ω_j for $j = 1,\ldots,4$ on $\partial\Omega^i_5$. We also take $n = v$ on the surface of the manifold $\mathcal{M}$. Then, define $\widehat{\Phi} : \partial\Omega^i_5 \to [0,\pi]$ by

$$\widehat{\Phi}(r,\omega) = \cos^{-1}(n_3(r,\omega))\,.$$

Note that by taking the gradient of $\widehat{\Phi}$ and then applying the inequality from (6.3),

$$|\nabla\widehat{\Phi}|^2 = \frac{1}{1-n_3^2}|\nabla n_3|^2 \leq C|\nabla n|^2 \leq C\left|\frac{\partial n}{\partial r}\right|^2 + C|\nabla_\omega n|^2\,,$$

for some $C > 0$, so the Lipschitz constant of $\widehat{\Phi}$ will be proportional to the maximum of the sum of radial and tangential derivatives of n on $\partial\Omega_5^i$. On $\partial\Omega_1$, we can see that

$$\left|\frac{\partial n}{\partial r}\right| \leq \frac{1}{\eta^2}\left|\frac{\partial n^*}{\partial \tilde{r}}\right|^2 \leq \frac{Ce^{-\sqrt[4]{24}\tilde{r}}}{\eta^2} \leq \frac{C}{\eta^2} \quad \text{and} \quad |\nabla_\omega n|^2 \leq C_{\delta,\kappa}\,,$$

using (4.3) and (6.4). Then on $\partial\Omega_2$, we were able to estimate the derivatives by

$$\left|\frac{\partial n}{\partial r}\right| \leq \frac{C}{H^2\eta^2} \leq \frac{C}{\eta^2} \quad \text{and} \quad |\nabla_\omega n|^2 \leq \widetilde{C}_{\delta,\kappa}\,.$$

Looking at $\partial\Omega_3$ and using both (6.5) and (6.8),

$$\left|\frac{\partial n}{\partial r}\right|^2 \leq \frac{C}{\eta^2}\left(\frac{1}{1+h^2}\right) \leq \frac{C}{\eta^2} \quad \text{and} \quad |\nabla_\omega n|^2 \leq \frac{C}{(\delta')^2|v|^2+\eta^2h^2} \leq \frac{C}{(\delta')^2} \leq C_\delta\,.$$

On $\partial\Omega_4$, we also saw from (6.9) and (6.11) that

$$\left|\frac{\partial n}{\partial r}\right|^2 \leq \frac{C}{\eta^2} \quad \text{and} \quad |\nabla_\omega n|^2 \leq \frac{C}{(\delta')^2|v|^2+\eta^2} \leq \frac{C}{(\delta')^2} \leq C_\delta\,,$$

so it remains to bound the gradient on the intersection of the boundary of Ω_5^i with $\mathcal{M}$ and the boundary with the exterior region where $Q_{\xi,\eta}^\delta = Q_\infty$. On $\mathcal{M}$ it holds that $n = v$, so $|\nabla_\omega n| = |\nabla_\omega v| \leq \widetilde{C}_{\delta,\kappa}$. Finally in the exterior region, $Q_{\xi,\eta}^\delta = Q_\infty$, so along this boundary, $\widehat{\Phi}$ is constant, thus the Lipschitz constant here is zero. We can see that this means $\widehat{\Phi}$ is Lipschitz on $\partial\Omega_5^i$, with a Lipschitz constant

$$\mathcal{L}_{\eta,\delta} \leq \sqrt{\frac{C}{\eta^2} + C_\delta}$$

for some constant C_δ which depends on $\delta > 0$ but not on η. So just as we have done in the spherical case, applying Theorem 2.10.43 from [9], we can extend $\widehat{\Phi}$ to all of Ω_5^i and $\widehat{\Phi}$ remains Lipschitz on this region, with the same Lipschitz constant $\mathcal{L}_{\eta,\delta}$. We can now define n on Ω_5^i by

$$n(r,\omega) = \left(\frac{v_1(\omega)\sin\widehat{\Phi}(r,\omega)}{\sqrt{1-(v_3(\omega))^2}}, \frac{v_2(\omega)\sin\widehat{\Phi}(r,\omega)}{\sqrt{1-(v_3(\omega))^2}}, \cos\widehat{\Phi}(r,\omega)\right)\,.$$

We note that n in this region is of a very similar form to n on Ω_4, so we can use the same computations to see that using (6.9),

$$\left|\frac{\partial n}{\partial r}\right|^2 = \left|\frac{\partial \widehat{\Phi}}{\partial r}\right|^2 \leq |\nabla \widehat{\Phi}|^2 \leq \mathcal{L}^2_{\eta,\delta} \leq \frac{C}{\eta^2} + C_\delta \,.$$

Next for the tangential derivatives we use (6.11) to get the estimate,

$$|\nabla_\omega n|^2 \leq |\nabla_\omega v|^2 + |\nabla_\omega \widehat{\Phi}|^2 \leq \frac{C}{\eta^2} + C_\delta \,.$$

Now again using that g is bounded, we estimate the energy in this region by

$$\eta E_{\xi,\eta}(Q^\delta_{\xi,\eta}; \Omega^i_5) \leq \int_{\Omega^i_5} \left(\eta |\nabla n|^2 + \frac{1}{\eta} g(n)\right) dx \leq \int_{\Omega^i_5} \frac{C}{\eta} + \eta C_\delta \, dx \leq CH|\mathcal{R}^\delta_i|(C + \eta^2 C_\delta) \,.$$

Therefore,

$$\limsup_{\delta\to 0} \left(\limsup_{\xi,\eta\to 0} \; \eta E_{\xi,\eta}(Q^\delta_{\xi,\eta}; \Omega^i_5)\right) = 0 \,,$$

so the energy in all of Ω_5 is negligible, i.e.

$$\limsup_{\delta\to 0} \left(\limsup_{\xi,\eta\to 0} \; \eta E_{\xi,\eta}(Q^\delta_{\xi,\eta}; \Omega_5)\right) = 0 \,.$$

Conclusion: Now we are able to put all of the regions together as follows,

$$\eta E_{\xi,\eta}(Q^\delta_{\xi,\eta}; \mathcal{C}_{2H\eta}(\mathcal{M}^+)) = \sum_{k=1}^{5} \eta E_{\xi,\eta}(Q^\delta_{\xi,\eta}; \Omega_k) \,,$$

therefore,

$$\limsup_{H\to\infty} \Big(\limsup_{\delta\to 0} \Big(\limsup_{\xi,\eta\to 0} \sum_{k=1}^{5} \eta E_{\xi,\eta}(Q^\delta_{\xi,\eta}; \Omega_k)\Big)\Big) \leq \int_{\mathcal{M}^+} D_\infty(Q^*_b(\omega)) \, d\omega \,.$$

The same construction for $Q^\delta_{\xi,\eta}$ works on $\mathcal{C}_{2H\eta}(\mathcal{M}^-)$, so we get the same upper bound. Then using that $D_\infty(Q^*_b(\omega)) = 0$ for $\omega \in \mathcal{M}^0$, we have,

$$\limsup_{\xi,\eta\to 0} \; \eta E_{\xi,\eta}(Q^\delta_{\xi,\eta}) \leq \int_{\mathcal{M}} D_\infty(Q^*_b(\omega)) \, d\omega \,.$$

$\square$

7 Open Questions

A next step would be to obtain the results for the lower and upper bounds for a more general class of manifolds by removing the restrictions on $\mathcal{M}_d = \{\omega \in \mathcal{M} : \nu(\omega) = \pm e_3\}$. Since $\mathcal{M}_d$ is a level set of ν, it is made up of finitely many connected sets, but these sets need not be only isolated points and curves of finite length. In fact the sets could even have positive measure, but this provides additional complications which were not addressed in this thesis.

Another question which may be of interest is given a manifold $\mathcal{M}$ what is its optimal orientation in terms of minimizing the energy of the system. Using the energy estimates from this thesis, we can quantify the limiting energy, given a manifold $\mathcal{M}$ and we expect to obtain a new minimization problem from this which can be further analyzed.

Something worth noting is that in the spherical case, for the lower bound, the boundary data did not need to be C^1 except at finitely many points. For the general manifold, we needed this assumption due to the finite length scale we were examining. However, it may be possible using a different approach to drop this assumption on the regularity of boundary data.

Finally, we dealt exclusively with the case of

$$\frac{\eta}{\xi} \to \lambda = \infty$$

but another interesting case is when $\lambda \in [0, \infty)$. The difficulty here is that minimizers of F_λ need not be uniaxial a.e., so it is much more difficult to construct a recovery sequence. As well, many of the strategies we used for the lower bound on the general manifold heavily relied upon $\lambda = \infty$ and would break down in the case where λ is finite.

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