



**HAL**  
open science

# TORUS-LIKE SOLUTIONS FOR THE LANDAU-DE GENNES MODEL. PART I: THE LYUKSYUTOV REGIME

Federico Dipasquale, Vincent Millot, Adriano Pisante

► **To cite this version:**

Federico Dipasquale, Vincent Millot, Adriano Pisante. TORUS-LIKE SOLUTIONS FOR THE LANDAU-DE GENNES MODEL. PART I: THE LYUKSYUTOV REGIME. Archive for Rational Mechanics and Analysis, In press. hal-02458774v1

**HAL Id: hal-02458774**

**<https://hal.science/hal-02458774v1>**

Submitted on 28 Jan 2020 (v1), last revised 29 Oct 2020 (v2)

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# TORUS-LIKE SOLUTIONS FOR THE LANDAU-DE GENNES MODEL. PART I: THE LYUKSYUTOV REGIME

FEDERICO DIPASQUALE, VINCENT MILLOT, AND ADRIANO PISANTE

ABSTRACT. We study global minimizers of a continuum Landau-De Gennes energy functional for nematic liquid crystals, in three-dimensional domains. Assuming smooth and uniaxial (e.g. homeotropic) boundary conditions and a corresponding physically relevant norm constraint (Lyuksyutov constraint), we prove full regularity up to the boundary for the (constrained) minimizers. As a consequence, in a relevant range of parameters (which we call *Lyuksyutov regime*), we show that unconstrained minimizers do not exhibit isotropic melting. In the case of a nematic droplet, the radial hedgehog is even shown to be an unstable equilibrium. Finally, we describe a class of boundary data including radial anchoring for which constrained or unconstrained minimizers are smooth configurations whose biaxiality level sets carry nontrivial topology. Results of this paper will be largely employed and refined in the next of our series. In particular in [16], where we prove that biaxiality level sets are generically finite unions of tori for smooth equilibrium configurations minimizing the energy in a restricted axially symmetric class.

## CONTENTS

1. Introduction	1
2. Small energy regularity theory: a tool box	9
2.1. Monotonicity formulae	10
2.2. Reflection across the boundary	15
2.3. The $\varepsilon$ -regularity theorem	21
2.4. Higher order regularity	26
2.5. Bochner inequality and uniform regularity estimates	30
3. Regularity of minimizers under norm constraint	33
3.1. Monotonicity formulae	33
3.2. Compactness of blow-ups and smallness of the scaled energy	33
3.3. Full regularity	38
4. LdG-minimizers in the Lyuksyutov regime	39
4.1. A priori estimates	39
4.2. Lyuksyutov regime and absence of isotropic melting	40
4.3. Instability of the melting hedgehog	42
5. Topology of minimizers	46
References	50

## 1. INTRODUCTION

Nematic liquid crystals are mesophases of matter between the liquid and the solid phases. Nematic molecules typically have elongated shape, approximately rod-like, and can flow freely, like in a liquid, which forces their long axes to align locally along some common direction. This feature is the key for the extreme responsivity of nematics to external stimuli, which in turn is the reason why they are so useful in technological applications. Macroscopic configurations of nematics are usually described by continuum theories, the most successful being the phenomenological Landau-de Gennes (LdG) theory ([61, 13, 2, 45]) which accounts for the most convincing description of the experimentally observed optical defects [31, 35]. In the present paper, we study minimizers of the Landau-de Gennes energy functional in three dimensional domains under topologically nontrivial boundary conditions (e.g. radial anchoring). The goal here is to shed some light on the emergence

---

*Date:* January 28, 2020.

*Key words and phrases.* Liquid crystals; axisymmetric torus solutions; harmonic maps.

of topological structure in the so-called biaxial surfaces associated to energy minimizing configurations, proving some mathematically rigorous results on the nature of the defects which, at least in model geometries, is expected to be of torus type [49, 32, 19, 33].

According to the (LdG) theory, we let  $\mathcal{M}_{3 \times 3}(\mathbb{R})$  be the real vector space made of  $3 \times 3$ -matrices, and we consider its 5-dimensional subspace

$$\mathcal{S}_0 := \left\{ Q = (Q_{ij}) \in \mathcal{M}_{3 \times 3}(\mathbb{R}) : Q = Q^t, \operatorname{tr}(Q) = 0 \right\},$$

where  $Q^t$  denotes the transpose of  $Q$ , and  $\operatorname{tr}(Q)$  the trace of  $Q$ . The space  $\mathcal{S}_0$  is endowed with the Hilbertian structure given by the usual (Frobenius) inner product. Since the matrices under consideration are symmetric, the inner product and the induced norm are given by

$$P : Q := \sum_{i,j=1}^3 P_{ij} Q_{ij} = \operatorname{tr}(PQ) \quad \text{and} \quad |Q|^2 = \operatorname{tr}(Q^2).$$

Upon the choice of an orthonormal basis,  $\mathcal{S}_0$  can be identified with the Euclidean space  $\mathbb{R}^5$ . In particular,

$$\left\{ Q \in \mathcal{S}_0 : |Q| = 1 \right\} = \mathbb{S}^4.$$

Let  $\Omega \subseteq \mathbb{R}^3$  a bounded domain with (at least)  $C^1$ -smooth boundary, and  $\mathbf{Q} : \Omega \rightarrow \mathcal{S}_0$  a configuration in the Sobolev space  $W^{1,2}(\Omega; \mathcal{S}_0)$ . We consider the Landau-de Gennes energy functional of the form

$$\mathcal{F}_{\text{LG}}(\mathbf{Q}) = \int_{\Omega} \frac{L}{2} |\nabla \mathbf{Q}|^2 + F_B(\mathbf{Q}) \, dx, \quad (1.1)$$

i.e., with the one-constant approximation for the elastic energy density with parameter  $L > 0$  and quartic polynomial bulk potential

$$F_B(\mathbf{Q}) := -\frac{a^2}{2} \operatorname{tr}(\mathbf{Q}^2) - \frac{b^2}{3} \operatorname{tr}(\mathbf{Q}^3) + \frac{c^2}{4} (\operatorname{tr}(\mathbf{Q}^2))^2, \quad (1.2)$$

where  $a, b$  and  $c$  are material-dependent strictly positive constants. It is convenient to subtract-off an additive constant and introduce

$$\tilde{F}_B(\mathbf{Q}) := F_B(\mathbf{Q}) - \min_{\mathcal{S}_0} F_B, \quad (1.3)$$

so that the potential becomes nonnegative.

In order to discuss the qualitative properties of energy minimizing configurations (such as isotropic/nematic phase transition, biaxial escape), we find convenient to modify the usual definition of biaxiality parameter as follows.

**Definition 1.1.** For any  $Q \in \mathcal{S}_0 \setminus \{0\}$ , we define the *signed biaxiality* parameter of  $Q$  as

$$\tilde{\beta}(Q) := \sqrt{6} \frac{\operatorname{tr}(Q^3)}{|Q|^3} \in [-1, 1]. \quad (1.4)$$

Observe that if the matrix  $Q$  has a spectrum  $\sigma(Q) = \{\lambda_1, \lambda_2, \lambda_3\} \subseteq \mathbb{R}$ , and we order the eigenvalues increasingly, then  $\tilde{\beta}(Q) = \pm 1$  iff the minimal/maximal eigenvalue is double (purely positive/negative uniaxial phase),  $\tilde{\beta}(Q) = 0$  iff  $\lambda_2 = 0$  and  $\lambda_1 = -\lambda_3$  (maximal biaxial phase), and  $Q = 0$  iff  $\lambda_1 = \lambda_2 = \lambda_3$  (isotropic phase).

It turns out that the potential is minimal when the signed biaxiality is maximal, and  $\tilde{F}_B(Q) = 0$  iff  $Q \in \mathcal{Q}_{\min}$ , i.e., if  $Q$  is in the vacuum-manifold of positive uniaxial matrices

$$\mathcal{Q}_{\min} := \left\{ Q \in \mathcal{S}_0 : Q = s_+ \left( n \otimes n - \frac{1}{3} I \right), \quad n \in \mathbb{S}^2 \right\}, \quad (1.5)$$

where

$$s_+ := \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2} \quad (1.6)$$

is the positive root of the characteristic equation

$$2c^2t^2 - b^2t - 3a^2 = 0. \quad (1.7)$$

Notice that, up to a multiplicative constant,  $\mathcal{Q}_{\min} \sim \mathbb{R}P^2$ , therefore it has nontrivial topology. In particular, there are nontrivial homotopy groups  $\pi_2(\mathcal{Q}_{\min}) = \mathbb{Z}$  and  $\pi_1(\mathcal{Q}_{\min}) = \mathbb{Z}_2$ , which are

relevant for the presence of topological defects. The corresponding energy functional is

$$\tilde{\mathcal{F}}_{LG}(\mathbf{Q}) := \int_{\Omega} \frac{L}{2} |\nabla \mathbf{Q}|^2 + \tilde{F}_B(\mathbf{Q}) \, dx, \quad (1.8)$$

which is the sum of two nonnegative term, penalizing respectively spatial variations and deviations from the vacuum manifold  $\mathcal{Q}_{\min}$ .

We rescale a tensor by setting

$$\mathbf{Q} =: s_+ \sqrt{\frac{2}{3}} Q.$$

In this way, the vacuum manifold becomes exactly the real projective plane  $\mathbb{R}P^2 = \mathbb{S}^2/\{\pm 1\}$ , where  $\mathbb{R}P^2 \subseteq \mathbb{S}^4$  is embedded as in (1.5), i.e., through the so-called *Veronese immersion*. We rewrite the energy functional as

$$\tilde{\mathcal{F}}_{LG}(\mathbf{Q}) = \frac{2}{3} s_+^2 L \mathcal{F}_{\lambda, \mu}(Q), \quad (1.9)$$

with

$$\mathcal{F}_{\lambda, \mu}(Q) := \int_{\Omega} \frac{1}{2} |\nabla Q|^2 + \lambda W(Q) + \frac{\mu}{4} (1 - |Q|^2)^2 \, dx. \quad (1.10)$$

The reduced parameters  $\lambda$  and  $\mu$  are given by

$$\lambda := \sqrt{\frac{2}{3}} \frac{b^2 s_+}{L} > 0, \quad \mu := \frac{a^2}{L} > 0,$$

and the reduced smooth potential  $W : \mathcal{S}_0 \rightarrow \mathbb{R}$  is nonnegative and vanishes exactly on  $\mathbb{R}P^2$ . More precisely, in view of (1.6)-(1.7), the potential  $W$  is explicitly given by

$$W(Q) = \frac{1}{3\sqrt{6}} \left( |Q|^3 - \sqrt{6} \operatorname{tr}(Q^3) \right) + \frac{1}{12\sqrt{6}} (3|Q|^2 + 2|Q| + 1)(|Q| - 1)^2, \quad (1.11)$$

or equivalently,

$$W(Q) = \frac{1}{4\sqrt{6}} |Q|^4 - \frac{1}{3} \operatorname{tr}(Q^3) + \frac{1}{12\sqrt{6}}. \quad (1.12)$$

The structure relations (1.10) and (1.11) suggests that, in a regime where  $\mu$  is large, the energy  $\mathcal{F}_{\lambda, \mu}$  favours rescaled configurations of approximatively unit norm.

In this paper, we first make the fundamental assumption that the norm of any admissible configuration is given by the constant value proper of the vacuum manifold [41], i.e.,

$$|\mathbf{Q}(x)| \equiv \sqrt{\frac{2}{3}} s_+ \quad (\text{Lyuksyutov constraint}). \quad (1.13)$$

Under the Lyuksyutov constraint, the energy functional takes the form

$$\tilde{\mathcal{F}}_{LG}(\mathbf{Q}) = \frac{2}{3} s_+^2 L \mathcal{E}_{\lambda}(Q)$$

for rescaled tensors  $Q \in W^{1,2}(\Omega; \mathbb{S}^4)$ , where

$$\mathcal{E}_{\lambda}(Q) := \int_{\Omega} \frac{1}{2} |\nabla Q|^2 + \lambda W(Q) \, dx. \quad (1.14)$$

The restriction of the potential  $W : \mathcal{S}_0 \rightarrow \mathbb{R}$  to  $\mathbb{S}^4$  is given by

$$W(Q) = \frac{1}{3\sqrt{6}} \left( 1 - \tilde{\beta}(Q) \right) \quad \forall Q \in \mathbb{S}^4. \quad (1.15)$$

In particular,  $W$  is nonnegative on  $\mathbb{S}^4$ ,  $\{W = 0\} \cap \mathbb{S}^4 = \mathbb{R}P^2$  and  $\nabla_{\tan} W(Q) = 0$  for any  $Q \in \mathbb{R}P^2$ . As a consequence, when further restricted to the subspace of uniaxial configurations  $W^{1,2}(\Omega; \mathbb{R}P^2)$ , the energy functional (1.14) reduces to the Dirichlet integral, i.e., the Frank-Oseen energy in the one-constant approximation. For an account on the qualitative properties of defects in the Frank-Oseen model, we refer the interested reader to e.g. [1, 8].

A critical point  $Q_{\lambda} \in W^{1,2}(\Omega; \mathbb{S}^4)$  of  $\mathcal{E}_{\lambda}$  among  $\mathbb{S}^4$ -valued maps satisfies in the sense of distributions in  $\Omega$  the Euler-Lagrange equation

$$\Delta Q_{\lambda} + |\nabla Q_{\lambda}|^2 Q_{\lambda} = \lambda \nabla_{\tan} W(Q_{\lambda}), \quad (1.16)$$

with the tangential gradient of  $W$  along  $\mathbb{S}^4 \subseteq \mathcal{S}_0$  given by

$$\nabla_{\tan} W(Q) = - \left( Q^2 - \frac{1}{3} I - \operatorname{tr}(Q^3) Q \right).$$

Notice that the left hand side of (1.16) is the so-called *tension field* of  $Q$ , a tangent field along  $Q$  in  $\mathbb{S}^4$ , and equation (1.16) is nothing but the harmonic map equation for  $\mathbb{S}^4$ -valued map with the extra term  $\lambda \nabla_{\tan} W(Q)$  as a source term. Any tensor field  $Q$  which is weakly harmonic among  $\mathbb{S}^4$ -valued maps and lying in the subspace  $W^{1,2}(\Omega; \mathbb{R}P^2)$  is also weakly harmonic among maps in  $W^{1,2}(\Omega; \mathbb{R}P^2)^1$ , and provides a solution to (1.16). Since everywhere discontinuous weakly harmonic maps among maps in  $W^{1,2}(\Omega; \mathbb{R}P^2)$  do exist (see [51]), we expect smoothness of solutions to (1.16) to fail in general, and to prove regularity we shall rely in an essential way on energy minimality.

We consider the minimization of the energy functional  $\mathcal{E}_\lambda$  among maps in  $W^{1,2}(\Omega; \mathbb{S}^4)$  satisfying a Dirichlet boundary condition (strong anchoring) in the sense of traces. We fix a Lipschitz (at least) boundary trace  $Q_b \in \text{Lip}(\partial\Omega; \mathbb{S}^4)$ , and we consider the set of admissible configurations

$$\mathcal{A}_{Q_b}(\Omega) := \left\{ Q \in W^{1,2}(\Omega; \mathcal{S}_0) : Q|_{\partial\Omega} = Q_b, |Q| = 1 \text{ a.e. in } \Omega \right\} \subseteq W^{1,2}(\Omega; \mathbb{S}^4), \quad (1.17)$$

which is nonempty by [28]. Hence, one can fix a reference extension  $\bar{Q}_b \in \mathcal{A}_{Q_b}(\Omega)$ , which, as a matter of fact, can be chosen in  $C^0(\bar{\Omega}; \mathbb{S}^4)$ , or even smooth in the interior since  $\pi_2(\mathbb{S}^4) = 0$  (so that density of smooth maps in  $\mathcal{A}_{Q_b}(\Omega)$  holds). By the direct method in the Calculus of Variations, it is routine to show that there exist minimizers  $Q_\lambda \in \mathcal{A}_{Q_b}(\Omega)$  of  $\mathcal{E}_\lambda$ . Requiring the boundary condition to be at least  $C^{1,1}$ -regular allows some smoothness up to the boundary for the corresponding minimizers. Indeed, the first result of our paper is the following regularity theorem.

**Theorem 1.2.** *Assume that  $\partial\Omega$  is of class  $C^3$  and  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ . If  $Q_\lambda$  is a minimizer of  $\mathcal{E}_\lambda$  in the class  $\mathcal{A}_{Q_b}(\Omega)$ , then  $Q_\lambda \in C^\omega(\Omega) \cap C^{1,\alpha}(\bar{\Omega})$  for every  $\alpha \in (0, 1)$ . If in addition,  $Q_b \in C^{2,\delta}(\partial\Omega; \mathbb{S}^4)$  for some  $\delta > 0$ , then  $Q_\lambda \in C^2(\bar{\Omega}; \mathbb{S}^4)$ , and, finally, if  $\Omega$  is a domain with analytic boundary and  $Q_b \in C^\omega(\partial\Omega; \mathbb{S}^4)$ , then  $Q_\lambda \in C^\omega(\bar{\Omega}; \mathbb{S}^4)$ .*

The proof of this theorem is based on ideas and techniques from the regularity theory of harmonic maps, starting from the pioneering papers [55, 56, 57], as summarized in the books [58, 47, 38]. The crucial point is to obtain Lipschitz continuity, while higher order regularity follows from standard Calderon-Zygmund and Schauder theories and the analyticity results in [46]. Both for the interior and for the boundary regularity, the main steps are : 1) monotonicity formulae; 2) strong compactness of blow-ups; 3) constancy of blow-up limits (Liouville property); 4) continuity under smallness of the scaled energy ( $\varepsilon$ -regularity); 5) Lipschitz continuity. Within this general scheme, our proof presents some differences and simplifications we want to comment on. The monotonicity formula here is not obtained by inner variations but instead by a penalty approximation which is, to our knowledge, new. More precisely, we relax the norm constraint, and passing to the limit in monotonicity formulae for approximated problems, we obtain interior and boundary monotonicity formulae. The validity of the latter requires the Lipschitz assumption on  $Q_b$  as in the harmonic map case (see e.g. [11]). Strong compactness of blow-ups is obtained by construction of comparison maps arguing as in [58] for harmonic maps again. Indeed, the perturbed Dirichlet energy  $\mathcal{E}_\lambda$  is treated as in [48] with techniques based on the Luckhaus interpolation lemma [40], both in the interior and near the boundary. As strong limits of blow-ups are degree-zero homogeneous and minimizing harmonic maps into  $\mathbb{S}^4$ , i.e.  $Q_*(x) = \omega(x/|x|)$  for some harmonic sphere  $\omega: \mathbb{S}^2 \rightarrow \mathbb{S}^4$ , their constancy in the interior case directly follows from [57]. At a boundary point, limits of blow-ups are of the form  $Q_*(x) = \omega^+(x/|x|)$  with  $x_3 > 0$  (up to rotations in the domain), for some harmonic half-sphere  $\omega^+: \mathbb{S}_+^2 \rightarrow \mathbb{S}^4$  with constant trace on  $\partial\mathbb{S}_+^2$ . The constancy of those  $\omega^+$  is derived in a way similar to [56]. We emphasize that boundary regularity is not deduced from minimality, but instead by a reflection argument and the  $2d$ -interior regularity result for weakly harmonic maps from [26], and constancy of  $\omega^+$  follows from [36] as in [56]. Since our argument for boundary regularity does not rely on energy minimality, it will be possible to apply it also in the symmetric case we consider in our companion papers [15, 16]. Our approach to  $\varepsilon$ -regularity treats in a unified way the interior and the boundary case, adapting for the latter the clever reflection argument devised in [53] for harmonic maps (under the same regularity assumptions on  $\partial\Omega$  and  $Q_b$ ). Moreover, Hölder-continuity under smallness of the scaled energy is not deduced as usual from Hardy-BMO duality as in [17], or using the integrability by compensation due to the hidden

<sup>1</sup>Observe that the converse implication is not true in general, because the Veronese immersion is minimal but it is not totally geodesic, and the tension field of  $Q$  in  $\mathbb{S}^4$  could be purely orthogonal to  $\mathbb{R}P^2$  but nonzero. Thus, if  $Q$  is weakly harmonic among map in the space  $W^{1,2}(\Omega; \mathbb{R}P^2)$ , i.e., it is a critical point of the Frank-Oseen energy, then it does not solve (1.16) in general. Hence it is not a critical point of the Landau-de Gennes energy under norm constraint.

antisymmetric structure of the quadratic gradient term in (1.16) as in [52] for harmonic maps. In the present paper, we adapt to our context the elementary iteration approach introduced in [10], based on the divergence structure of the quadratic gradient term and the decay properties of the BMO seminorm together with the integral characterization of Hölder-continuous functions due to Campanato. Finally, Lipschitz continuity is obtained using the harmonic replacement argument of [54] for harmonic maps.

With Theorem 1.2 at hand, we now remove the norm constraint (1.13), and we consider the full energy functional (1.10). We minimize  $\mathcal{F}_{\lambda,\mu}$  over maps in  $W^{1,2}(\Omega; \mathcal{S}_0)$  still satisfying a Dirichlet boundary condition (strong anchoring) in the sense of traces. Given a Lipschitz boundary trace  $Q_b \in \text{Lip}(\partial\Omega; \mathcal{S}_0)$ , existence of minimizers  $Q_\lambda^\mu \in W^{1,2}(\Omega; \mathcal{S}_0)$  follows again from the direct method in the Calculus of Variations. In addition, applying usual interior and boundary regularity for semilinear elliptic equations to the Euler-Lagrange equation satisfied by critical points of  $\mathcal{F}_{\lambda,\mu}$  (see (4.1)), we can infer that  $Q_\lambda^\mu \in C^\alpha(\bar{\Omega}; \mathcal{S}_0) \cap C^\omega(\Omega; \mathcal{S}_0)$  for some  $\alpha \in (0, 1)$ . At this stage, we are interested in the asymptotic behaviour of minimizers  $Q_\lambda^\mu$  in the range of parameters (that we call *Lyuksyutov regime*)

$$\lambda = \sqrt{\frac{2}{3}} \frac{b^2 s_+}{L} \equiv \text{const}, \quad \mu = \frac{a^2}{L} \rightarrow +\infty. \quad (1.18)$$

Particular cases are given by  $a^2 \rightarrow \infty$ ,  $b^2 \sim |a|^{-1}$  or  $L \rightarrow 0$ ,  $b^2 \sim L$ . These regimes resemble the low-temperature limit and the small elastic constant limit, respectively. For further discussions on this aspect and related asymptotic limits, we refer to Remark 4.11 and [18].

Under these restrictions on the parameters, the last term in  $\mathcal{F}_{\lambda,\mu}$  acts as a penalty approximation of the norm constraint (1.13), and it is natural to expect convergence of the family  $\{\mathcal{F}_{\lambda,\mu}\}_\mu$  to the functional  $\mathcal{E}_\lambda$  (in the sense of  $\Gamma$ -convergence, see e.g. [7]), and that minimizers of  $\mathcal{F}_{\lambda,\mu}$  converge to minimizers of  $\mathcal{E}_\lambda$ .

**Theorem 1.3.** *Assume that  $\partial\Omega$  is of class  $C^3$  and  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ . There exist minimizers  $Q_\lambda^\mu$  of  $\mathcal{F}_{\lambda,\mu}$  in the class  $W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$ , and any such  $Q_\lambda^\mu$  belongs to  $C^\omega(\Omega) \cap C^{1,\alpha}(\bar{\Omega})$  for every  $\alpha \in (0, 1)$ . In addition, as  $\mu \rightarrow \infty$  with  $\lambda$  constant (Lyuksyutov regime), the following holds:*

- (1) *there exists  $Q_\lambda \in W^{1,2}(\Omega; \mathbb{S}^4)$  minimizing  $\mathcal{E}_\lambda$  in the class  $\mathcal{A}_{Q_b}(\Omega)$  such that, up to a subsequence,  $Q_\lambda^\mu \rightarrow Q_\lambda$  strongly in  $W^{1,2}(\Omega; \mathcal{S}_0)$ ;*
- (2)  *$\mathcal{F}_{\lambda,\mu}(Q_\lambda^\mu) \rightarrow \mathcal{E}_\lambda(Q_\lambda)$  and  $\mu \int_\Omega (1 - |Q_\lambda^\mu|^2)^2 dx \rightarrow 0$ ;*
- (3)  *$|Q_\lambda^\mu| \rightarrow 1$  uniformly in  $\bar{\Omega}$ .*

*In particular, for each  $\lambda > 0$ , there exists a value  $\mu_\lambda = \mu_\lambda(\lambda, \Omega, Q_b) > 0$  such that for  $\mu > \mu_\lambda$ , any minimizer  $Q_\lambda^\mu$  of  $\mathcal{F}_{\lambda,\mu}$  satisfies  $|Q_\lambda^\mu| > 0$  in  $\bar{\Omega}$ , i.e., minimizers do not exhibit the isotropic phase.*

In this theorem, existence and regularity properties of minimizers  $Q_\lambda^\mu$  have already been recalled in the discussion above. Claim (1) and (2) can be seen as a standard consequence of the  $\Gamma$ -convergence of the family  $\{\mathcal{F}_{\lambda,\mu}\}_\mu$  to  $\mathcal{E}_\lambda$ , although for the reader's convenience such notion is not explicitly used in the proof (but just mentioned here for readers familiar with it). As a matter of fact, the claims rely on a sharp two-sided bound on the energies  $\{\mathcal{F}_{\lambda,\mu}(Q_\lambda^\mu)\}_\mu$ , the lower semicontinuity property of the energy functionals (i.e., the  $\Gamma$ -liminf inequality), the construction of trial sequences (i.e., the recovery sequences for the  $\Gamma$ -limsup inequality), and the standard weak compactness in  $W^{1,2}$  coming from the equicoercivity of the energies (i.e., the compactness in  $\Gamma$ -convergence). As a consequence, minimum points strongly converge to minimum points in  $W^{1,2}$ , and the two claims follow as the upper and the lower bound mentioned above coincide. The second claim tells us in particular that the limiting map must be  $\mathbb{S}^4$ -valued as a direct consequence of Fatou's Lemma. Finally, claim (3) is by far the most interesting as it guarantees that the isotropic phase is avoided by energy minimizing configurations  $Q_\lambda^\mu$  in the Lyuksyutov regime (as already proved in [9] and [12, 27] in the low-temperature limit in 2D and 3D, respectively). Our proof of this property is based in a crucial way on Theorem 1.2. Indeed, smoothness of the limiting minimizer  $Q_\lambda$  and the strong  $W^{1,2}$ -convergence yield smallness of the scaled energy of  $Q_\lambda^\mu$  at a sufficiently small scale. Combining monotonicity formulae with elliptic regularity in a way similar to [44], we are then able to show that  $|Q_\lambda^\mu|$  has to converge to one uniformly as  $\mu \rightarrow \infty$ .

To illustrate our results so far, let us now consider the model case of a nematic droplet, i.e.,  $\Omega = \{|x| < 1\}$  is the unit ball. The outer unit normal to the boundary is  $\vec{n}(x) = x/|x|$ , and a

natural boundary datum is the so called *radial anchoring*, namely

$$Q_b(x) = \sqrt{\frac{3}{2}} \left( \frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}I \right). \quad (1.19)$$

Since  $\vec{n}: \partial\Omega \rightarrow \mathbb{S}^2$  is harmonic, the homogeneous extension  $\bar{H}(x) = Q_b(x/|x|)$  (the *constant-norm hedgehog*) is a weakly harmonic map from  $\Omega$  into  $\mathbb{R}P^2$ , and it is an energy minimizer of  $\mathcal{E}_\lambda$  for its own boundary value in  $W^{1,2}(\Omega; \mathbb{R}P^2)$  by the lifting property of  $W^{1,2}$ -maps in  $\mathbb{R}P^2$  in [3] and the celebrated result in [8]. Moreover, a direct computation shows that  $\bar{H}$  is also a weak solution to (1.16), i.e., a critical point of  $\mathcal{E}_\lambda$ . As  $\bar{H}$  is singular at the origin, Theorem 1.2 tells us that  $\bar{H}$  is not minimizing  $\mathcal{E}_\lambda$  in the class  $\mathcal{A}_{Q_b}(\Omega)$ . We shall prove in Proposition 4.7 that  $\bar{H}$  is in fact strictly unstable, employing an argument similar to [57], an explicit computation of the second variation of energy, and a perturbation localized near the origin.

Still in the case of a nematic droplet subject to radial anchoring, the energy functional  $\mathcal{F}_{\lambda,\mu}$  has an  $O(3)$ -equivariant (radial) critical point commonly known as *radial hedgehog*

$$H_\lambda^\mu(x) := s_\lambda^\mu(|x|) \left( \frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}I \right), \quad 0 < |x| < 1. \quad (1.20)$$

This solution is obtained from a unique function  $s_\lambda^\mu(|x|)$  increasing from 0 to  $\sqrt{3/2}$  solving an ODE with the prescribed values at  $|x| = 0$  and  $|x| = 1$ , see e.g. [43, 30] and the references therein. It turns out to be the unique uniaxial critical point of  $\mathcal{F}_{\lambda,\mu}$  w.r.to arbitrary (not necessarily uniaxial) perturbations, see [34]. As the origin is an isotropic point, Theorem 1.3 shows that  $H_\lambda^\mu$  does not minimize  $\mathcal{F}_{\lambda,\mu}$  in the class  $W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$ , at least for  $\mu$  large enough. Thus, biaxial escape must occur for minimizers. Using the strong convergence of  $H_\lambda^\mu$  to  $\bar{H}$  as  $\mu \rightarrow \infty$ , we are able to pass to the limit in the second variation of  $\mathcal{F}_{\lambda,\mu}$  at  $H_\lambda^\mu$ , and we infer in Theorem 4.8 the instability of  $H_\lambda^\mu$  w.r.to biaxial perturbations for  $\mu$  large enough. Both properties are the counterpart in the Lyuksyutov regime of the instability of the radial hedgehog in the low-temperature limit (essentially  $a^2 \rightarrow \infty$ ) already proved in [29] (see also [20, 43]) together with the (infinitesimal) biaxial escape phenomenon obtained there.

Once the smoothness of  $Q_\lambda$  and the absence of isotropic phase for  $Q_\lambda^\mu$  are established, we can discuss for both cases the topological properties related to the presence of biaxial phase, and the way they are connected with the topology of the vacuum manifold. The starting point is that, under the assumption  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ ,  $Q_\lambda$  and  $Q_\lambda^\mu$  are configurations satisfying the hypothesis

$$(HP_0) \quad Q \in C^1(\bar{\Omega}; \mathcal{S}_0 \setminus \{0\}) \cap C^\omega(\Omega; \mathcal{S}_0).$$

The first assumption at the boundary that we impose on a configuration  $Q: \bar{\Omega} \rightarrow \mathcal{S}_0 \setminus \{0\}$  is the following

$$(HP_1) \quad \bar{\beta} := \min_{x \in \partial\Omega} \tilde{\beta} \circ Q(x) > -1.$$

The case  $\bar{\beta} = 1$  occurs for the main and most natural example of boundary condition, which is (in view of the embedding  $\mathbb{R}P^2 \subseteq \mathbb{S}^4$ )

$$Q_b(x) = \sqrt{\frac{3}{2}} \left( v(x) \otimes v(x) - \frac{1}{3}I \right) \quad \text{for all } x \in \partial\Omega, \quad v \in C^1(\partial\Omega; \mathbb{S}^2). \quad (1.21)$$

In particular, if  $\partial\Omega$  is of class  $C^2$ , the choice  $v(x) = \vec{n}(x)$  (the outer unit normal to the boundary  $\partial\Omega$ ) corresponds to the so-called *homeotropic* boundary condition (or *radial anchoring*).

If  $\Omega \subseteq \mathbb{R}^3$  is a bounded open set with boundary of class at least  $C^1$ , we know that  $\partial\Omega$  is a finite union of embedded  $C^1$ -surfaces. More precisely,  $\partial\Omega = \cup_{i=1}^N S_i$  where the surfaces  $S_i$  are of class (at least)  $C^1$ , disjoint, embedded, connected, orientable, and boundaryless. The second assumption we make on (the boundary of)  $\Omega$  is

$$(HP_2) \quad \Omega \text{ is connected and simply connected.}$$

Under this assumption, each surface  $S_i$  has zero genus, so it is an embedded sphere (see Lemma 5.1). The domain  $\Omega$  is thus a topological ball with finitely many disjoint closed balls removed from its interior. By assumption  $(HP_1)$ , the maximal eigenvalue  $\lambda_{\max}(x)$  of  $Q(x)$  is simple for every  $x \in \partial\Omega$ . Hence there exists a corresponding well defined  $C^1$ -smooth eigenspace map  $V_{\max} \in C^1(\partial\Omega; \mathbb{R}P^2)$ ,

and this map has a (nonunique) lifting  $v_{\max} \in C^1(\partial\Omega; \mathbb{S}^2)$  since each surface  $S_i$  has zero genus. To enforce the emergence of topology in the minimizers, we finally make a third assumption

$$(HP_3) \quad \deg(v_{\max}, \partial\Omega) = \sum_{i=1}^N \deg(v_{\max}, S_i) \text{ is odd.}$$

Notice that this property depends only on the map  $V_{\max}$ , it does not depend on the choice of the lifting  $v_{\max}$ . In case of radial anchoring (i.e.,  $Q_b$  of the form (1.21) with  $v = \vec{n} = v_{\max}$ ), it is satisfied whenever  $N$  is odd, that is whenever  $\partial\Omega$  has an odd number of connected components (or, equivalently, if the domain  $\Omega$  is a topological ball with an even number of disjoint closed ball removed from its interior).

In order to emphasize the consequence of assumptions  $(HP_0)$ - $(HP_3)$  on a configuration  $Q$  satisfying  $Q = Q_b$  on  $\partial\Omega$ , let us assume for a moment that  $Q_b$  takes values into the vacuum manifold, i.e.,  $Q_b \in C^1(\partial\Omega; \mathbb{R}P^2)$ . First, observe that  $Q_b$  has a lifting by  $(HP_2)$ , i.e.,  $Q_b$  is of the form (1.21). Moreover, any lifting  $v \in C^1(\partial\Omega; \mathbb{S}^2)$  of  $Q_b$  admits a finite energy extension  $\bar{v} \in W^{1,2}(\Omega; \mathbb{S}^2)$  (see e.g. [28]), but no continuous extension because of assumption  $(HP_3)$ . As a consequence,  $Q_b$  admits an extension  $\bar{Q}_b \in W^{1,2}(\Omega; \mathbb{R}P^2)$  of the form

$$\bar{Q}_b(x) = \sqrt{\frac{3}{2}} \left( \bar{v}(x) \otimes \bar{v}(x) - \frac{1}{3}I \right). \quad (1.22)$$

In view of [3] and  $(HP_3)$ , any extension  $\bar{Q}_b \in W^{1,2}(\Omega; \mathbb{R}P^2)$  of  $Q_b$  is in fact of the form (1.22) for a suitable (necessarily) discontinuous map  $\bar{v} \in W^{1,2}(\Omega; \mathbb{S}^2)$ . The configuration  $Q$  being smooth and without isotropic phase by assumption  $(HP_0)$ , it cannot be purely uniaxial (i.e.,  $\mathbb{R}P^2$ -valued) and *biaxial escape* must occur for purely topological reasons.

To describe the way a configuration  $Q$  encodes some topological information, we shall make use of the biaxiality function as follows.

**Definition 1.4.** For a configuration  $Q \in C^0(\bar{\Omega}; \mathcal{S}_0 \setminus \{0\})$  we define its *biaxiality function*  $\beta := \tilde{\beta} \circ Q$  and for each  $t \in [-1, 1]$  the associated *biaxiality regions* as the closed subsets of  $\bar{\Omega}$  given by

$$\{\beta \leq t\} := \{x \in \bar{\Omega} : \tilde{\beta} \circ Q(x) \leq t\} \quad \text{and} \quad \{\beta \geq t\} := \{x \in \bar{\Omega} : \tilde{\beta} \circ Q(x) \geq t\}, \quad (1.23)$$

where  $\tilde{\beta}$  is the signed biaxiality parameter (1.4). The corresponding *biaxial surfaces* are defined as

$$\{\beta = t\} := \{x \in \bar{\Omega} : \tilde{\beta} \circ Q(x) = t\}.$$

Observe that if  $t \in (-1, 1)$  is a regular value of  $\beta$ , then biaxial surfaces are smooth surfaces inside  $\bar{\Omega}$ , possibly with boundary which is anyway smooth and contained in  $\partial\Omega$ . Moreover, the regions in (1.23) are homotopically equivalent to their interior  $\{\beta < t\}$  and  $\{\beta > t\}$ , since the biaxial surfaces are actually smooth and serve as their common boundary.

We now introduce a notion of “mutual linking”, a property that will (partially) encode the topological nontriviality of the biaxiality regions.

**Definition 1.5.** Let  $A, B \subseteq \bar{\Omega}$  be two compact subset. The sets  $A$  and  $B$  are said to be *mutually linked*<sup>2</sup> if  $A$  is not contractible in  $\bar{\Omega} \setminus B$  and  $B$  is not contractible in  $\bar{\Omega} \setminus A$ .

To illustrate this definition, let us discuss again the case of a nematic droplet. If  $\Omega$  is the unit ball and  $Q_b$  is the hedgehog boundary data (1.19), we expect the minimizers  $Q_\lambda$  or  $Q_\lambda^\mu$  to be axially symmetric around a fixed axis (in a sense made precise below). In particular, we expect their biaxiality regions (1.23) to be axially symmetric as well. More precisely,  $\{\beta < t\}$  with  $t \in (-1, 1)$  should be an increasing family of axially symmetric solid tori, and the complementary regions  $\{\beta > t\}$  should be kind of distance neighborhoods from the boundary  $\partial\Omega$  with cylindrical neighborhoods of the symmetry axis added. In the extreme case  $t = \pm 1$ , we expect  $\{\beta = -1\}$  to be a circle with axial symmetry, and  $\{\beta = 1\}$  to be the sphere  $\partial\Omega$  with the segment connecting the two antipodal points lying on the symmetry axis added. Clearly sub and superlevel of the biaxiality function should be mutually linked in the sense of Definition 1.5 above. This conjectural picture is supported by numerical simulations as already detailed in [49, 32, 19, 33], where authors

<sup>2</sup>As an example, if  $\Omega$  is the unit ball,  $A$  is an unknotted embedded copy of  $\mathbb{S}^1$  into  $\Omega$ , and  $B = \bar{\Omega} \setminus A_\delta$  with  $A_\delta$  a sufficiently small tubular neighborhood of  $A$ , then  $A$  and  $B$  are mutually linked.

refer to it as the **“torus solution”** of the Landau-de Gennes model. For the nematic droplet with radial anchoring, the situation clearly reminds the one corresponding to the Hopf fibration

$$\mathbb{C} \times \mathbb{C} \supseteq \mathbb{S}^3 \xrightarrow{\Phi} \mathbb{S}^2 \subseteq \mathbb{C} \times \mathbb{R}, \quad \Phi(z_1, z_2) = (2z_1\bar{z}_2, |z_1|^2 - |z_2|^2),$$

where the subsets  $\{|z_1|^2 - |z_2|^2 > t\}$  and  $\{|z_1|^2 - |z_2|^2 < t\}$  with  $t \in (-1, 1)$  form a decomposition of  $\mathbb{S}^3$  into two disjoint mutually linked solid tori (a so-called Heegaard splitting).

The weak counterpart of the conjectural picture described in the example above is the main topological result of the paper.

**Theorem 1.6.** *Let  $\Omega \subseteq \mathbb{R}^3$  be a bounded connected open set with boundary of class  $C^3$ , and assume that either  $Q = Q_\lambda$  is a minimizer of  $\mathcal{E}_\lambda$  as in Theorem 1.2 or  $Q = Q_\lambda^\mu$  is a minimizer of  $\mathcal{F}_{\lambda,\mu}$  as in Theorem 1.3, so that  $(HP_0)$  holds. If assumptions  $(HP_1)$ - $(HP_3)$  also hold (e.g., suppose that  $\Omega$  is connected and simply connected,  $\partial\Omega$  has an odd number of connected components, and that  $Q_b(x) = \sqrt{3}/2(\vec{n}(x) \otimes \vec{n}(x) - \frac{1}{3}I)$  is the radial anchoring), then the biaxiality regions associated to the configuration  $Q$  satisfy:*

- 1) *the set of singular values of  $\beta = \tilde{\beta} \circ Q$  in  $[-1, \bar{\beta}]$  is at most countable, and it can accumulate only at  $\bar{\beta}$ ; moreover, for any regular value  $-1 < t < \bar{\beta}$  of  $\beta$  the set  $\{\beta = t\} \subseteq \Omega$  is a smooth surface with a connected component of positive genus;*
- 2) *for any  $-1 \leq t_1 < t_2 < \bar{\beta}$ , the sets  $\{\beta \leq t_1\} \subseteq \Omega$  and  $\{\beta \geq t_2\} \subseteq \bar{\Omega}$  are nonempty, compact, and not simply connected;*
- 3) *if in addition  $Q \in C^\omega(\bar{\Omega})$  and  $\bar{\beta} = 1$ , then the set of critical values is finite and  $\{\beta = 1\} \subseteq \bar{\Omega}$  is nonempty, compact, and not simply connected; in particular  $\{\beta = 1\} \cap \Omega$  is not empty;*
- 4) *for any  $-1 \leq t_1 < t_2 < \bar{\beta}$ , if the interval  $(t_1, t_2)$  contains no critical value, then  $\{\beta \leq t_1\}$  and  $\{\beta \geq t_2\}$  are mutually linked.*

Claim 1) on discreteness of the set of singular values is a consequence of the analytic Morse-Sard theorem from [59]. The rest of the claim together with claim 2) is proved by contradiction using a degree-counting argument. The key observation is that on each spherical component of a biaxial surface  $\{\beta = t\}$ , the pull back bundle  $E = v_{\max}^* F$  of the tangent bundle  $F = T\mathbb{S}^2 \rightarrow \mathbb{S}^2$  under the lifting  $v_{\max}$  of the eigenspace map  $V_{\max}$  must be trivial (hence its Euler number vanishes). Then the contradiction coming essentially from  $(HP_3)$  ensures that some  $S_i$  has positive genus. The argument for 2) and 3) above holds for regular values  $t \in (-1, \bar{\beta})$ , and the extension to arbitrary values is based on the analytic regularity of  $Q$  and the Lojasiewicz retraction theorem [39] (it is the only instance where this property is used). Finally, the linking property in 4) follows easily by contradiction using a deformation of the biaxial regions along the positive/negative gradient flow of  $\beta$ . We expect analogous properties to hold also for  $t \in (\bar{\beta}, 1)$ , but this case seems to be more subtle since the biaxial surfaces meet the boundary  $\partial\Omega$ , and we do not have rigorous result in this direction at present.

As the conclusions of the theorem are weak counterparts of the properties conjectured for the torus solution on a nematic droplet, we refer to such solutions on a general domain as **“torus-like solutions”**. It is a very challenging open problem to obtain a precise estimate on the genus of the surfaces  $S_i$ , if any. Any control on it should depend on a subtle role of the genus in giving a possible lower order correction term in the energy expansion of the minimizing configurations.

In our subsequent papers [15] and [16] of the series, we continue this analysis focusing on axially symmetric configurations. Letting  $\mathbb{S}^1$  act by rotation around the vertical axis on an  $\mathbb{S}^1$ -invariant domain  $\Omega \subseteq \mathbb{R}^3$ , and on  $\mathcal{S}_0$  by the induced action  $\mathcal{S}_0 \ni A \mapsto R^t A R \in \mathcal{S}_0$ ,  $R \in \mathbb{S}^1$ , we consider Sobolev maps  $Q \in W^{1,2}(\Omega; \mathcal{S}_0)$  satisfying the equivariance property

$$Q(Rx) = R^t Q(x) R \quad \forall R \in \mathbb{S}^1. \quad (1.24)$$

Minimizing the energy functional (1.14) or (1.10) in the appropriate class of equivariant configurations will provide minimizers which are either smooth and nowhere vanishing or with singularities/isotropic points, depending on the geometry of the domain and on the chosen boundary data. In case such defects are not present, we will be able to show that the level sets of the signed biaxiality parameter are generically finite union of axially symmetric tori. On the other hand, when singularities/isotropic points occur, the regularity/absence of isotropic phase results of the present paper will show that axial symmetry of minimizers is not inherited from the boundary condition, and axial symmetry breaking and nonuniqueness phenomena must occur. Such phenomena were

already proved in [1] for minimizers of the Frank-Oseen energy, and our results are the natural counterpart for the Landau-de Gennes model, in agreement with the numerical simulations in [14].

**Acknowledgements.** We would like to thank Eugene Gartland for having pointed out to us the reference [18] and suggested to discuss the validity of our results for non-dimensionalized forms of the Landau-de Gennes energy.

## 2. SMALL ENERGY REGULARITY THEORY: A TOOL BOX

The aim of this section is to provide several regularity estimates, both in the interior and at the boundary, for weak solutions of (1.16) under certain general conditions. We emphasize that the material developed here is not restricted to minimizers of the energy functional  $\mathcal{E}_\lambda$ , but it applies to rather general critical points satisfying suitable *energy monotonicity formulae*. With this respect, we shall make a crucial use of the results of this section in our companion papers [15, 16] where we considered solutions obtained by minimization of  $\mathcal{E}_\lambda$  in restricted (symmetric) classes.

Before going further, let us precise for completeness the (usual) notion of critical point of  $\mathcal{E}_\lambda$  over the nonlinear space  $W^{1,2}(\Omega; \mathbb{S}^4)$ , and show that critical points are exactly the distributional solutions of (1.16) belonging to  $W^{1,2}(\Omega; \mathbb{S}^4)$ .

**Definition 2.1.** A map  $Q_\lambda \in W^{1,2}(\Omega; \mathbb{S}^4)$  is said to be a critical point of  $\mathcal{E}_\lambda$  if

$$\left[ \frac{d}{dt} \mathcal{E}_\lambda \left( \frac{Q_\lambda + t\Phi}{|Q_\lambda + t\Phi|} \right) \right]_{t=0} = 0$$

for every  $\Phi \in C_c^1(\Omega; \mathcal{S}_0)$ .

The Euler-Lagrange equation for critical points of  $\mathcal{E}_\lambda$  reads as follows.

**Proposition 2.2.** *A map  $Q_\lambda \in W^{1,2}(\Omega; \mathbb{S}^4)$  is a critical point of  $\mathcal{E}_\lambda$  if and only if*

$$\int_{\Omega} \nabla Q_\lambda : \nabla \Phi \, dx = \lambda \int_{\Omega} Q_\lambda^2 : \Phi \, dx \quad (2.1)$$

for every  $\Phi \in W^{1,2}(\Omega; Q_\lambda^* T\mathbb{S}^4)$  compactly supported in  $\Omega$  (i.e., for every  $\Phi \in W^{1,2}(\Omega; \mathcal{S}_0)$  compactly supported in  $\Omega$  and satisfying  $\Phi(x) \in T_{Q_\lambda(x)}\mathbb{S}^4$  for a.e.  $x \in \Omega$ ), or equivalently, if and only if

$$-\Delta Q_\lambda = |\nabla Q_\lambda|^2 Q_\lambda + \lambda \left( Q_\lambda^2 - \frac{1}{3} I - \text{tr}(Q_\lambda^3) Q_\lambda \right) \quad \text{in } \mathcal{D}'(\Omega). \quad (2.2)$$

*Proof. Step 1.* Given  $Q \in W^{1,2}(\Omega; \mathbb{S}^4)$ , let us consider  $\Phi \in C_c^1(\Omega; \mathcal{S}_0)$ , and set for  $t$  small enough,

$$Q_t := \frac{Q + t\Phi}{|Q + t\Phi|} \in W^{1,2}(\Omega; \mathcal{S}_0).$$

Classically (see e.g. [58, Section 2.2]), we have

$$\left[ \frac{d}{dt} \int_{\Omega} \frac{1}{2} |\nabla Q_t|^2 \, dx \right]_{t=0} = \int_{\Omega} (\nabla Q : \nabla \Phi - |\nabla Q|^2 Q : \Phi) \, dx.$$

On the other hand, a straightforward computations yields

$$\left[ \frac{d}{dt} \int_{\Omega} W(Q_t) \, dx \right]_{t=0} = - \int_{\Omega} (Q^2 : \Phi - \text{tr}(Q^3) Q : \Phi) \, dx,$$

and thus

$$\begin{aligned} \left[ \frac{d}{dt} \mathcal{E}_\lambda \left( \frac{Q + t\Phi}{|Q + t\Phi|} \right) \right]_{t=0} &= \int_{\Omega} \nabla Q : \nabla \Phi \, dx - \int_{\Omega} |\nabla Q|^2 Q : \Phi \, dx \\ &\quad - \lambda \int_{\Omega} (Q^2 : \Phi - \text{tr}(Q^3) Q : \Phi) \, dx. \end{aligned} \quad (2.3)$$

*Step 2.* Assume that  $Q_\lambda \in W^{1,2}(\Omega; \mathbb{S}^4)$  is a critical point of  $\mathcal{E}_\lambda$ . We consider  $\Phi \in W^{1,2}(\Omega; Q_\lambda^* T\mathbb{S}^4)$  compactly supported in  $\Omega$ , and prove that (2.1) holds. By a standard truncation argument, we can assume that  $\Phi \in L^\infty(\Omega)$ . By a usual approximation argument, we can find a sequence  $\{\Phi_k\} \subseteq C_c^1(\Omega; \mathcal{S}_0)$  such that  $\Phi_k \rightarrow \Phi$  a.e. in  $\Omega$  and strongly in  $W^{1,2}(\Omega)$ , and satisfying  $\|\Phi_k\|_{L^\infty(\Omega)} \leq \|\Phi\|_{L^\infty(\Omega)}$ . Then we deduce from Step 1 and the criticality of  $Q_\lambda$  that

$$\int_{\Omega} \nabla Q_\lambda : \nabla \Phi_k \, dx = \int_{\Omega} |\nabla Q_\lambda|^2 Q_\lambda : \Phi_k \, dx + \lambda \int_{\Omega} (Q_\lambda^2 : \Phi_k - \text{tr}(Q_\lambda^3) Q_\lambda : \Phi_k) \, dx. \quad (2.4)$$

Since  $Q_\lambda : \Phi = 0$  a.e. in  $\Omega$ , we deduce by dominated convergence that  $|\nabla Q_\lambda|^2 Q_\lambda : \Phi_k \rightarrow 0$  and  $(Q_\lambda^2 : \Phi_k - \text{tr}(Q_\lambda^3) Q_\lambda : \Phi_k) \rightarrow Q_\lambda^2 : \Phi$  in  $L^1(\Omega)$ . Hence, letting  $k \rightarrow \infty$  in (2.4) leads to (2.1).

*Step 3.* Assume that  $Q_\lambda \in W^{1,2}(\Omega; \mathbb{S}^4)$  satisfies (2.1), and fix an arbitrary  $\Phi \in C_c^1(\Omega; \mathcal{M}_{3 \times 3}^{\text{sym}}(\mathbb{R}))$ . Define  $\Phi_0 := \Phi - \frac{1}{3}(\Phi : I)I \in C_c^1(\Omega; \mathcal{S}_0)$ . Noticing that

$$\Phi_0 - (Q_\lambda : \Phi_0)Q_\lambda \in W_0^{1,2}(\Omega; Q_\lambda^* T\mathbb{S}^4),$$

we infer from (2.1) that

$$\int_\Omega \nabla Q_\lambda : \nabla \Phi_0 dx = \int_\Omega |\nabla Q_\lambda|^2 Q_\lambda : \Phi_0 dx + \lambda \int_\Omega (Q_\lambda^2 : \Phi_0 - \text{tr}(Q_\lambda^3) Q_\lambda : \Phi_0) dx. \quad (2.5)$$

Since  $Q_\lambda : I = \text{tr}(Q_\lambda) = 0$  and  $|Q_\lambda|^2 = \text{tr}(Q_\lambda^2) = 1$ , this last identity leads to

$$\int_\Omega \nabla Q_\lambda : \nabla \Phi dx = \int_\Omega |\nabla Q_\lambda|^2 Q_\lambda : \Phi dx + \lambda \int_\Omega \left( Q_\lambda^2 - \frac{1}{3}I - \text{tr}(Q_\lambda^3) Q_\lambda \right) : \Phi dx,$$

and (2.2) follows.

*Step 4.* Finally, if  $Q_\lambda \in W^{1,2}(\Omega; \mathbb{S}^4)$  satisfies (2.2), then (2.5) holds for every  $\Phi_0 \in C_c^1(\Omega; \mathcal{S}_0)$ . In view of (2.3), it implies that  $Q_\lambda$  is indeed a critical point of  $\mathcal{E}_\lambda$ .  $\square$

**Remark 2.3.** If a map  $Q_\lambda \in W^{1,2}(\Omega; \mathbb{S}^4)$  is a minimizer of  $\mathcal{E}_\lambda$  among all  $Q \in W^{1,2}(\Omega; \mathbb{S}^4)$  such that  $Q - Q_\lambda$  is compactly supported in  $\Omega$ , then  $Q_\lambda$  is a critical point of  $\mathcal{E}_\lambda$  by the first order condition for minimality. In particular, if  $Q_\lambda$  is minimizing  $\mathcal{E}_\lambda$  over  $\mathcal{A}_{Q_b}(\Omega)$ , then  $Q_\lambda$  satisfies (2.2) (or equivalently (2.1)).

**2.1. Monotonicity formulae.** In this subsection, our goal is (essentially) to derive the aforementioned monotonicity formulae for certain critical points of  $\mathcal{E}_\lambda$ . Concerning minimizers, such formulae can be classically obtained by inner variations of the energy. However this argument can not be used when considering energy minimizers over symmetric classes as we do in [15, 16]. To circumvent this difficulty, we consider critical points of  $\mathcal{E}_\lambda$  which can be (strongly) approximated by critical points of a suitable Ginzburg-Landau functional in which the constraint to be  $\mathbb{S}^4$ -valued is relaxed. In this way, the approximate solution is smooth enough to derive the monotonicity formulae from the Euler-Lagrange equation, and we conclude by taking the limit in the approximation parameter. This procedure applies of course to minimizers (as we shall see in Section 3), but also to the symmetric solutions of (1.16) considered in [15, 16]. Let us now describe it in details.

Given a bounded open set  $\Omega \subseteq \mathbb{R}^3$ , a reference map  $Q_{\text{ref}} \in \mathcal{A}_{Q_b}(\Omega)$  and a small parameter  $\varepsilon \in (0, \lambda^{-1/2})$ , we consider the energy functional  $\mathcal{G}\mathcal{L}_\varepsilon(Q_{\text{ref}}; \cdot)$  defined over  $W^{1,2}(\Omega; \mathcal{S}_0)$  by

$$\mathcal{G}\mathcal{L}_\varepsilon(Q_{\text{ref}}; Q) := \mathcal{E}_\lambda(Q) + \frac{1}{4\varepsilon^2} \int_\Omega (1 - |Q|^2)^2 dx + \frac{1}{2} \int_\Omega |Q - Q_{\text{ref}}|^2 dx. \quad (2.6)$$

If  $Q_{\text{ref}}$  can be achieved as a (strong) limit of critical points of  $\mathcal{G}\mathcal{L}_\varepsilon(Q_{\text{ref}}; \cdot)$  when  $\varepsilon \rightarrow 0$ , then  $Q_{\text{ref}}$  satisfies the monotonicity formulae stated in the following proposition.

**Proposition 2.4.** *Assume that  $\partial\Omega$  is of class  $C^3$  and  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ . Let  $Q_{\text{ref}} \in \mathcal{A}_{Q_b}(\Omega)$ . For each  $\varepsilon > 0$ , let  $Q_\varepsilon \in W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$  be a critical point of the functional  $\mathcal{G}\mathcal{L}_\varepsilon(Q_{\text{ref}}; \cdot)$ . If*

$$Q_\varepsilon \xrightarrow{\varepsilon \rightarrow 0} Q_{\text{ref}} \text{ in } L^2(\Omega), \text{ and } \mathcal{G}\mathcal{L}_\varepsilon(Q_{\text{ref}}; Q_\varepsilon) \xrightarrow{\varepsilon \rightarrow 0} \mathcal{E}_\lambda(Q_{\text{ref}}), \quad (2.7)$$

then  $Q_{\text{ref}}$  satisfies

1) *the Interior Monotonicity Formula:*

$$\frac{1}{r} \mathcal{E}_\lambda(Q_{\text{ref}}, B_r(x_0)) - \frac{1}{\rho} \mathcal{E}_\lambda(Q_{\text{ref}}, B_\rho(x_0)) = \int_{B_r(x_0) \setminus B_\rho(x_0)} \frac{1}{|x - x_0|} \left| \frac{\partial Q_{\text{ref}}}{\partial |x - x_0|} \right|^2 dx + 2\lambda \int_\rho^r \left( \frac{1}{t^2} \int_{B_t(x_0)} W(Q_{\text{ref}}) dx \right) dt \quad (2.8)$$

for every  $x_0 \in \Omega$  and every  $0 < \rho < r \leq \text{dist}(x_0, \partial\Omega)$ ;

2) *the Boundary Monotonicity Inequality: there exist two constants  $C_\Omega > 0$  and  $\mathbf{r}_\Omega > 0$  (depending only on  $\Omega$ ) such that*

$$\begin{aligned} & \frac{1}{r} \mathcal{E}_\lambda(Q_{\text{ref}}, B_r(x_0) \cap \Omega) - \frac{1}{\rho} \mathcal{E}_\lambda(Q_{\text{ref}}, B_\rho(x_0) \cap \Omega) \geq -(r - \rho) K_\lambda(Q_{\text{b}}, Q_{\text{ref}}) \\ & + \int_{(B_r(x_0) \setminus B_\rho(x_0)) \cap \Omega} \frac{1}{|x - x_0|} \left| \frac{\partial Q_{\text{ref}}}{\partial |x - x_0|} \right|^2 dx + 2\lambda \int_\rho^r \left( \frac{1}{t^2} \int_{B_t(x_0) \cap \Omega} W(Q_{\text{ref}}) dx \right) dt \end{aligned} \quad (2.9)$$

for every  $x_0 \in \partial\Omega$  and every  $0 < \rho < r < \mathbf{r}_\Omega$ , where

$$K_\lambda(Q_{\text{b}}, Q_{\text{ref}}) := C_\Omega \left( \|\nabla_{\text{tan}} Q_{\text{b}}\|_{L^\infty(\partial\Omega)}^2 + \lambda \|W(Q_{\text{b}})\|_{L^1(\partial\Omega)} + \|\nabla Q_{\text{ref}}\|_{L^2(\Omega)}^2 \right).$$

*Proof. Step 1: Euler-Lagrange equation, regularity, and convergence.* Since  $Q_\varepsilon$  is a critical point of  $\mathcal{G}\mathcal{L}_\varepsilon(Q_{\text{ref}}; \cdot)$  over  $W_{Q_{\text{b}}}^{1,2}(\Omega; \mathcal{S}_0)$ , it satisfies the Euler-Lagrange equation

$$\begin{cases} -\Delta Q_\varepsilon = \lambda \left( Q_\varepsilon^2 - \frac{1}{3} |Q_\varepsilon|^2 I - \frac{1}{\sqrt{6}} |Q_\varepsilon|^2 Q_\varepsilon \right) + \frac{1}{\varepsilon^2} (1 - |Q_\varepsilon|^2) Q_\varepsilon - (Q_\varepsilon - Q_{\text{ref}}) & \text{in } \Omega, \\ Q_\varepsilon = Q_{\text{b}} & \text{on } \partial\Omega. \end{cases} \quad (2.10)$$

This equation can be easily derived from outer variations noticing that the term  $\frac{1}{3} |Q_\varepsilon|^2 I$  corresponds to the Lagrange multiplier associated to the traceless constraint and using the expression (1.12) for the potential  $W$ . By the Sobolev embedding  $W^{1,2}(\Omega) \hookrightarrow L^6(\Omega)$ , we have  $Q_\varepsilon \in L^6(\Omega)$ , which implies that  $\Delta Q_\varepsilon \in L^2(\Omega)$ . Note that the regularity assumption on  $Q_{\text{b}}$  and  $\partial\Omega$  ensures that  $Q_{\text{b}}$  admits a  $C^{1,1}$  extension (with values in  $\mathcal{S}_0$ ) to the whole domain  $\Omega$  (see the material in Subsection 2.2). By elliptic regularity, we thus have  $Q_\varepsilon \in W^{2,2}(\Omega)$ , see e.g. [22, Theorem 8.12]. In particular,  $Q_\varepsilon \in W^{1,6}(\Omega)$  and thus  $Q_\varepsilon \in L^\infty(\Omega)$  by the Sobolev embedding  $W^{1,6}(\Omega) \hookrightarrow L^\infty(\Omega)$ . Hence,  $\Delta Q_\varepsilon \in L^\infty(\Omega)$ , and by elliptic regularity again, we have  $Q_\varepsilon \in C^{1,\alpha}(\bar{\Omega})$  for every  $\alpha \in (0, 1)$ , see e.g. [22, Theorem 8.34].

We now claim that assumption (2.7) implies that

$$Q_\varepsilon \xrightarrow{\varepsilon \rightarrow 0} Q_{\text{ref}} \text{ strongly in } W^{1,2}(\Omega), \text{ and } \frac{1}{\varepsilon^2} \int_\Omega (1 - |Q_\varepsilon|^2)^2 dx \xrightarrow{\varepsilon \rightarrow 0} 0.$$

Indeed, we first infer from (2.7) that  $\{Q_\varepsilon\}_{\varepsilon > 0}$  remains bounded in  $W^{1,2}(\Omega)$  as  $\varepsilon \rightarrow 0$ . Therefore, given an arbitrary sequence  $\varepsilon_n \rightarrow 0$ , we have  $Q_{\varepsilon_n} \rightharpoonup Q_{\text{ref}}$  weakly in  $W^{1,2}(\Omega)$ . In particular,  $Q_{\varepsilon_n} \rightarrow Q_{\text{ref}}$  in  $L^4(\Omega)$  by the compact Sobolev embedding  $W^{1,2}(\Omega) \hookrightarrow L^4(\Omega)$ . As a consequence,  $\int_\Omega W(Q_{\varepsilon_n}) dx \rightarrow \int_\Omega W(Q_{\text{ref}}) dx$ . On the other hand, by (2.7) and lower semi-continuity of the Dirichlet integral, we have

$$\begin{aligned} \mathcal{E}_\lambda(Q_{\text{ref}}) & \leq \liminf_{n \rightarrow \infty} \mathcal{E}_\lambda(Q_{\varepsilon_n}) \leq \limsup_{n \rightarrow \infty} \mathcal{E}_\lambda(Q_{\varepsilon_n}) \\ & \leq \lim_{n \rightarrow \infty} \left( \mathcal{E}_\lambda(Q_{\varepsilon_n}) + \frac{1}{4\varepsilon_n^2} \int_\Omega (1 - |Q_{\varepsilon_n}|^2)^2 dx \right) = \mathcal{E}_\lambda(Q_{\text{ref}}). \end{aligned}$$

Hence  $\frac{1}{\varepsilon_n^2} \int_\Omega (1 - |Q_{\varepsilon_n}|^2)^2 dx \rightarrow 0$ , and  $\|\nabla Q_{\varepsilon_n}\|_{L^2(\Omega)} \rightarrow \|\nabla Q_{\text{ref}}\|_{L^2(\Omega)}$ . This latter fact, combined with the  $W^{1,2}$ -weak convergence, implies the  $W^{1,2}$ -strong convergence of  $Q_{\varepsilon_n}$  toward  $Q_{\text{ref}}$ .

*Step 2: Interior Monotonicity Formula.* Without loss of generality, we may assume that  $x_0 = 0$ . Let us take the inner product of (2.10) with  $(x \cdot \nabla) Q_\varepsilon$ , and integrate by parts over the ball  $B_t$  of radius  $t \in (\rho, r)$ . It yields

$$\begin{aligned} & -\frac{1}{2} \int_{B_t} |\nabla Q_\varepsilon|^2 dx + \frac{t}{2} \int_{\partial B_t} |\nabla Q_\varepsilon|^2 d\mathcal{H}^2 - \lambda \int_{B_t} W(Q_\varepsilon) dx + \lambda t \int_{\partial B_t} W(Q_\varepsilon) d\mathcal{H}^2 \\ & - \frac{1}{4\varepsilon^2} \int_{B_t} (1 - |Q_\varepsilon|^2)^2 dx + \frac{t}{4\varepsilon^2} \int_{\partial B_t} (1 - |Q_\varepsilon|^2)^2 d\mathcal{H}^2 - \frac{1}{2} \int_{B_t} |Q_\varepsilon - Q_{\text{ref}}|^2 dx + \frac{t}{2} \int_{\partial B_t} |Q_\varepsilon - Q_{\text{ref}}|^2 d\mathcal{H}^2 \\ & = t \int_{\partial B_t} \left| \frac{\partial Q_\varepsilon}{\partial |x|} \right|^2 d\mathcal{H}^2 + 2\lambda \int_{B_t} W(Q_\varepsilon) dx + \frac{1}{2\varepsilon^2} \int_{B_t} (1 - |Q_\varepsilon|^2)^2 dx \\ & \quad + \int_{B_t} |Q_\varepsilon - Q_{\text{ref}}|^2 dx - \int_{B_t} (Q_\varepsilon - Q_{\text{ref}}) : ((x \cdot \nabla) Q_{\text{ref}}) dx. \end{aligned}$$

Dividing both sides by  $t^2$ , we obtain

$$\begin{aligned} \frac{d}{dt} \left( \frac{1}{t} \mathcal{G}\mathcal{L}_\varepsilon(Q_{\text{ref}}; Q_\varepsilon, B_t) \right) &= \frac{1}{t} \int_{\partial B_t} \left| \frac{\partial Q_\varepsilon}{\partial |x|} \right|^2 d\mathcal{H}^2 + \frac{2\lambda}{t^2} \int_{B_t} W(Q_\varepsilon) dx \\ &+ \frac{1}{2\varepsilon^2 t^2} \int_{B_t} (1 - |Q_\varepsilon|^2)^2 dx + \frac{1}{t^2} \int_{B_t} |Q_\varepsilon - Q_{\text{ref}}|^2 dx - \frac{1}{t^2} \int_{B_t} (Q_\varepsilon - Q_{\text{ref}}) : ((x \cdot \nabla) Q_{\text{ref}}) dx. \end{aligned}$$

Integrating this identity between  $\rho$  and  $r$  yields

$$\begin{aligned} \frac{1}{r} \mathcal{G}\mathcal{L}_\varepsilon(Q_{\text{ref}}; Q_\varepsilon, B_r) - \frac{1}{\rho} \mathcal{G}\mathcal{L}_\varepsilon(Q_{\text{ref}}; Q_\varepsilon, B_\rho) &= \int_{B_r \setminus B_\rho} \frac{1}{|x|} \left| \frac{\partial Q_\varepsilon}{\partial |x|} \right|^2 dx \\ &+ 2\lambda \int_\rho^r \left( \frac{1}{t^2} \int_{B_t} W(Q_\varepsilon) dx \right) dt + \frac{1}{2\varepsilon^2} \int_\rho^r \left( \frac{1}{t^2} \int_{B_t} (1 - |Q_\varepsilon|^2)^2 dx \right) dt \\ &+ \int_\rho^r \left( \frac{1}{t^2} \int_{B_t} |Q_\varepsilon - Q_{\text{ref}}|^2 dx \right) dt - \int_\rho^r \left( \frac{1}{t^2} \int_{B_t} (Q_\varepsilon - Q_{\text{ref}}) : ((x \cdot \nabla) Q_{\text{ref}}) dx \right) dt. \end{aligned}$$

In view of the convergences established in Step 1, letting  $\varepsilon \rightarrow 0$  in this last identity leads to (2.8).

*Step 3: Boundary Monotonicity Inequality.* We first claim that there exists a constant  $C_\Omega > 0$  depending only on  $\Omega$  such that

$$\begin{aligned} \int_{\partial\Omega} \left| \frac{\partial Q_\varepsilon}{\partial \nu} \right|^2 d\mathcal{H}^2 &\leq C_\Omega \left( \|\nabla_{\tan} Q_b\|_{L^2(\partial\Omega)}^2 + \lambda \|W(Q_b)\|_{L^1(\partial\Omega)} \right. \\ &\quad \left. + \|\nabla Q_\varepsilon\|_{L^2(\Omega)}^2 + \|\nabla Q_{\text{ref}}\|_{L^2(\Omega)}^2 + \|Q_\varepsilon - Q_{\text{ref}}\|_{L^2(\Omega)}^2 \right). \end{aligned} \quad (2.11)$$

To prove this estimate, let us introduce  $\Phi_\Omega \in C^{2,\alpha}(\bar{\Omega})$  the unique solution of

$$\begin{cases} -\Delta \Phi_\Omega = 1 & \text{in } \Omega, \\ \Phi_\Omega = 0 & \text{on } \partial\Omega, \end{cases}$$

see e.g. [22, Theorem 6.14]. We consider  $V : \bar{\Omega} \rightarrow \mathbb{R}^3$  the  $C^{1,\alpha}$ -vector field given by  $V := -\nabla \Phi_\Omega$ . Note that  $V = (V \cdot \nu)\nu$  on  $\partial\Omega$  (since  $\Phi_\Omega$  is constant on  $\partial\Omega$ ), where  $\nu$  is outer unit normal on  $\partial\Omega$ . Taking the inner product of (2.10) with  $(V \cdot \nabla)Q_\varepsilon$ , and integrating by parts over  $\Omega$  leads to

$$\begin{aligned} \frac{1}{2} \int_{\partial\Omega} \left| \frac{\partial Q_\varepsilon}{\partial \nu} \right|^2 (V \cdot \nu) d\mathcal{H}^2 \\ + \int_\Omega \left( \frac{1}{2} |\nabla Q_\varepsilon|^2 + \lambda W(Q_\varepsilon) + \frac{1}{4\varepsilon^2} (1 - |Q_\varepsilon|^2)^2 + \frac{1}{2} |Q_\varepsilon - Q_{\text{ref}}|^2 \right) \text{div}(V) dx \\ = \frac{1}{2} \int_{\partial\Omega} |\nabla_{\tan} Q_b|^2 (V \cdot \nu) d\mathcal{H}^2 + \lambda \int_{\partial\Omega} W(Q_b) (V \cdot \nu) d\mathcal{H}^2 \\ + \int_\Omega \sum_{i,j=1}^3 (\partial_i Q_\varepsilon : \partial_j Q_\varepsilon) \partial_j V_i dx + \int_\Omega (Q_\varepsilon - Q_{\text{ref}}) : (V \cdot \nabla) Q_{\text{ref}} dx, \end{aligned}$$

since  $Q_\varepsilon = Q_{\text{ref}} = Q_b$  on  $\partial\Omega$  and  $|Q_b| = 1$ . Using  $\text{div}(V) = 1$  in  $\Omega$ , we deduce that

$$\begin{aligned} \int_{\partial\Omega} \left| \frac{\partial Q_\varepsilon}{\partial \nu} \right|^2 (V \cdot \nu) d\mathcal{H}^2 &\leq C \|V\|_{C^1(\Omega)} \left( \|\nabla_{\tan} Q_b\|_{L^2(\partial\Omega)}^2 + \lambda \|W(Q_b)\|_{L^1(\partial\Omega)} + \|\nabla Q_\varepsilon\|_{L^2(\Omega)}^2 \right. \\ &\quad \left. + \|\nabla Q_{\text{ref}}\|_{L^2(\Omega)}^2 + \|Q_\varepsilon - Q_{\text{ref}}\|_{L^2(\Omega)}^2 \right), \end{aligned}$$

for some universal constant  $C > 0$ . On the other hand, by the Hopf lemma, there is a constant  $\mathbf{c}_\Omega^0 > 0$  depending only on  $\Omega$  such that  $V \cdot \nu \geq \mathbf{c}_\Omega^0$  on  $\partial\Omega$ , and (2.11) follows.

We now fix  $x_0 \in \partial\Omega$ . By the smoothness assumption on  $\partial\Omega$ , there are two constants  $\mathbf{r}_\Omega > 0$  and  $\mathbf{c}_\Omega^1 > 0$  (depending only on  $\Omega$ ) such that for every  $t \in (0, \mathbf{r}_\Omega)$ ,

$$\mathcal{H}^2(B_t(x_0) \cap \partial\Omega) \leq \mathbf{c}_\Omega^1 t^2, \quad \text{and} \quad |(x - x_0) \cdot \nu(x)| \leq \mathbf{c}_\Omega^1 t^2 \quad \text{on } B_t(x_0) \cap \partial\Omega. \quad (2.12)$$

In what follows, we assume without loss of generality that  $x_0 = 0$ . Let us fix  $0 < \rho < r < \mathbf{r}_\Omega$ . Taking once again the inner product of (2.10) with  $(x \cdot \nabla)Q_\varepsilon$ , we integrate the result by parts in

$B_t \cap \Omega$  with  $t \in (\rho, r)$ . Similarly to Step 2, it yields (after dividing by  $t^2$ )

$$\begin{aligned} \frac{d}{dt} \left( \frac{1}{t} \mathcal{G}\mathcal{L}_\varepsilon(Q_{\text{ref}}; Q_\varepsilon, B_t \cap \Omega) \right) &= \frac{1}{t} \int_{\Omega \cap \partial B_t} \left| \frac{\partial Q_\varepsilon}{\partial |x|} \right|^2 d\mathcal{H}^2 + \frac{2\lambda}{t^2} \int_{\Omega \cap B_t} W(Q_\varepsilon) dx \\ &+ \frac{1}{2\varepsilon^2 t^2} \int_{B_t} (1 - |Q_\varepsilon|^2)^2 dx + \frac{1}{t^2} \int_{\Omega \cap B_t} |Q_\varepsilon - Q_{\text{ref}}|^2 dx - \frac{1}{t^2} \int_{\Omega \cap B_t} (Q_\varepsilon - Q_{\text{ref}}) : ((x \cdot \nabla) Q_{\text{ref}}) dx \\ &\quad - \frac{1}{2t^2} \int_{B_t \cap \partial \Omega} |\nabla Q_\varepsilon|^2 (x \cdot \nu) d\mathcal{H}^2 + \frac{1}{t^2} \int_{B_t \cap \partial \Omega} \frac{\partial Q_\varepsilon}{\partial \nu} : ((x \cdot \nabla) Q_\varepsilon) d\mathcal{H}^2 \\ &\quad - \frac{\lambda}{t^2} \int_{B_t \cap \partial \Omega} W(Q_b)(x \cdot \nu) d\mathcal{H}^2. \end{aligned} \quad (2.13)$$

Note that we used once again  $Q_\varepsilon = Q_{\text{ref}} = Q_b$  on  $\partial \Omega$ , and  $|Q_b| = 1$ . Next, if we denote by  $(\tau_1, \tau_2)$  an orthonormal basis of the tangent space of  $\partial \Omega$  at  $x$ , we have

$$\begin{aligned} -\frac{1}{2} \int_{B_t \cap \partial \Omega} |\nabla Q_\varepsilon|^2 (x \cdot \nu) d\mathcal{H}^2 + \int_{B_t \cap \partial \Omega} \frac{\partial Q_\varepsilon}{\partial \nu} : ((x \cdot \nabla) Q_\varepsilon) d\mathcal{H}^2 &= \frac{1}{2} \int_{B_t \cap \partial \Omega} \left| \frac{\partial Q_\varepsilon}{\partial \nu} \right|^2 (x \cdot \nu) d\mathcal{H}^2 \\ &\quad - \frac{1}{2} \int_{B_t \cap \partial \Omega} \left| \frac{\partial Q_b}{\partial \tau_1} \right|^2 (x \cdot \nu) d\mathcal{H}^2 - \frac{1}{2} \int_{B_t \cap \partial \Omega} \left| \frac{\partial Q_b}{\partial \tau_2} \right|^2 (x \cdot \nu) d\mathcal{H}^2 \\ &\quad + \int_{B_t \cap \partial \Omega} \frac{\partial Q_\varepsilon}{\partial \nu} : \frac{\partial Q_b}{\partial \tau_1} (x \cdot \tau_1) d\mathcal{H}^2 + \int_{B_t \cap \partial \Omega} \frac{\partial Q_\varepsilon}{\partial \nu} : \frac{\partial Q_b}{\partial \tau_2} (x \cdot \tau_2) d\mathcal{H}^2. \end{aligned}$$

Then we infer from (2.12) that

$$\begin{aligned} -\frac{1}{2} \int_{B_t \cap \partial \Omega} |\nabla Q_\varepsilon|^2 (x \cdot \nu) d\mathcal{H}^2 + \int_{B_t \cap \partial \Omega} \frac{\partial Q_\varepsilon}{\partial \nu} : ((x \cdot \nabla) Q_\varepsilon) d\mathcal{H}^2 &\geq \\ &\quad - C_\Omega t^2 (\|\partial_\nu Q_\varepsilon\|_{L^2(\partial \Omega)}^2 + \|\nabla_{\tan} Q_b\|_{L^\infty(\partial \Omega)}^2), \end{aligned} \quad (2.14)$$

for a constant  $C_\Omega > 0$  depending only on the constants  $\mathbf{r}_\Omega$  and  $\mathbf{c}_\Omega^1$ . Still by (2.12), we have

$$\int_{B_t \cap \partial \Omega} W(Q_b)(x \cdot \nu) d\mathcal{H}^2 \leq C_\Omega t^2 \int_{\partial \Omega} W(Q_b) d\mathcal{H}^2. \quad (2.15)$$

Inserting (2.14), (2.15), and (2.11) in (2.13), and integrating the resulting inequality between  $\rho$  and  $r$  yields

$$\begin{aligned} \frac{1}{r} \mathcal{G}\mathcal{L}_\varepsilon(Q_{\text{ref}}; Q_\varepsilon, B_r \cap \Omega) - \frac{1}{\rho} \mathcal{G}\mathcal{L}_\varepsilon(Q_{\text{ref}}; Q_\varepsilon, B_\rho \cap \Omega) &\geq -(r - \rho) \tilde{K}_\lambda(Q_b, Q_{\text{ref}}, Q_\varepsilon) \\ &\quad + \int_{(B_r \setminus B_\rho) \cap \Omega} \frac{1}{|x|} \left| \frac{\partial Q_\varepsilon}{\partial |x|} \right|^2 dx + 2\lambda \int_\rho^r \left( \frac{1}{t^2} \int_{B_t \cap \Omega} W(Q_\varepsilon) dx \right) dt \\ &\quad + \frac{1}{2\varepsilon^2} \int_\rho^r \left( \frac{1}{t^2} \int_{B_t \cap \Omega} (1 - |Q_\varepsilon|^2)^2 dx \right) dt + \int_\rho^r \left( \frac{1}{t^2} \int_{B_t \cap \Omega} |Q_\varepsilon - Q_{\text{ref}}|^2 dx \right) dt \\ &\quad - \int_\rho^r \left( \frac{1}{t^2} \int_{B_t \cap \Omega} (Q_\varepsilon - Q_{\text{ref}}) : ((x \cdot \nabla) Q_{\text{ref}}) dx \right) dt, \end{aligned}$$

where

$$\begin{aligned} \tilde{K}_\lambda(Q_b, Q_{\text{ref}}, Q_\varepsilon) &:= C_\Omega \left( \|\nabla_{\tan} Q_b\|_{L^\infty(\partial \Omega)}^2 + \lambda \|W(Q_b)\|_{L^1(\partial \Omega)} \right. \\ &\quad \left. + \|\nabla Q_\varepsilon\|_{L^2(\Omega)}^2 + \|\nabla Q_{\text{ref}}\|_{L^2(\Omega)}^2 + \|Q_\varepsilon - Q_{\text{ref}}\|_{L^2(\Omega)}^2 \right), \end{aligned}$$

and  $C_\Omega > 0$  is a constant depending only on  $\mathbf{r}_\Omega$ ,  $\mathbf{c}_\Omega^1$ ,  $(\mathbf{c}_\Omega^0)^{-1} \|\nabla \Phi_\Omega\|_{C^1(\Omega)}$ , and the (2-dimensional) measure of  $\partial \Omega$ . In view of the convergences established in Step 1, letting  $\varepsilon \rightarrow 0$  in this last inequality leads to (2.9).  $\square$

**Remark 2.5** (Specific geometry [16]). In our companion paper [16], we consider a domain  $\Omega$  and a boundary condition  $Q_b$  for which the following situation occurs:  $0 \in \partial \Omega$ ,  $B_1 \cap \Omega = B_1 \cap \{x_3 > 0\}$ , and  $Q_b$  is constant on  $B_1 \cap \partial \Omega = B_1 \cap \{x_3 = 0\}$ . In this situation, the boundary monotonicity

inequality (2.9) for points on  $B_1 \cap \partial\Omega$  becomes an equality of the following form: for every point  $x_0 \in B_1 \cap \partial\Omega$  and every  $0 < \rho < r < 1 - |x_0|$ ,

$$\frac{1}{r} \mathcal{E}_\lambda(Q_{\text{ref}}, B_r(x_0) \cap \Omega) - \frac{1}{\rho} \mathcal{E}_\lambda(Q_{\text{ref}}, B_\rho(x_0) \cap \Omega) = \int_{(B_r(x_0) \setminus B_\rho(x_0)) \cap \Omega} \frac{1}{|x - x_0|} \left| \frac{\partial Q_{\text{ref}}}{\partial |x - x_0|} \right|^2 dx + 2\lambda \int_\rho^r \left( \frac{1}{t^2} \int_{B_t(x_0) \cap \Omega} W(Q_{\text{ref}}) dx \right) dt.$$

Indeed, it suffices to notice that  $(x - x_0) \cdot \nu = 0$  and  $\nabla_{\text{tan}} Q_b = 0$  on  $B_1 \cap \partial\Omega$ , and then use this facts in identity (2.13).

One of the main consequences of the monotonicity formulae in Proposition 2.4 is a uniform control of the energy in small balls. Recalling that  $\bar{Q}_b \in \mathcal{A}_{Q_b}(\Omega)$  is a given  $\mathbb{S}^4$ -valued extension to the domain  $\Omega$  of the boundary condition  $Q_b$ , we have

**Lemma 2.6.** *Assume that  $\partial\Omega$  is of class  $C^3$  and  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ . If  $Q_{\text{ref}} \in \mathcal{A}_{Q_b}(\Omega)$  satisfies the monotonicity formulae (2.8) and (2.9) with*

$$K_\lambda(Q_b, Q_{\text{ref}}) \leq C_\Omega (\|\nabla_{\text{tan}} Q_b\|_{L^\infty(\partial\Omega)}^2 + \lambda \|W(Q_b)\|_{L^1(\partial\Omega)} + \mathcal{E}_\lambda(\bar{Q}_b))$$

for some constant  $C_\Omega > 0$  depending only on  $\Omega$ , then

(1) for every  $x_0 \in \Omega$  and  $r \in (0, \text{dist}(x_0, \partial\Omega))$ ,

$$\sup_{B_\rho(x) \subseteq B_{r/2}(x_0)} \frac{1}{\rho} \mathcal{E}_\lambda(Q_{\text{ref}}, B_\rho(x)) \leq \frac{2}{r} \mathcal{E}_\lambda(Q_{\text{ref}}, B_r(x_0));$$

(2) there exist two constants  $\mathbf{r}_\Omega^{(1)} > 0$  (depending only on  $\Omega$ ) and  $C_{Q_b}^\lambda$  (depending only on  $\Omega$ ,  $Q_b$ ,  $\lambda \|W(Q_b)\|_{L^1(\partial\Omega)}$ , and  $\mathcal{E}_\lambda(\bar{Q}_b)$ ) such that for every  $x_0 \in \partial\Omega$  and  $r \in (0, \mathbf{r}_\Omega^{(1)})$ ,

$$\sup_{B_\rho(x) \subseteq B_{r/6}(x_0)} \frac{1}{\rho} \mathcal{E}_\lambda(Q_{\text{ref}}, B_\rho(x) \cap \Omega) \leq \frac{4}{r} \mathcal{E}_\lambda(Q_{\text{ref}}, B_r(x_0) \cap \Omega) + C_{Q_b}^\lambda r. \quad (2.16)$$

*Proof. Step 1: proof of (1).* We assume without loss of generality that  $x_0 = 0$ , and we consider an arbitrary ball  $B_\rho(x) \subseteq B_{r/2}$ . By the interior monotonicity formula (2.8), we have

$$\frac{1}{\rho} \mathcal{E}_\lambda(Q_{\text{ref}}, B_\rho(x)) \leq \frac{1}{\rho + |x|} \mathcal{E}_\lambda(Q_{\text{ref}}, B_{\rho+|x|}(x)) \leq \frac{1}{\rho + |x|} \mathcal{E}_\lambda(Q_{\text{ref}}, B_{2(\rho+|x|)}) \leq \frac{2}{r} \mathcal{E}_\lambda(Q_{\text{ref}}, B_r),$$

and the claim is proved.

*Step 2: proof of (2).* We choose  $\mathbf{r}_\Omega^{(1)} \in (0, \mathbf{r}_\Omega)$  (where  $\mathbf{r}_\Omega$  is given by Proposition 2.4) in such a way that the nearest point projection  $\pi_\Omega$  on  $\partial\Omega$  is well defined in the  $\mathbf{r}_\Omega^{(1)}$ -tubular neighborhood of  $\partial\Omega$ . Once again, we may assume that  $x_0 = 0$ , and we consider  $B_\rho(x) \subseteq B_{r/6}$ . We now distinguish different cases.

Assume first that  $x \in \partial\Omega$ . Then, we deduce from the boundary monotonicity inequality (2.9) that

$$\begin{aligned} \frac{1}{\rho} \mathcal{E}_\lambda(Q_{\text{ref}}, B_\rho(x) \cap \Omega) &\leq \frac{1}{\rho + |x|} \mathcal{E}_\lambda(Q_{\text{ref}}, B_{\rho+|x|}(x) \cap \Omega) + C_{Q_b}^\lambda |x| \\ &\leq \frac{1}{\rho + |x|} \mathcal{E}_\lambda(Q_{\text{ref}}, B_{2(\rho+|x|)} \cap \Omega) + C_{Q_b}^\lambda r \leq \frac{2}{r} \mathcal{E}_\lambda(Q_{\text{ref}}, B_r \cap \Omega) + C_{Q_b}^\lambda r. \end{aligned}$$

Next, for  $x \notin \partial\Omega$  and  $|x - \pi_\Omega(x)| \leq \rho$ , we have  $2\rho + |\pi_\Omega(x)| \leq r/2$  so that

$$\frac{1}{\rho} \mathcal{E}_\lambda(Q_{\text{ref}}, B_\rho(x) \cap \Omega) \leq \frac{1}{\rho} \mathcal{E}_\lambda(Q_{\text{ref}}, B_{2\rho}(\pi_\Omega(x)) \cap \Omega) \leq \frac{4}{r} \mathcal{E}_\lambda(Q_{\text{ref}}, B_r \cap \Omega) + C_{Q_b}^\lambda r,$$

by the previous inequality.

Finally, for  $x \in \Omega$  and  $|x - \pi_\Omega(x)| > \rho$ , we have  $B_\rho(x) \subseteq \Omega$  and thus

$$\frac{1}{\rho} \mathcal{E}_\lambda(Q_{\text{ref}}, B_\rho(x)) \leq \frac{1}{|x - \pi_\Omega(x)|} \mathcal{E}_\lambda(Q_{\text{ref}}, B_{|x - \pi_\Omega(x)|}(x)) \leq \frac{4}{r} \mathcal{E}_\lambda(Q_{\text{ref}}, B_r \cap \Omega) + C_{Q_b}^\lambda r,$$

where we have used again the previous inequality,  $|x - \pi_\Omega(x)| \leq r/6$ , and  $|\pi_\Omega(x)| \leq r/6$ .  $\square$

**Remark 2.7** (Specific geometry [16]). As already mentioned in Remark 2.5, we consider in our companion paper [16] a situation where  $0 \in \partial\Omega$ ,  $B_1 \cap \Omega = B_1 \cap \{x_3 > 0\}$ ,  $Q_b$  is constant on  $B_1 \cap \partial\Omega = B_1 \cap \{x_3 = 0\}$ . In this case, if  $Q_{\text{ref}} \in \mathcal{A}_{Q_b}(\Omega)$  satisfies the boundary monotonicity formula in Remark 2.5, then we can repeat the argument in Lemma 2.6 above to obtain

$$\sup_{B_\rho(x) \subseteq B_{1/6}} \frac{1}{\rho} \mathcal{E}_\lambda(Q_{\text{ref}}, B_\rho(x) \cap \Omega) \leq 4\mathcal{E}_\lambda(Q_{\text{ref}}, B_1 \cap \Omega) \quad (2.17)$$

instead of (2.16) (with  $x_0 = 0$  and  $r = 1$ ).

**2.2. Reflection across the boundary.** To obtain regularity estimates at the boundary for critical points of  $\mathcal{E}_\lambda$  in the class  $\mathcal{A}_{Q_b}(\Omega)$ , we rely on arguments developed by C. Scheven in [53]. The main idea is to construct a suitable reflection across the boundary taking into account the prescribed boundary condition  $Q_b$  in such a way that the reflected critical point satisfies an equation similar in nature to (2.2) in a larger domain. Boundary regularity can then be treated as an interior regularity problem. The aim of this subsection is to construct such reflection and to derive the resulting equation in the extended domain. We proceed as follows.

We still assume that the boundary of the bounded open set  $\Omega \subseteq \mathbb{R}^3$  is of class  $C^3$ . In this way, we can find a small number  $\delta_\Omega > 0$  such that the nearest point projection  $\pi_\Omega$  on  $\partial\Omega$  is well defined and of class  $C^2$  in the  $(2\delta_\Omega)$ -tubular neighborhood of  $\partial\Omega$  (see e.g. [58, Chapter 2, Section 2.12.3]). We set for  $\delta \in (0, 2\delta_\Omega]$ ,

$$\begin{aligned} U_\delta &:= \{x \in \mathbb{R}^3 : \text{dist}(x, \partial\Omega) < \delta\}, \\ U_\delta^{\text{ex}} &:= \{x \in U_\delta : (x - \pi_\Omega(x)) \cdot \nu(\pi_\Omega(x)) > 0\}, \\ U_\delta^{\text{in}} &:= U_\delta \setminus \overline{U_\delta^{\text{ex}}}, \end{aligned}$$

where  $\nu$  denotes the outer unit normal vector field on  $\partial\Omega$ . Choosing  $\delta_\Omega$  smaller if necessary, we can assume that

$$\Omega \cap B_{2\delta_\Omega}(x) = U_{2\delta_\Omega}^{\text{in}} \cap B_{2\delta_\Omega}(x) \quad \forall x \in \partial\Omega.$$

The *geodesic reflection* across  $\partial\Omega$  is the involutive  $C^2$ -diffeomorphism  $\sigma_\Omega : U_{2\delta_\Omega} \rightarrow U_{2\delta_\Omega}$  given by

$$\sigma_\Omega(x) := 2\pi_\Omega(x) - x.$$

It satisfies

$$\sigma_\Omega(U_\delta^{\text{in}}) = U_\delta^{\text{ex}} \quad \forall \delta \in (0, 2\delta_\Omega), \text{ and } \sigma_\Omega(x) = x \quad \forall x \in \partial\Omega.$$

Being involutive, its (matrix) differential satisfies

$$D\sigma_\Omega(\sigma_\Omega(x))D\sigma_\Omega(x) = I \quad \forall x \in U_{2\delta_\Omega}. \quad (2.18)$$

Moreover, for every  $x \in \partial\Omega$  we have

$$D\sigma_\Omega(x)v = 2\mathbf{p}_x(v) - v \quad \forall v \in \mathbb{R}^3,$$

where  $\mathbf{p}_x$  denotes the orthogonal projection of  $\mathbb{R}^3$  onto the tangent plane  $T_x(\partial\Omega)$ , i.e., in this case  $D\sigma_\Omega(x)$  is the (linear) reflection across the tangent plane  $T_x(\partial\Omega)$ . In particular,

$$D\sigma_\Omega(x)(D\sigma_\Omega(x))^t = D\sigma_\Omega(x)D\sigma_\Omega(x) = I \quad \forall x \in \partial\Omega, \quad (2.19)$$

where  $I$  is the identity matrix. We now extend the domain  $\Omega$  to the domain

$$\widehat{\Omega} := \Omega \cup U_{\delta_\Omega} = \overline{\Omega} \cup U_{\delta_\Omega}^{\text{ex}}, \quad (2.20)$$

and we simplify the notation by setting

$$U := U_{\delta_\Omega}, \quad U^{\text{ex}} := U_{\delta_\Omega}^{\text{ex}}, \quad U^{\text{in}} := U_{\delta_\Omega}^{\text{in}}.$$

On the extended domain  $\widehat{\Omega}$ , we consider the Lipschitz continuous field of symmetric  $3 \times 3$ -matrices

$$A(x) = \left( a_{kl}(x) \right)_{k,l=1}^3 := \begin{cases} |J(\sigma_\Omega(x))| D\sigma_\Omega(\sigma_\Omega(x)) (D\sigma_\Omega(\sigma_\Omega(x)))^t & \text{if } x \in \widehat{\Omega} \setminus \Omega, \\ I & \text{otherwise,} \end{cases} \quad (2.21)$$

where  $J(\sigma_\Omega)$  denotes the Jacobian determinant of  $\sigma_\Omega$ . Note that the continuity of  $A$  across  $\partial\Omega$  follows from (2.19). In addition, (2.18) implies that  $A$  is uniformly elliptic, i.e.,

$$m_\Omega I \leq A(x) \leq M_\Omega I \quad \forall x \in \widehat{\Omega}$$

in the sense of quadratic forms for some constants  $m_\Omega > 0$  and  $M_\Omega > 0$  depending only on  $\Omega$ .

Let us now consider for any given  $(Q_1, Q_2) \in \mathcal{S}_0 \times \mathcal{S}_0$  their tensor product  $Q_1 \otimes Q_2$  as the linear mapping  $Q_1 \otimes Q_2: \mathcal{S}_0 \rightarrow \mathcal{S}_0$  defined by

$$(Q_1 \otimes Q_2)P := (P : Q_2)Q_1$$

for any  $P \in \mathcal{S}_0$ . The *geodesic reflection* on  $\mathbb{S}^4 \subseteq \mathcal{S}_0$  with respect to a point  $N \in \mathbb{S}^4$  is given by the linear mapping  $(2N \otimes N - \text{id})$ , where  $\text{id}$  denotes the identity map on  $\mathcal{S}_0$ . Note that  $(2N \otimes N - \text{id})$  is simply the orthogonal symmetry with respect to  $\langle N \rangle$  which is the identity along  $\langle N \rangle$  and minus the identity along any orthogonal direction to  $N$ . In particular, it is involutive, isometric, and symmetric. Given a boundary data  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ , we consider the mapping  $\Sigma: U \rightarrow \text{GL}(\mathcal{S}_0)$  of class  $C^{1,1}$  given by

$$\Sigma(x) := 2Q_b(\pi_\Omega(x)) \otimes Q_b(\pi_\Omega(x)) - \text{id}.$$

Notice that by construction  $\partial_\nu \Sigma \equiv 0$  on  $\partial\Omega$ , as  $\partial_\nu \pi_\Omega(x) = 0$  for any  $x \in \partial\Omega$ .

With the help of  $\Sigma$ , we define the extension procedure of maps in  $\mathcal{A}_{Q_b}(\Omega)$  to the domain  $\widehat{\Omega}$  as follows: to a map  $Q \in \mathcal{A}_{Q_b}(\Omega)$  we associate  $\widehat{Q} \in W^{1,2}(\widehat{\Omega}; \mathbb{S}^4)$  given by

$$\widehat{Q}(x) := \begin{cases} Q(x) & \text{if } x \in \Omega, \\ \Sigma(x)Q(\sigma_\Omega(x)) & \text{if } x \in \widehat{\Omega} \setminus \Omega. \end{cases} \quad (2.22)$$

Note that  $\widehat{Q}$  indeed belongs to  $W^{1,2}(\widehat{\Omega})$  since  $\Sigma Q \circ \sigma_\Omega = \Sigma Q = \Sigma Q_b = Q_b$  on  $\partial\Omega$ .

$\triangle$  If no confusion arises, we shall simply write  $Q$  instead of  $\widehat{Q}$  the extension of a map  $Q$ .

In what follows, we also denote for  $P, Q \in W^{1,2}(\widehat{\Omega}; \mathcal{S}_0)$ ,

$$\langle \nabla P, \nabla Q \rangle_A := \sum_{i,j=1}^3 (A \nabla P_{ij}) \cdot \nabla Q_{ij} = \sum_{k,l=1}^3 a_{kl} \partial_k P : \partial_l Q \quad \text{and} \quad |\nabla Q|_A^2 := \langle \nabla Q, \nabla Q \rangle_A,$$

where  $A$  is the matrix field defined in (2.21).

We are now in position to present the equation satisfied by the extension to  $\widehat{\Omega}$  of a critical point of  $\mathcal{E}_\lambda$  in the class  $\mathcal{A}_{Q_b}(\Omega)$ .

**Proposition 2.8.** *Assume that  $\partial\Omega$  is of class  $C^3$  and  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ . If  $Q_\lambda \in \mathcal{A}_{Q_b}(\Omega)$  is a critical point of  $\mathcal{E}_\lambda$ , then*

$$-\text{div}(A \nabla Q_\lambda) = |\nabla Q_\lambda|_A^2 Q_\lambda + G_\lambda(x, Q_\lambda, \nabla Q_\lambda) \quad \text{in } \mathcal{D}'(\widehat{\Omega}), \quad (2.23)$$

where  $G_\lambda: \widehat{\Omega} \times \mathbb{S}^4 \times (\mathcal{S}_0)^3 \rightarrow \mathcal{S}_0$  is a Carathéodory<sup>3</sup> map, and

$$|G_\lambda(x, Q, \xi)| \leq C_{Q_b}(1 + \lambda + |\xi|) \quad \forall (x, Q, \xi) \in \widehat{\Omega} \times \mathbb{S}^4 \times (\mathcal{S}_0)^3, \quad (2.24)$$

for a constant  $C_{Q_b} > 0$  depending only on  $\Omega$  and  $Q_b$ .

The proof of Proposition 2.8 essentially rests on the following lemma.

**Lemma 2.9.** *Assume that  $\partial\Omega$  is of class  $C^3$  and  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ . If  $Q_\lambda \in \mathcal{A}_{Q_b}(\Omega)$  is a critical point of  $\mathcal{E}_\lambda$ , then*

$$\begin{aligned} \int_{\widehat{\Omega}} \langle \nabla Q_\lambda, \nabla \Phi \rangle_A dx &= \lambda \int_{\Omega} Q_\lambda^2 : \Phi dx \\ &+ \lambda \int_{U^{\text{ex}}} ((Q_\lambda \Sigma Q_\lambda) : \Phi) f(x) dx + \int_{U^{\text{ex}}} F(x, Q_\lambda, \nabla Q_\lambda) : \Phi dx \end{aligned} \quad (2.25)$$

for every  $\Phi \in W^{1,2}(\widehat{\Omega}; Q_\lambda^* T\mathbb{S}^4)$  compactly supported in  $\widehat{\Omega}$ , where the function  $f: U^{\text{ex}} \rightarrow \mathbb{R}$  is continuous, the map  $F: U^{\text{ex}} \times \mathbb{S}^4 \times (\mathcal{S}_0)^3 \rightarrow \mathcal{S}_0$  is Carathéodory, and

$$0 \leq f(x) \leq C_\Omega \quad \text{and} \quad |F(x, Q, \xi)| \leq C_{Q_b}(1 + |\xi|) \quad \forall (x, Q, \xi) \in U^{\text{ex}} \times \mathbb{S}^4 \times (\mathcal{S}_0)^3,$$

for some constants  $C_\Omega > 0$  (depending only on  $\Omega$ ) and  $C_{Q_b} > 0$  (depending only on  $\Omega$  and  $Q_b$ ).

*Proof.* If  $\Phi \in W^{1,2}(\widehat{\Omega}; Q_\lambda^* T\mathbb{S}^4)$  is compactly supported in  $\Omega$ , then (2.25) reduces to (2.1). Therefore, it suffices to consider the case where  $\Phi$  is compactly supported in  $U$ . Following the argument in [53], we decompose  $\Phi$  into its equivariant and anti-equivariant parts with respect to the involution  $\Phi(x) \rightarrow \Sigma(x)\Phi(\sigma_\Omega(x))$ , defined for  $x \in U$  by

$$\Phi^e(x) := \frac{1}{2} \left( \Phi(x) + \Sigma(x)\Phi(\sigma_\Omega(x)) \right) \quad \text{and} \quad \Phi^a(x) := \frac{1}{2} \left( \Phi(x) - \Sigma(x)\Phi(\sigma_\Omega(x)) \right).$$

<sup>3</sup> $G(\cdot, Q, \xi)$  is measurable for every  $(Q, \xi) \in \mathbb{S}^4 \times (\mathcal{S}_0)^3$ , and  $G(x, \cdot, \cdot)$  is continuous for a.e.  $x \in \widehat{\Omega}$ .

Here equivariance is understood in terms of the joint reflections across the boundary and on  $\mathbb{S}^4$ . Thus, one simply obtains

$$\Phi^e(\sigma_\Omega(x)) = \Sigma(x)\Phi^e(x) \quad \text{and} \quad \Phi^a(\sigma_\Omega(x)) = -\Sigma(x)\Phi^a(x) \quad \forall x \in U.$$

We shall prove (2.25) for  $\Phi^e$  and  $\Phi^a$  separately, starting with  $\Phi^a$ . To this purpose, we consider  $Q_\lambda$  as extended to the whole  $U$  as in (2.22) and we also introduce for  $x \in U$ ,

$$Q_\lambda^*(x) := Q_\lambda(\sigma_\Omega(x)) = \Sigma(x)Q_\lambda(x).$$

We start from the identity

$$\begin{aligned} \int_{U^{\text{ex}}} \langle \nabla Q_\lambda, \nabla \Phi^a \rangle_A dx &= \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} \partial_k (\Sigma Q_\lambda^*) : \partial_l \Phi^a dx \\ &= \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} (\Sigma \partial_k Q_\lambda^*) : \partial_l \Phi^a dx + \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} ((\partial_k \Sigma) Q_\lambda^*) : \partial_l \Phi^a dx \\ &=: I + II. \end{aligned} \tag{2.26}$$

To compute the  $II$ -term, we integrate by parts. Since  $A$  is the identity matrix on  $\partial\Omega$  and  $\partial_\nu \Sigma = 0$  on  $\partial\Omega$ , the boundary term vanishes, and we are left with

$$\begin{aligned} II &= - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} \partial_l [a_{kl} (\partial_k \Sigma) Q_\lambda^*] : \Phi^a dx = - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} \partial_l [a_{kl} (\partial_k \Sigma) \Sigma Q_\lambda] : \Phi^a dx \\ &= - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} (\partial_l a_{kl}) ((\partial_k \Sigma) \Sigma Q_\lambda) : \Phi^a dx - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} ((\partial_k^2 \Sigma) \Sigma Q_\lambda) : \Phi^a dx \\ &\quad - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} ((\partial_k \Sigma) (\partial_l \Sigma) Q_\lambda) : \Phi^a dx - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} ((\partial_k \Sigma) \Sigma \partial_l Q_\lambda) : \Phi^a dx. \end{aligned} \tag{2.27}$$

Concerning the  $I$ -term, we use the anti-equivariance of  $\Phi^a$  to derive

$$\begin{aligned} I &= \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} \partial_k Q_\lambda^* : (\Sigma \partial_l \Phi^a) dx \\ &= \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} \partial_k Q_\lambda^* : \partial_l (\Sigma \Phi^a) dx - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} \partial_k Q_\lambda^* : ((\partial_l \Sigma) \Phi^a) dx \\ &= - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} \partial_k (Q_\lambda \circ \sigma_\Omega) : \partial_l (\Phi^a \circ \sigma_\Omega) dx - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} ((\partial_l \Sigma) \partial_k (\Sigma Q_\lambda)) : \Phi^a dx \\ &= - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} \partial_k (Q_\lambda \circ \sigma_\Omega) : \partial_l (\Phi^a \circ \sigma_\Omega) dx - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} ((\partial_l \Sigma) (\partial_k \Sigma) Q_\lambda) : \Phi^a dx \\ &\quad - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} ((\partial_l \Sigma) \Sigma \partial_k Q_\lambda) : \Phi^a dx. \end{aligned} \tag{2.28}$$

Next we change variables in the first term of the last identity, and by (2.18) we obtain

$$\begin{aligned}
& - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} \partial_k (Q_\lambda \circ \sigma_\Omega) : \partial_l (\Phi^a \circ \sigma_\Omega) dx = - \sum_{i,j=1}^3 \int_{U^{\text{ex}}} A \nabla (Q_{\lambda,ij} \circ \sigma_\Omega) \cdot \nabla (\Phi_{ij}^a \circ \sigma_\Omega) dx \\
& = - \sum_{i,j=1}^3 \int_{U^{\text{ex}}} [D\sigma_\Omega(x) A(x) (D\sigma_\Omega(x))^{\dagger}] \nabla Q_{\lambda,ij}(\sigma_\Omega(x)) \cdot \nabla \Phi_{ij}^a(\sigma_\Omega(x)) dx \\
& = - \sum_{i,j=1}^3 \int_{U^{\text{ex}}} \nabla Q_{\lambda,ij}(\sigma_\Omega(x)) \cdot \nabla \Phi_{ij}^a(\sigma_\Omega(x)) |J(\sigma_\Omega(x))| dx \\
& = - \sum_{i,j=1}^3 \int_{U^{\text{in}}} \nabla Q_{\lambda,ij} \cdot \nabla \Phi_{ij}^a dx \\
& = - \int_{U^{\text{in}}} \langle \nabla Q_\lambda, \nabla \Phi^a \rangle_A dx. \tag{2.29}
\end{aligned}$$

Since  $\Sigma^2 = \text{id}$ , we have the identities everywhere (resp. a.e.) in  $U$ ,

$$(\partial_k \Sigma) \Sigma + \Sigma (\partial_k \Sigma) = 0 \text{ and } (\partial_k^2 \Sigma) \Sigma + (\partial_k \Sigma) (\partial_l \Sigma) + (\partial_l \Sigma) (\partial_k \Sigma) + \Sigma (\partial_{kl}^2 \Sigma) = 0,$$

so that gathering (2.26), (2.27), (2.28), and (2.29) yields

$$\begin{aligned}
\int_{U^{\text{ex}}} \langle \nabla Q_\lambda, \nabla \Phi^a \rangle_A dx & = - \int_{U^{\text{in}}} \langle \nabla Q_\lambda, \nabla \Phi^a \rangle_A dx \\
& + \sum_{k,l=1}^3 \int_{U^{\text{ex}}} \Sigma \left( (a_{kl} \partial_{kl}^2 \Sigma + \partial_l a_{kl} \partial_k \Sigma) Q_\lambda + 2a_{kl} (\partial_k \Sigma) \partial_l Q_\lambda \right) : \Phi^a dx.
\end{aligned}$$

Consequently,

$$\int_U \langle \nabla Q_\lambda, \nabla \Phi^a \rangle_A dx = \int_{U^{\text{ex}}} F(x, Q_\lambda, \nabla Q_\lambda) : \Phi^a dx \tag{2.30}$$

with

$$F(x, Q_\lambda, \nabla Q_\lambda) := \sum_{k,l=1}^3 \Sigma(x) \left( (a_{kl}(x) \partial_{kl}^2 \Sigma(x) + \partial_l a_{kl}(x) \partial_k \Sigma(x)) Q_\lambda + 2a_{kl}(x) \partial_k \Sigma(x) \partial_l Q_\lambda \right).$$

Clearly,  $F : U^{\text{ex}} \times \mathbb{S}^4 \times (\mathcal{S}_0)^3 \rightarrow \mathcal{S}_0$  is Carathéodory and it is sublinear in its third argument because  $\Sigma \in C^{1,1}$  and  $|Q_\lambda| \leq 1$  in  $U$ .

It now remains to perform the computations with the equivariant part  $\Phi^e$ . First, we observe that  $\Phi^e = 0$  on  $\partial\Omega$ . Indeed, since the function  $(Q_\lambda : \Phi)$  belongs to  $W^{1,1}(U)$ , it has a trace on  $\partial\Omega$ , and this trace is equal to the inner product of the traces on  $\partial\Omega$ . Since  $(Q_\lambda : \Phi) = 0$  in  $U$ , and  $Q_\lambda = Q_b$  on  $\partial\Omega$ , we infer that  $(Q_b : \Phi) = 0$  on  $\partial\Omega$ . Hence  $\Sigma \Phi = -\Phi$  on  $\partial\Omega$ , which yields  $\Phi^e = 0$  on  $\partial\Omega$ . As a consequence,  $\Phi^e \in W_0^{1,2}(U^{\text{in}}; \mathcal{S}_0)$ . Moreover, for a.e.  $x \in U^{\text{in}}$ ,

$$\Phi^e(x) : Q_\lambda(x) = \frac{1}{2} \Phi(\sigma_\Omega(x)) : (\Sigma(x) Q_\lambda(x)) = \frac{1}{2} \Phi(\sigma_\Omega(x)) : Q_\lambda(\sigma_\Omega(x)) = 0,$$

and thus  $\Phi^e \in W_0^{1,2}(U^{\text{in}}; Q_\lambda^* T\mathcal{S}^4)$ . Thanks to the regularity of  $\partial\Omega$ , (2.1) holds for every test functions in  $W_0^{1,2}(\Omega; Q_\lambda^* T\mathcal{S}^4)$  by approximation. Therefore,

$$\int_{U^{\text{in}}} \langle \nabla Q_\lambda, \nabla \Phi^e \rangle_A dx = \int_{U^{\text{in}}} \nabla Q_\lambda : \nabla \Phi^e dx = \lambda \int_{U^{\text{in}}} Q_\lambda^2 : \Phi^e dx. \tag{2.31}$$

Next, from the definition of  $Q_\lambda^*$  we have an identity analogous to (2.26), namely

$$\begin{aligned}
\int_{U^{\text{ex}}} \langle \nabla Q_\lambda, \nabla \Phi^e \rangle_A dx & = \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} (\Sigma \partial_k Q_\lambda^*) : \partial_l \Phi^e dx + \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} ((\partial_k \Sigma) Q_\lambda^*) : \partial_l \Phi^e dx \\
& =: III + IV. \tag{2.32}
\end{aligned}$$

The computations of  $IV$  are identical to the ones of  $II$  in (2.27), with  $\Phi^e$  instead of  $\Phi^a$ . Similarly, we can compute  $III$  in a way similar to (2.28), thus using the equivariance of  $\Phi^e$  and the change

of variable as in (2.29) we obtain

$$\begin{aligned} III &= \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} \partial_k (Q_\lambda \circ \sigma_\Omega) : \partial_l (\Phi^e \circ \sigma_\Omega) dx - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} ((\partial_l \Sigma)(\partial_k \Sigma) Q_\lambda) : \Phi^e dx \\ &\quad - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} ((\partial_l \Sigma) \Sigma \partial_k Q_\lambda) : \Phi^e dx \\ &= \int_{U^{\text{in}}} \langle \nabla Q_\lambda, \nabla \Phi^e \rangle_A dx - \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} ((\partial_l \Sigma)(\partial_k \Sigma) Q_\lambda) : \Phi^e dx \end{aligned} \quad (2.33)$$

$$- \sum_{k,l=1}^3 \int_{U^{\text{ex}}} a_{kl} ((\partial_l \Sigma) \Sigma \partial_k Q_\lambda) : \Phi^e dx \quad (2.34)$$

Summing up the contributions for *III* and *IV*, in view of the identities for  $\Sigma$  and its derivatives we infer

$$\int_{U^{\text{ex}}} \langle \nabla Q_\lambda, \nabla \Phi^e \rangle_A dx = \int_{U^{\text{in}}} \langle \nabla Q_\lambda, \nabla \Phi^e \rangle_A dx + \int_{U^{\text{ex}}} F(x, Q_\lambda, \nabla Q_\lambda) : \Phi^e dx, \quad (2.35)$$

with the same  $F$  as in (2.30).

Combining (2.31) and (2.35) leads to

$$\int_U \langle \nabla Q_\lambda, \nabla \Phi^e \rangle_A dx = 2\lambda \int_{U^{\text{in}}} Q_\lambda^2 : \Phi^e dx + \int_{U^{\text{ex}}} F(x, Q_\lambda, \nabla Q_\lambda) : \Phi^e dx. \quad (2.36)$$

Finally, summing (2.30) with (2.36), we are led to

$$\begin{aligned} \int_U \langle \nabla Q_\lambda, \nabla \Phi \rangle_A dx &= 2\lambda \int_{U^{\text{in}}} Q_\lambda^2 : \Phi dx + \int_{U^{\text{ex}}} F(x, Q_\lambda, \nabla Q_\lambda) : \Phi dx \\ &= \lambda \int_{U^{\text{in}}} Q_\lambda^2 : \Phi dx + \lambda \int_{U^{\text{in}}} Q_\lambda^2 : (\Sigma \Phi \circ \sigma_\Omega) dx \\ &\quad + \int_{U^{\text{ex}}} F(x, Q_\lambda, \nabla Q_\lambda) : \Phi dx. \end{aligned} \quad (2.37)$$

Changing variables once again, we derive

$$\begin{aligned} \int_{U^{\text{in}}} Q_\lambda^2 : (\Sigma \Phi \circ \sigma_\Omega) dx &= \int_{U^{\text{in}}} [\Sigma Q_\lambda^2(\sigma_\Omega(x))] : \Phi(\sigma_\Omega(x)) dx \\ &= \int_{U^{\text{ex}}} ((\Sigma Q_\lambda^2) : \Phi) f(x) dx, \end{aligned} \quad (2.38)$$

with  $f := |J(\sigma_\Omega)|$ . Combining (2.37) and (2.38), the conclusion follows.  $\square$

*Proof of Proposition 2.8.* Starting from Lemma 2.9, we proceed as in the proof of Proposition 2.2. Given  $\Phi \in C_c^\infty(\widehat{\Omega}; \mathcal{M}_{3 \times 3}^{\text{sym}}(\mathbb{R}))$ , we consider  $\Phi_0 := \Phi - \frac{1}{3}(\Phi : I)I \in C_c^\infty(\widehat{\Omega}; \mathcal{S}_0)$  and

$$\Phi_* := \Phi_0 - (Q_\lambda : \Phi_0) Q_\lambda \in W^{1,2}(\widehat{\Omega}; Q_\lambda^* TS^4).$$

Since  $\Phi_*$  is compactly supported in  $\widehat{\Omega}$ , (2.25) applies. On the other hand, direct computations yield

$$\begin{aligned} \int_{\widehat{\Omega}} \langle \nabla Q_\lambda, \nabla \Phi_* \rangle_A dx &= \int_{\widehat{\Omega}} \langle \nabla Q_\lambda, \nabla \Phi_0 \rangle_A dx - \int_{\widehat{\Omega}} |\nabla Q_\lambda|_A^2 Q_\lambda : \Phi_0 dx \\ &= \int_{\widehat{\Omega}} \langle \nabla Q_\lambda, \nabla \Phi \rangle_A dx - \int_{\widehat{\Omega}} |\nabla Q_\lambda|_A^2 Q_\lambda : \Phi dx, \end{aligned} \quad (2.39)$$

and

$$\begin{aligned} \lambda \int_{\Omega} Q_\lambda^2 : \Phi_* dx + \lambda \int_{U^{\text{ex}}} ((\Sigma Q_\lambda^2) : \Phi_*) f(x) dx + \int_{U^{\text{ex}}} F(x, Q_\lambda, \nabla Q_\lambda) : \Phi_* dx \\ = \int_{\Omega} G_\lambda(x, Q_\lambda, \nabla Q_\lambda) : \Phi dx, \end{aligned} \quad (2.40)$$

with

$$\begin{aligned} G_\lambda(x, Q_\lambda, \nabla Q_\lambda) &:= \lambda \chi_\Omega(x) \left[ Q_\lambda^2 - \frac{1}{3} I - \text{tr}(Q_\lambda^3) Q_\lambda \right] \\ &\quad + \lambda \chi_{U^{\text{ex}}}(x) f(x) \left[ \Sigma Q_\lambda^2 - \frac{1}{3} \text{tr}(\Sigma Q_\lambda^2) I - \text{tr}(\Sigma Q_\lambda^3) Q_\lambda \right] \\ &\quad + \chi_{U^{\text{ex}}}(x) \left[ F(x, Q_\lambda, \nabla Q_\lambda) - \frac{1}{3} \text{tr}(F(x, Q_\lambda, \nabla Q_\lambda)) I - \text{tr}(F(x, Q_\lambda, \nabla Q_\lambda) Q_\lambda) Q_\lambda \right]. \end{aligned}$$

Combining (2.25), (2.39), and (2.40) leads to the conclusion.  $\square$

Before closing the subsection, we provide a counterpart to Lemma 2.6 for reflected maps.

**Lemma 2.10.** *Assume that  $\partial\Omega$  is of class  $C^3$  and  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ . Let  $Q_{\text{ref}} \in \mathcal{A}_{Q_b}(\Omega)$  satisfying conclusion (2.16) in Lemma 2.6. There exist two constants  $\mathbf{r}_\Omega^{(2)} > 0$  and  $\kappa = \kappa_\Omega \in (0, 1)$  depending only on  $\Omega$  such that for every  $x_0 \in \partial\Omega$  and  $r \in (0, \mathbf{r}_\Omega^{(2)})$ ,*

$$\sup_{B_\rho(x) \subseteq B_{\kappa r}(x_0)} \frac{1}{\rho} \int_{B_\rho(x)} |\nabla \widehat{Q}_{\text{ref}}|^2 dx \leq \frac{C_\Omega}{r} \mathcal{E}_\lambda(Q_{\text{ref}}, B_r(x_0) \cap \Omega) + C_{Q_b}^\lambda r, \quad (2.41)$$

where  $C_\Omega > 0$  only depends on  $\Omega$ , and  $C_{Q_b}^\lambda > 0$  only depends on  $\Omega$ ,  $Q_b$ ,  $\lambda \|W(Q_b)\|_{L^1(\partial\Omega)}$ , and  $\mathcal{E}_\lambda(\bar{Q}_b)$ .

*Proof.* Set  $\kappa := \frac{1}{6} \min(\|D\sigma_\Omega\|_{L^\infty(U)}^{-1}, 1)$ , and  $\mathbf{r}_\Omega^{(2)} := \min(\mathbf{r}_\Omega^{(1)}, \delta_\Omega)$ , where  $\mathbf{r}_\Omega^{(1)} > 0$  is given by Lemma 2.6. Given a point  $x_0 \in \partial\Omega$  and a radius  $r \in (0, \mathbf{r}_\Omega^{(2)})$ , we apply (2.16) to estimate in a ball  $B_\rho(x) \subseteq B_{\kappa r}(x_0)$ ,

$$\begin{aligned} \frac{1}{\rho} \int_{B_\rho(x)} |\nabla \widehat{Q}_{\text{ref}}|^2 dx &= \frac{1}{\rho} \int_{B_\rho(x) \cap \Omega} |\nabla Q_{\text{ref}}|^2 dx + \frac{1}{\rho} \int_{B_\rho(x) \cap U^{\text{ex}}} |\nabla \widehat{Q}_{\text{ref}}|^2 dx \\ &\leq \frac{4}{r} \mathcal{E}_\lambda(Q_{\text{ref}}, B_r(x_0) \cap \Omega) + \frac{1}{\rho} \int_{B_\rho(x) \cap U^{\text{ex}}} |\nabla \widehat{Q}_{\text{ref}}|^2 dx + C_{Q_b}^\lambda r. \end{aligned} \quad (2.42)$$

Using the facts that  $\Sigma(x)$  is isometric for every  $x \in U$  and  $|Q_{\text{ref}}| = 1$ , we estimate

$$\begin{aligned} \int_{B_\rho(x) \cap U^{\text{ex}}} |\nabla \widehat{Q}_{\text{ref}}|^2 dx &= \int_{B_\rho(x) \cap U^{\text{ex}}} |\nabla(\Sigma Q_{\text{ref}} \circ \sigma_\Omega)|^2 dx \\ &\leq 2 \int_{B_\rho(x) \cap U^{\text{ex}}} |\nabla(Q_{\text{ref}} \circ \sigma_\Omega)|^2 dx + C_{Q_b} \rho^3 \leq C_\Omega \int_{\sigma_\Omega(B_\rho(x)) \cap U^{\text{in}}} |\nabla Q_{\text{ref}}|^2 dx + C_{Q_b} \rho^3, \end{aligned}$$

where the last inequality follows from a change of variables. Setting  $y := \sigma_\Omega(x)$ , we observe that  $\sigma_\Omega(B_\rho(x)) \cap U^{\text{in}} \subseteq B_{\rho/(6\kappa)}(y) \cap U^{\text{in}}$  and  $B_{\rho/(6\kappa)}(y) \subseteq B_{r/6}(x_0)$ , and consequently

$$\begin{aligned} \frac{1}{\rho} \int_{B_\rho(x) \cap U^{\text{ex}}} |\nabla \widehat{Q}_{\text{ref}}|^2 dx &\leq \frac{C_\Omega}{\rho} \int_{B_{\rho/(6\kappa)}(y) \cap \Omega} |\nabla Q_{\text{ref}}|^2 dx + C_{Q_b} \rho^2 \\ &\leq \frac{C_\Omega}{r} \mathcal{E}_\lambda(Q_{\text{ref}}, B_r(x_0) \cap \Omega) + C_{Q_b}^\lambda r, \end{aligned} \quad (2.43)$$

thanks again to (2.16). The result now follows from (2.42) and (2.43).  $\square$

**Remark 2.11** (Specific geometry [16]). Recall from Remark 2.7 that we shall consider in [16] the following situation:  $0 \in \partial\Omega$ ,  $B_1 \cap \Omega = B_1 \cap \{x_3 > 0\}$ , and  $Q_b$  is constant on  $B_1 \cap \partial\Omega = B_1 \cap \{x_3 = 0\}$ . In this case,  $\Sigma$  is constant in  $B_1$ , and  $\sigma_\Omega(x) = (x_1, x_2, -x_3) =: \bar{x}$  for every  $x = (x_1, x_2, x_3) \in B_1$ . Hence  $|\nabla \widehat{Q}_{\text{ref}}(x)|^2 = |\nabla Q_{\text{ref}}(\bar{x})|^2$  for every  $x \in B_1 \cap \{x_3 < 0\}$ . As a consequence, if  $Q_{\text{ref}}$  satisfies conclusion (2.17) in Remark 2.7, then

$$\sup_{B_\rho(x) \subseteq B_{1/6}} \frac{1}{\rho} \mathcal{E}_\lambda(\widehat{Q}_{\text{ref}}, B_\rho(x)) \leq 8 \mathcal{E}_\lambda(Q_{\text{ref}}, B_1 \cap \Omega),$$

instead of (2.41) (with  $x_0 = 0$  and  $r = 1$ ).

**2.3. The  $\varepsilon$ -regularity theorem.** In this subsection, we present the main regularity estimate which provides local Hölder regularity for weak solutions of (2.2) under a smallness assumption on the energy. To treat interior and boundary estimates in a unified way, we consider the case of a general system with diagonal principal part, corresponding to the scalar operator  $Lv = -\operatorname{div}(A\nabla v)$ , as it appears in Proposition 2.8.

**Theorem 2.12.** *Let  $r_0 \in (0, 1]$  and  $A : B_{r_0} \rightarrow \mathcal{M}_{3 \times 3}^{\operatorname{sym}}(\mathbb{R})$  be a Lipschitz field of symmetric matrices, and assume that  $A$  is uniformly elliptic (i.e.,  $mI \leq A \leq MI$  for some constants  $m > 0$  and  $M > 0$ ). Let  $Q \in W^{1,2}(B_{r_0}; \mathbb{S}^4)$  and  $G \in L^2(B_{r_0}; \mathcal{S}_0)$  be such that*

$$-\operatorname{div}(A\nabla Q) = |\nabla Q|_A^2 Q + G \quad \text{in } \mathcal{D}'(B_{r_0}). \quad (2.44)$$

*There exist two constants  $\varepsilon_A > 0$  and  $C_A > 0$ , and an exponent  $\alpha = \alpha(A) \in (0, 1)$  depending only on the Lipschitz norm of  $A$  in  $B_{r_0}$  and the ellipticity bounds  $m$  and  $M$  such that the condition*

$$\sup_{B_r(\bar{x}) \subseteq B_{r_0}} \left( \frac{1}{r} \int_{B_r(\bar{x})} |\nabla Q|^2 dx + r \int_{B_r(\bar{x})} |G|^2 dx \right) \leq \varepsilon_A \quad (2.45)$$

*implies  $Q \in C^{0,\alpha}(\overline{B}_{r_0/2})$  with  $[Q]_{C^{0,\alpha}(\overline{B}_{r_0/2})} \leq C_A r_0^{-\alpha}$ .*

We postpone the proof of this theorem as we require some preliminary lemmas. To this purpose, let us first recall the notion of *function of bounded mean oscillation*. Given an open ball  $B \subseteq \mathbb{R}^d$ , a function  $u \in L^1(B)$  belongs to the space  $\operatorname{BMO}(B)$  if

$$\|u\|_{\operatorname{BMO}(B)} := \sup_{\overline{B}_\rho(y) \subseteq B} \int_{B_\rho(y)} \left| u - \int_{B_\rho(y)} u \right| dx < +\infty,$$

where the supremum is taken over closed balls  $\overline{B}_\rho(y)$  as above. Analogously, for  $p > 1$  a function  $u \in L^p(B)$  belongs to the space  $\operatorname{BMO}^p(B)$  if

$$\|u\|_{\operatorname{BMO}^p(B)}^p := \sup_{\overline{B}_\rho(y) \subseteq B} \int_{B_\rho(y)} \left| u - \int_{B_\rho(y)} u \right|^p dx < +\infty,$$

where as above the supremum is taken over closed balls  $\overline{B}_\rho(y)$ . It is well known that taking closed cubes inside  $B$  or closed balls  $\overline{B}_\rho(y)$  such that  $B_{2\rho}(y) \subseteq B$  gives equivalent definitions where the previous quantities are equivalent norms (see [60]).

A first ingredient coming into play is the classical John-Nirenberg inequality, see e.g. [25, Chapter 19].

**Lemma 2.13** (John-Nirenberg inequality). *For every  $1 < p < \infty$ , there exists a constant  $C_p > 1$  depending only on  $p$  and the dimension such that*

$$\frac{1}{C_p} \|u\|_{\operatorname{BMO}(B)}^p \leq \|u\|_{\operatorname{BMO}^p(B)}^p \leq C_p \|u\|_{\operatorname{BMO}(B)}^p$$

for every  $u \in \operatorname{BMO}(B)$ .

The second result is a standard scaling-invariant local regularity estimate for solutions of linear elliptic PDE's. Since the result is standard but we were not able to find a reference in the literature we sketch the proof for the reader's convenience.

**Lemma 2.14.** *For  $d \geq 3$ , let  $A : \tilde{\Omega} \subseteq \mathbb{R}^d \rightarrow \mathcal{M}_{d \times d}(\mathbb{R})$  be a Lipschitz field of symmetric matrices, and assume that  $A$  is uniformly elliptic (i.e.,  $mI \leq A \leq MI$  in  $\tilde{\Omega}$  for some constants  $m > 0$  and  $M > 0$ ). Let  $f \in L^2(\tilde{\Omega}; \mathbb{R}^d)$ ,  $g \in L^2(\tilde{\Omega})$  and for each  $B_r \subseteq \tilde{\Omega}$ ,  $0 < r \leq 1$ , consider  $u \in W_0^{1,2}(B_r)$  the (unique) weak solution of*

$$\begin{cases} -\operatorname{div}(A\nabla u) = \operatorname{div} f + g & \text{in } B_r, \\ u = 0 & \text{on } \partial B_r. \end{cases}$$

*For every  $q \in (\frac{d}{d-1}, 2)$ , there exists a constant  $C_A = C_A(q)$  depending only on  $q$ ,  $d$  and the Lipschitz norm of  $A$  in  $\tilde{\Omega}$  (i.e., not on the radius  $r$ ) such that*

$$\|\nabla u\|_{L^q(B_r)} \leq C_A \left( \|f\|_{L^q(B_r)} + \|g\|_{L^{\frac{dq}{d+q}}(B_r)} \right).$$

*Proof.* (Sketch) Since all the norms in the inequality have the same scaling properties and the Lipschitz norm of  $A$  is decreasing under scaling with factor  $r \leq 1$  we may assume  $r = 1$ . Then the estimate for  $q = 2$  just follows testing with  $u$ , integrating by parts and using Sobolev inequality. The case  $q \in (2, d)$  follows from the case  $q = 2$  and the combination of [22, Theorem 9.15] for the case  $f \equiv 0$  with [23, Theorem 10.17] for the case  $g \equiv 0$ . Finally, standard duality arguments give the desired conclusion in the dual range of exponents  $q \in (\frac{d}{d-1}, 2)$ .  $\square$

The final ingredient is the following local gradient estimate for  $A$ -harmonic functions.

**Lemma 2.15.** *For  $d \geq 2$ , let  $A : \tilde{\Omega} \subseteq \mathbb{R}^d \rightarrow \mathcal{M}_{d \times d}(\mathbb{R})$  be a Lipschitz field of symmetric matrices, and assume that  $A$  is uniformly elliptic (i.e.,  $mI \leq A \leq MI$  in  $\tilde{\Omega}$  for some constants  $m > 0$  and  $M > 0$ ). If  $B_r \subseteq \tilde{\Omega}$ ,  $0 < r \leq 1$ , and  $u \in W^{1,2}(B_r)$  satisfies in the weak sense*

$$-\operatorname{div}(A\nabla u) = 0 \quad \text{in } B_r, \quad (2.46)$$

then  $u \in C^1(B_r)$  and

$$\sup_{B_{r/4}} |\nabla u|^2 \leq \frac{C_A}{r^2} \int_{\partial B_r} |u - \xi|^2 dx \quad \forall \xi \in \mathbb{R},$$

for some constant  $C_A > 0$  depending only on  $d$  and the Lipschitz norm of  $A$  in  $\tilde{\Omega}$  (i.e., not on the radius  $r$ ).

*Proof.* Since  $u - \xi$  also solves (2.46), we may assume that  $\xi = 0$ . By standard elliptic regularity theory,  $u$  is of class  $C^{1,\alpha}$  locally inside  $B_r$ , and the following estimate holds (see e.g. [21, Theorem 5.19])

$$\sup_{B_{r/4}} |\nabla u|^2 \leq C_A \int_{B_{r/2}} |\nabla u|^2 dx.$$

On the other hand, Caccioppoli's inequality (see e.g. [21, Theorem 4.4]) yields

$$\int_{B_{r/2}} |\nabla u|^2 dx \leq \frac{C_A}{r^2} \int_{B_r} |u|^2 dx,$$

so that

$$\sup_{B_{r/4}} |\nabla u|^2 \leq \frac{C_A}{r^2} \int_{B_r} |u|^2 dx. \quad (2.47)$$

Next we observe that  $|u|^2 \in W^{1,1}(B_r)$  satisfies (in the  $W^{-1,1}$ -sense)

$$-\operatorname{div}(A\nabla |u|^2) = -2(A\nabla u) \cdot \nabla u \leq 0 \quad \text{in } B_r. \quad (2.48)$$

According to [22, Theorem 9.15], there exists a unique strong solution  $\varphi$  of

$$\begin{cases} -\operatorname{div}(A\nabla \varphi) = 1 & \text{in } B_r, \\ \varphi = 0 & \text{on } \partial B_r, \end{cases}$$

which belongs to  $W^{2,p}(B_r)$  for every  $p < \infty$ . In particular,  $\varphi \in C^1(\overline{B_r})$  by Sobolev embedding whenever  $p > d$ , and an elementary scaling argument (using  $r \leq 1$ ) leads to

$$\|\nabla \varphi\|_{L^\infty(B_r)} \leq C_A r, \quad (2.49)$$

for some constant  $C_A > 0$  depending only on  $d$  and the Lipschitz norm of  $A$  in  $\tilde{\Omega}$  (and independent of  $r$ ). Moreover,  $\varphi \geq 0$  in  $B_r$  by the maximum principle.

Next we write  $|u|^2 = -|u|^2 \operatorname{div}(A\nabla \varphi)$ , and we integrate by parts over  $B_r$  to obtain

$$\int_{B_r} |u|^2 dx = \int_{B_r} (A\nabla |u|^2) \cdot \nabla \varphi dx - \int_{\partial B_r} |u|^2 (A\nabla \varphi) \cdot \nu dx \leq C_A r \int_{\partial B_r} |u|^2 dx, \quad (2.50)$$

thanks to (2.48) and (2.49). Gathering (2.47) and (2.50) yields the announced conclusion.  $\square$

*Proof of Theorem 2.12.* We start with some useful pointwise identities which hold a.e. in the domain and which allow to perform the so-called Helein's trick and rewrite the quadratic term in the right hand side of (2.44) in divergence form.

From the identity  $|Q|^2 = 1$ , we first infer that  $Q : \partial_k Q = 0$  for each  $k \in \{1, 2, 3\}$ . As a consequence,

$$\sum_{k,l=1}^3 Q_{kl} (A\nabla Q_{ij}) \cdot \nabla Q_{kl} = 0 \quad \forall i, j \in \{1, 2, 3\},$$

which in turn implies that

$$|\nabla Q|_A^2 Q_{ij} = \sum_{k,l=1}^3 Q_{ij} (A\nabla Q_{kl}) \cdot \nabla Q_{kl} = \sum_{k,l=1}^3 B_{ij}^{kl} \cdot \nabla Q_{kl},$$

with the vector fields

$$B_{ij}^{kl} := Q_{ij} (A\nabla Q_{kl}) - Q_{kl} (A\nabla Q_{ij}) \in L^2(B_{r_0}; \mathbb{R}^3), \quad i, j, k, l \in \{1, 2, 3\}. \quad (2.51)$$

We now claim that in view of the previous pointwise identities for every  $i, j, k, l \in \{1, 2, 3\}$ ,

$$\operatorname{div} B_{ij}^{kl} = G_{kl} Q_{ij} - G_{ij} Q_{kl} \quad \text{in } \mathcal{D}'(B_{r_0}). \quad (2.52)$$

Indeed, given a test function  $\varphi \in \mathcal{D}(B_{r_0})$ , we integrate by parts using equation (2.44) to obtain

$$\begin{aligned} \int_{B_1} B_{ij}^{kl} \cdot \nabla \varphi \, dx &= \int_{B_1} (A\nabla Q_{kl}) \cdot \nabla (Q_{ij} \varphi) \, dx - \int_{B_1} (A\nabla Q_{ij}) \cdot \nabla (Q_{kl} \varphi) \, dx \\ &= \int_{B_1} G_{kl} Q_{ij} \varphi \, dx - \int_{B_1} G_{ij} Q_{kl} \varphi \, dx, \end{aligned}$$

and the claim follows.

We may now write in the sense of distributions

$$B_{ij}^{kl} \cdot \nabla Q_{kl} = \operatorname{div}(Q_{kl} B_{ij}^{kl}) + Q_{kl}^2 G_{ij} - G_{kl} Q_{kl} Q_{ij},$$

in such a way that for each  $i, j \in \{1, 2, 3\}$

$$-\operatorname{div}(A\nabla Q_{ij}) = \operatorname{div}(Q : B_{ij}) + (Q : Q) G_{ij} - (G : Q) Q_{ij} \quad \text{in } W^{-1,2}(B_{r_0}),$$

where  $B_{ij} \in L^2(B_{r_0}; (\mathcal{S}_0)^3)$  are matrix-valued vector fields given by  $B_{ij} := (B_{ij}^{kl})_{k,l=1}^3$  as defined in (2.51).

Finally, if  $T \in \mathcal{S}_0$  is a constant matrix, we have for every  $i, j \in \{1, 2, 3\}$ ,

$$-\operatorname{div}(A\nabla Q_{ij}) = \operatorname{div}((Q - T) : B_{ij}) + F_{ij} \quad \text{in } W^{-1,2}(B_{r_0}), \quad (2.53)$$

with  $F_{ij} := (Q : (Q - T)) G_{ij} - (G : (Q - T)) Q_{ij} \in L^2(B_{r_0})$ .

Let  $\sigma \in (0, 1/8]$  be a constant to be specified later. We fix  $x_0 \in B_{r_0/2}$  and  $t \in (0, r_0/2)$  such that  $B_t(x_0) \subseteq B_{r_0}$ , and then arbitrary  $\bar{x} \in B_{\sigma t}(x_0)$  and  $r \in (0, t)$  such that  $B_{\sigma r}(\bar{x}) \subseteq B_{\sigma t}(x_0)$ . Note that  $B_r(\bar{x}) \subseteq B_t(x_0) \subseteq B_{r_0}$ , and thus assumption (2.45) yields

$$\sup_{0 < \rho \leq r} \left( \frac{1}{\rho} \int_{B_\rho(\bar{x})} |\nabla Q|^2 \, dx + \rho \int_{B_\rho(\bar{x})} |G|^2 \, dx \right) \leq \varepsilon_A. \quad (2.54)$$

Define

$$T := \int_{B_r(\bar{x})} Q \, dx \in \mathcal{S}_0.$$

By a standard average argument based on Fubini's theorem, we can find a good radius  $\bar{r} \in (r/2, r)$  for which

$$\int_{\partial B_{\bar{r}}(\bar{x})} |Q - T|^2 \, d\mathcal{H}^2 \leq \frac{4}{r} \int_{B_r(\bar{x})} |Q - T|^2 \, dx. \quad (2.55)$$

Since  $Q \in W^{1/2,2}(\partial B_{\bar{r}}(\bar{x}); \mathcal{S}_0)$ , there exists a unique  $H \in W^{1,2}(B_{\bar{r}}(\bar{x}); \mathcal{S}_0)$  satisfying

$$\begin{cases} -\operatorname{div}(A\nabla H) = 0 & \text{in } B_{\bar{r}}(\bar{x}), \\ H = Q & \text{on } \partial B_{\bar{r}}(\bar{x}). \end{cases} \quad (2.56)$$

In addition, applying Lemma 2.15 with  $\tilde{\Omega} = B_{r_0}$  we infer that  $H$  belongs to  $C^1(B_{\bar{r}}(\bar{x}))$  and that

$$\sup_{B_{\bar{r}/4}(\bar{x})} |\nabla H|^2 \leq \frac{C_A}{\bar{r}^2} \int_{\partial B_{\bar{r}}(\bar{x})} |H - T|^2 \, d\mathcal{H}^2 = \frac{C_A}{\bar{r}^2} \int_{\partial B_{\bar{r}}(\bar{x})} |Q - T|^2 \, d\mathcal{H}^2 \leq \frac{C_A}{r^2} \int_{B_r(\bar{x})} |Q - T|^2 \, dx, \quad (2.57)$$

thanks to our choice of  $\bar{r}$  made in (2.55).

By (2.53) and (2.56), the map  $Q - H$  has components which solve

$$\begin{cases} -\operatorname{div}(A\nabla(Q_{ij} - H_{ij})) = \operatorname{div}((Q - T) : B_{ij}) + F_{ij} & \text{in } W^{-1,2}(B_{\bar{r}}(\bar{x})), \\ Q_{ij} - H_{ij} = 0 & \text{on } \partial B_{\bar{r}}(\bar{x}), \end{cases}$$

and our aim now is to apply Lemma 2.14. To this purpose, let us fix the exponents

$$q \in (3/2, 2) \quad \text{and} \quad s := \frac{3q}{3+q} \in (1, 6/5).$$

(One can choose for instance  $q = 7/4$ .) Using the identity  $|Q| = 1$  and Hölder's inequality, we estimate with the help of (2.54),

$$\begin{aligned} \|(Q - T) : B_{ij}\|_{L^q(B_{\bar{r}}(\bar{x}))} &\leq \|B_{ij}\|_{L^2(B_{\bar{r}}(\bar{x}))} \|Q - T\|_{L^{\frac{2q}{2-q}}(B_{\bar{r}}(\bar{x}))} \\ &\leq C_A \|\nabla Q\|_{L^2(B_{\bar{r}}(\bar{x}))} \|Q - T\|_{L^{\frac{2q}{2-q}}(B_{\bar{r}}(\bar{x}))} \\ &\leq C_A (\varepsilon_A \bar{r})^{1/2} \|Q - T\|_{L^{\frac{2q}{2-q}}(B_{\bar{r}}(\bar{x}))}, \end{aligned}$$

as well as

$$\begin{aligned} \|F_{ij}\|_{L^s(B_{\bar{r}}(\bar{x}))} &\leq C \|G\|_{L^2(B_{\bar{r}}(\bar{x}))} \|Q - T\|_{L^{\frac{6q}{6-q}}(B_{\bar{r}}(\bar{x}))} \\ &\leq C (\varepsilon_A / \bar{r})^{1/2} \|Q - T\|_{L^{\frac{6q}{6-q}}(B_{\bar{r}}(\bar{x}))} \\ &\leq C (\varepsilon_A \bar{r})^{1/2} \|Q - T\|_{L^{\frac{2q}{2-q}}(B_{\bar{r}}(\bar{x}))}. \end{aligned}$$

According to Lemma 2.14, we thus have

$$\|\nabla(Q - H)\|_{L^q(B_{\bar{r}}(\bar{x}))} \leq C_A (\varepsilon_A \bar{r})^{1/2} \|Q - T\|_{L^{\frac{2q}{2-q}}(B_{\bar{r}}(\bar{x}))}.$$

Since  $\bar{r} \in (r/2, r)$ , the previous estimate and the Sobolev inequality in  $W_0^{1,p}(B_{\bar{r}}(\bar{x}))$  yield

$$\begin{aligned} \left( \int_{B_{\bar{r}}(\bar{x})} |Q - H|^p dx \right)^{1/p} &\leq \frac{C}{\bar{r}^{3/p}} \|\nabla(Q - H)\|_{L^q(B_{\bar{r}}(\bar{x}))} \\ &\leq C_A \varepsilon_A^{1/2} \left( \int_{B_{\bar{r}}(\bar{x})} |Q - T|^{\frac{2q}{2-q}} dx \right)^{\frac{2-q}{2q}}, \end{aligned} \quad (2.58)$$

where  $p := q^* = \frac{3q}{3-q} > 2$  is the Sobolev exponent. Next we set

$$\bar{H} := \int_{B_{\sigma r}(\bar{x})} H dx \quad \text{and} \quad \bar{Q} := \int_{B_{\sigma r}(\bar{x})} Q dx,$$

and we infer from (2.57) and Hölder's inequality, as  $\bar{r} \in (r/2, r)$  and  $\frac{2q}{2-q} > 2$ , that

$$\left( \int_{B_{\sigma r}(\bar{x})} |H - \bar{H}|^p dx \right)^{1/p} \leq C \sigma r \sup_{B_{\bar{r}/4}(\bar{x})} |\nabla H| \leq C_A \sigma \left( \int_{B_{\bar{r}}(\bar{x})} |Q - T|^{\frac{2q}{2-q}} dx \right)^{\frac{2-q}{2q}}. \quad (2.59)$$

In view of (2.58) and (2.59), as  $\bar{r} \in (r/2, r)$  we may now deduce from Minkowski's inequality and the John-Nirenberg inequality in Lemma 2.13 that

$$\begin{aligned} \left( \int_{B_{\sigma r}(\bar{x})} |Q - \bar{H}|^p dx \right)^{1/p} &\leq C \sigma^{-3/p} \left( \int_{B_{\bar{r}}(\bar{x})} |Q - H|^p dx \right)^{1/p} + \left( \int_{B_{\sigma r}(\bar{x})} |H - \bar{H}|^p dx \right)^{1/p} \\ &\leq C_A (\sigma^{-3/p} \varepsilon_A^{1/2} + \sigma) \left( \int_{B_{\bar{r}}(\bar{x})} |Q - T|^{\frac{2q}{2-q}} dx \right)^{\frac{2-q}{2q}} \\ &\leq C_A (\sigma^{-3/p} \varepsilon_A^{1/2} + \sigma) \|Q\|_{\text{BMO}(B_t(x_0))}. \end{aligned} \quad (2.60)$$

It now follows from (2.58) and (2.60) together with Hölder's inequality and the John-Nirenberg inequality again that

$$\begin{aligned}
\int_{B_{\sigma r}(\bar{x})} |Q - \bar{Q}| dx &\leq \int_{B_{\sigma r}(\bar{x})} |Q - \bar{H}| dx + |\bar{H} - \bar{Q}| \\
&\leq \int_{B_{\sigma r}(\bar{x})} |Q - \bar{H}| dx + \int_{B_{\sigma r}(\bar{x})} |Q - H| dx \\
&\leq \left( \int_{B_{\sigma r}(\bar{x})} |Q - \bar{H}|^p dx \right)^{1/p} + C\sigma^{-3/p} \left( \int_{B_{\bar{x}}} |Q - H|^p dx \right)^{1/p} \\
&\leq C_A (\sigma^{-3/p} \varepsilon_A^{1/2} + \sigma) \|Q\|_{\text{BMO}(B_t(x_0))}.
\end{aligned}$$

Finally, taking the supremum over  $\bar{x}$  and  $r$ , we conclude that

$$\|Q\|_{\text{BMO}(B_{\sigma t}(x_0))} \leq C_A (\sigma^{-3/p} \varepsilon_A^{1/2} + \sigma) \|Q\|_{\text{BMO}(B_t(x_0))}.$$

We then choose  $\sigma \in (0, 1/8]$  and  $\varepsilon_A > 0$  small enough (depending only on  $A$ ) in such a way that

$$\|Q\|_{\text{BMO}(B_{\sigma t}(x_0))} \leq \frac{1}{2} \|Q\|_{\text{BMO}(B_t(x_0))}.$$

In view of the arbitrariness of  $t \in (0, r_0/2)$ , the inequality above holds for every  $t \in (0, r_0/2)$ . A classical iteration argument on the function  $t \mapsto \|Q\|_{\text{BMO}(B_t(x_0))}$  then shows that

$$\|Q\|_{\text{BMO}(B_t(x_0))} \leq \|Q\|_{\text{BMO}(B_{r_0/2}(x_0))} 2^\alpha r_0^{-\alpha} t^\alpha \leq 2^{\alpha+1} r_0^{-\alpha} t^\alpha \quad \forall t \in (0, r_0/2), \quad (2.61)$$

where  $\alpha \in (0, 1/3)$  is determined by  $\sigma^\alpha = 1/2$  (note that we have used the fact that  $|Q| = 1$  in the second inequality). In particular, (2.61) leads to

$$\int_{B_t(x_0)} \left| Q - \int_{B_t(x_0)} Q dy \right| dx \leq C r_0^{-\alpha} t^\alpha \quad \forall t \in (0, r_0/2).$$

In view of the arbitrariness of  $x_0 \in B_{r_0/2}$ , it implies that  $Q \in C^{0,\alpha}(\bar{B}_{r_0/2})$  with the announced estimate by Campanato's criterion, see e.g. [42, Theorem 6.1].  $\square$

Applying Theorem 2.12 to our main equation (2.2) yields the following interior regularity estimate.

**Corollary 2.16.** *Let  $Q_\lambda \in W^{1,2}(B_{r_0}; \mathbb{S}^4)$  be such that*

$$-\Delta Q_\lambda = |\nabla Q_\lambda|^2 Q_\lambda + \lambda \left( Q_\lambda^2 - \frac{1}{3} I - \text{tr}(Q_\lambda^3) Q_\lambda \right) \quad \text{in } \mathcal{D}'(B_{r_0}).$$

*There exist two universal constants  $\varepsilon_{\text{in}} > 0$  and  $\mathbf{r}_{\text{in}} > 0$  such that for every ball  $B_r(x_0) \subseteq B_{r_0}$  of radius  $0 < r < \mathbf{r}_{\text{in}}(1 + \lambda)^{-1/2}$ , the condition*

$$\sup_{B_\rho(x) \subseteq B_r(x_0)} \frac{1}{\rho} \int_{B_\rho(x)} |\nabla Q_\lambda|^2 dx \leq \varepsilon_{\text{in}}$$

*implies  $Q_\lambda \in C^{0,\alpha}(\bar{B}_{r/2}(x_0))$  with  $[Q_\lambda]_{C^{0,\alpha}(B_{r/2}(x_0))} \leq C r^{-\alpha}$  for some constants  $\alpha \in (0, 1)$  and  $C > 0$  independent of  $\lambda$ .*

*Proof.* Since  $Q_\lambda$  is a weak solution of (1.16), it solves (2.44) in  $B_r(x_0)$  with the matrix  $A = I$ , and  $G := \lambda(Q_\lambda^2 - \frac{1}{3}I - \text{tr}(Q_\lambda^3)Q_\lambda)$ . The map  $Q_\lambda$  being  $\mathbb{S}^4$ -valued, we have

$$\sup_{B_\rho(x) \subseteq B_r(x_0)} \rho \int_{B_\rho(x)} |G|^2 dx \leq C \frac{\mathbf{r}_{\text{in}}^4 \lambda^2}{(1 + \lambda)^2} \leq C \mathbf{r}_{\text{in}}^4,$$

for some universal constant  $C > 0$ . Hence, we can choose  $\varepsilon_{\text{in}}$  and  $\mathbf{r}_{\text{in}}$  small enough in such a way that (2.45) holds (with  $\varepsilon_A = \varepsilon_I$ ), and the conclusion follows from Theorem 2.12.  $\square$

Concerning boundary regularity estimates under a Dirichlet boundary condition, we apply the reflection procedure of the previous subsection, and then Theorem 2.12 to equation (2.23).

**Corollary 2.17.** *Assume that  $\partial\Omega$  is of class  $C^3$  and  $Q_{\text{b}} \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ . Let  $Q_\lambda \in \mathcal{A}_{Q_{\text{b}}}(\Omega)$  be a critical point of  $\mathcal{E}_\lambda$ , and  $\hat{Q}_\lambda$  its extension to  $\hat{\Omega}$  given by (2.22). There exist two constants  $\varepsilon_{\text{bd}} > 0$*

and  $\mathbf{r}_{\text{bd}} > 0$  depending only on  $\Omega$  and  $Q_{\text{b}}$  such that for every ball  $B_r(x_0) \subseteq \widehat{\Omega}$  with  $x_0 \in \partial\Omega$  and  $0 < r < \mathbf{r}_{\text{bd}}(1 + \lambda)^{-1/2}$ , the condition

$$\sup_{B_\rho(x) \subseteq B_r(x_0)} \frac{1}{\rho} \int_{B_\rho(x)} |\nabla \widehat{Q}_\lambda|^2 dx \leq \varepsilon_{\text{bd}}$$

implies  $\widehat{Q}_\lambda \in C^{0,\alpha}(\overline{B}_{r/2}(x_0))$  with  $[\widehat{Q}_\lambda]_{C^{0,\alpha}(B_{r/2}(x_0))} \leq C_{Q_{\text{b}}} r^{-\alpha}$  for some constants  $\alpha \in (0, 1)$  and  $C_{Q_{\text{b}}} > 0$  depending only on  $\Omega$  and  $Q_{\text{b}}$  (and not on  $\lambda$ ).

*Proof.* By Proposition 2.8,  $\widehat{Q}_\lambda$  solves (2.44) in  $B_r(x_0)$  with the matrix field  $A$  given by (2.21), and the map  $G$  given by  $G := G_\lambda(\cdot, \widehat{Q}_\lambda, \nabla \widehat{Q}_\lambda)$  where  $G_\lambda$  satisfies the growth condition (2.24). In particular,

$$\begin{aligned} \sup_{B_\rho(x) \subseteq B_r(x_0)} \rho \int_{B_\rho(x)} |G|^2 dx &\leq C_{Q_{\text{b}}} \sup_{B_\rho(x) \subseteq B_r(x_0)} \rho \int_{B_\rho(x)} ((1 + \lambda)^2 + |\nabla \widehat{Q}_\lambda|^2) dx \\ &\leq C_{Q_{\text{b}}} \mathbf{r}_{\text{bd}}^2 (\mathbf{r}_{\text{bd}}^2 + \varepsilon_{\text{bd}}), \end{aligned}$$

for a constant  $C_{Q_{\text{b}}} > 0$  depending only on  $\Omega$  and  $Q_{\text{b}}$ . Hence, we can choose  $\varepsilon_{\text{bd}}$  and  $\mathbf{r}_{\text{bd}}$  small enough in such a way that (2.45) holds, and the conclusion follows from Theorem 2.12.  $\square$

**2.4. Higher order regularity.** In this subsection, we improve Hölder continuity estimates from the previous one into Lipschitz estimates. Finally, we deduce analytic regularity both in the interior and at the boundary, whenever boundary data permit.

**Proposition 2.18.** *Let  $r \in (0, 1]$  and let  $A : B_r \rightarrow \mathcal{M}_{3 \times 3}^{\text{sym}}(\mathbb{R})$  be a Lipschitz field of symmetric matrices. Assume that  $A$  is uniformly elliptic, i.e.,  $mI \leq A \leq MI$  for some constants  $m > 0$  and  $M > 1$ . Let  $G : B_r \times \mathbb{S}^4 \times (\mathcal{S}_0)^3 \rightarrow \mathcal{S}_0$  be a Carathéodory map satisfying*

$$|G(x, q, \xi)| \leq C_*(\Lambda + |\xi|^2) \quad \forall (x, q, \xi) \in B_r \times \mathbb{S}^4 \times (\mathcal{S}_0)^3, \quad (2.62)$$

for some constants  $\Lambda > 0$  and  $C_* > 0$ . Let  $Q \in W^{1,2}(B_r; \mathbb{S}^4)$  be such that

$$-\text{div}(A \nabla Q) = G(x, Q, \nabla Q) \quad \text{in } \mathcal{D}'(B_r).$$

If  $Q \in C^{0,\alpha}(\overline{B}_r)$  for some  $\alpha \in (0, 1)$  and  $[Q]_{C^{0,\alpha}(B_r)} \leq \kappa r^{-\alpha}$ , then  $Q \in W^{1,\infty}(B_{r/2})$  and

$$r^2 \|\nabla Q\|_{L^\infty(B_{r/2})}^2 \leq C \left( \frac{1}{r} \int_{B_r} |\nabla Q|^2 dx + \Lambda r^2 \right),$$

for some constant  $C > 0$  depending only on  $\|A\|_{\text{Lip}(B_r)}$ ,  $m$ ,  $M$ ,  $C_*$ ,  $\alpha$ , and  $\kappa$ .

*Proof.* Let us fix an arbitrary point  $x_0 \in B_{r/2}$ , and set  $A_0 := A(x_0)$ ,  $r_1 := r/(2\sqrt{M}) < 1$ . We change variables by setting for  $x \in B_{r_1}$  (so that  $A_0^{1/2}x + x_0 \in B_{r/2}(x_0)$ ),

$$\bar{Q}(x) := Q \left( A_0^{1/2}x + x_0 \right).$$

Then  $\bar{Q} \in W^{1,2}(B_{r_1}; \mathbb{S}^4) \cap C^{0,\alpha}(\overline{B}_{r_1})$  satisfies  $[\bar{Q}]_{C^{0,\alpha}(B_{r_1})} \leq M^{\alpha/2} \kappa r_1^{-\alpha}$ , and it solves

$$-\text{div}(\bar{A} \nabla \bar{Q}) = \bar{G}(x, \bar{Q}, \nabla \bar{Q}) \quad \text{in } \mathcal{D}'(B_{r_1}), \quad (2.63)$$

with

$$\bar{A}(x) := A_0^{-1/2} A(A_0^{1/2}x + x_0) A_0^{-1/2}$$

and

$$\bar{G}(x, q, \xi) := G(A_0^{1/2}x + x_0, q, A_0^{-1/2}\xi).$$

We observe that  $\bar{A}$  is Lipschitz continuous in  $B_{r_1}$ , and

$$\frac{m}{M} I \leq \bar{A} \leq \frac{M}{m} I \quad \text{and} \quad \bar{A}(0) = I.$$

Concerning  $\bar{G}$ , it satisfies

$$|\bar{G}(x, q, \xi)| \leq \tilde{C}_*(\Lambda + |\xi|^2) \quad \forall (x, q, \xi) \in B_{r_1} \times \mathbb{S}^4 \times (\mathcal{S}_0)^3, \quad (2.64)$$

for some constant  $\tilde{C}_* > 0$  depending only on  $C_*$  and  $A$ .

We now fix an arbitrary radius  $\rho \in (0, r_1]$ , and we consider  $H \in W^{1,2}(B_\rho; \mathcal{S}_0) \cap C^0(\bar{B}_\rho)$  the (unique) solution of

$$\begin{cases} -\Delta H = 0 & \text{in } B_\rho, \\ H = \bar{Q} & \text{in } \partial B_\rho. \end{cases}$$

Representing  $H$  through the Poisson integral formula, one easily obtains

$$\text{osc}_{B_\rho} H = \text{osc}_{\partial B_\rho} \bar{Q} \leq Cr_1^{-\alpha} \rho^\alpha,$$

for some constant  $C > 0$  depending only  $A$  and  $\kappa$  (and  $\text{osc}$  is meant for oscillation). Since  $H - \bar{Q} = 0$  on  $\partial B_\rho$ , we deduce that

$$\sup_{B_\rho} |\bar{Q} - H| \leq \text{osc}_{B_\rho} \bar{Q} + \text{osc}_{B_\rho} H \leq Cr_1^{-\alpha} \rho^\alpha, \quad (2.65)$$

with  $C > 0$  depending only  $A$  and  $\kappa$ .

On the other hand, concerning the harmonic function  $H$ , we have  $H \in C^\infty(B_\rho)$  and also  $\Delta|\nabla H|^2 = 2|D^2 H|^2 \geq 0$ . Hence the function  $\rho \rightarrow \rho^{-2} \int_{|x|=\rho} |\nabla H|^2 d\mathcal{H}^2$  is nondecreasing, and in turn  $\rho \rightarrow \rho^{-3} \int_{B_\rho} |\nabla H|^2 dx$  is nondecreasing as well. As a consequence, since  $H$  is equal to  $\bar{Q}$  on  $\partial B_\rho$ , it satisfies

$$\int_{B_{\rho'}} |\nabla H|^2 dx \leq \int_{B_\rho} |\nabla H|^2 dx \leq \int_{B_\rho} |\nabla \bar{Q}|^2 dx \quad \forall \rho' \in (0, \rho). \quad (2.66)$$

We are now ready to estimate

$$\left( \int_{B_{\rho/2}} |\nabla \bar{Q}|_{\bar{A}}^2 dx \right)^{1/2} \leq \left( \int_{B_{\rho/2}} |\nabla H|_{\bar{A}}^2 dx \right)^{1/2} + C \left( \int_{B_\rho} |\nabla(\bar{Q} - H)|_{\bar{A}}^2 dx \right)^{1/2} =: I^{1/2} + CII^{1/2}, \quad (2.67)$$

and we shall treat separately the two terms  $I$  and  $II$ . Since  $A$  is Lipschitz and  $\bar{A}(0) = I$ , we have  $|\bar{A} - I| \leq C_A \rho$  in  $B_\rho$ , and we infer from (2.66) that

$$I \leq (1 + C_A \rho) \int_{B_{\rho/2}} |\nabla H|^2 dx \leq (1 + C_A \rho) \int_{B_\rho} |\nabla H|^2 dx \leq (1 + C_A r_1^{-\alpha} \rho^\alpha) \int_{B_\rho} |\nabla \bar{Q}|^2 dx,$$

where we have used that  $0 < \rho \leq r_1 \leq 1$ . Using again this property together with the ellipticity bounds on  $A$  and  $|\bar{A} - I| \leq C_A \rho$  in  $B_\rho$  we conclude,

$$\sqrt{I} \leq (1 + C_A r_1^{-\alpha/2} \rho^{\alpha/2}) \left( \int_{B_\rho} |\nabla \bar{Q}|_{\bar{A}}^2 dx \right)^{1/2}. \quad (2.68)$$

Next we write

$$II = \int_{B_\rho} \langle \nabla \bar{Q}, \nabla(\bar{Q} - H) \rangle_{\bar{A}} dx + \int_{B_\rho} \langle \nabla H, \nabla(H - \bar{Q}) \rangle_{\bar{A}} dx. \quad (2.69)$$

Since  $\bar{Q} - H \in W_0^{1,2}(B_\rho) \cap L^\infty$ , we can apply (2.63) and then deduce from (2.64) and (2.65) that

$$\int_{B_\rho} \langle \nabla \bar{Q}, \nabla(\bar{Q} - H) \rangle_{\bar{A}} dx = \int_{B_\rho} \bar{G}(x, \bar{Q}, \nabla \bar{Q}) : (\bar{Q} - H) dx \leq Cr_1^{-\alpha} \rho^\alpha \left( \int_{B_\rho} |\nabla \bar{Q}|^2 dx + \Lambda \right). \quad (2.70)$$

Since  $H$  is harmonic and  $\bar{Q} - H = 0$  on  $\partial B_\rho$ , we have  $\int_{B_\rho} \nabla H : \nabla(\bar{Q} - H) dx = 0$ , and consequently

$$\begin{aligned} \int_{B_\rho} \langle \nabla H, \nabla(H - \bar{Q}) \rangle_{\bar{A}} dx &\leq \int_{B_\rho} |\bar{A} - I| |\nabla H| |\nabla(H - \bar{Q})| dx \\ &\leq C_A \rho \left( \int_{B_\rho} |\nabla H|^2 dx + \int_{B_\rho} |\nabla \bar{Q}|^2 dx \right) \leq Cr_1^{-\alpha} \rho^\alpha \int_{B_\rho} |\nabla \bar{Q}|^2 dx, \end{aligned} \quad (2.71)$$

where we have used again  $|\bar{A} - I| \leq C_A \rho$  in  $B_\rho$ , (2.66), and  $0 < \rho \leq r_1 \leq 1$ . Combining now (2.69), (2.70), and (2.71) leads to

$$II \leq C_A r_1^{-\alpha} \rho^\alpha \left( \int_{B_\rho} |\nabla \bar{Q}|^2 dx + \Lambda \right).$$

As  $0 < \rho \leq r_1 \leq 1$ , in view of the ellipticity bounds of  $A$  and  $|\bar{A} - I| \leq C_A \rho$  in  $B_\rho$  we conclude

$$\sqrt{II} \leq C_A r_1^{-\alpha/2} \rho^{\alpha/2} \left( \int_{B_\rho} |\nabla \bar{Q}|_{\bar{A}}^2 dx + \Lambda \right)^{1/2}. \quad (2.72)$$

Combining (2.67) with (2.68) and (2.72), we obtain

$$\left( \int_{B_{\rho/2}} |\nabla \bar{Q}|_{\bar{A}}^2 dx \right)^{1/2} \leq (1 + C_A r_1^{-\alpha/2} \rho^{\alpha/2}) \left( \int_{B_\rho} |\nabla \bar{Q}|_{\bar{A}}^2 dx \right)^{1/2} + C_A \sqrt{\Lambda} r_1^{-\alpha/2} \rho^{\alpha/2}, \quad (2.73)$$

for a constant  $C_A > 0$  depending only on  $A$ ,  $C_*$ , and  $\kappa$  and for all  $0 < \rho \leq r_1 \leq 1$ .

In view of the arbitrariness of  $\rho$ , we can apply (2.73) with  $\rho_k := 2^{-k} r_1$  and  $k \in \mathbb{N}$ . It leads to

$$\left( \int_{B_{\rho_{k+1}}} |\nabla \bar{Q}|_{\bar{A}}^2 dx \right)^{1/2} \leq (1 + C_A 2^{-\alpha k/2}) \left( \int_{B_{\rho_k}} |\nabla \bar{Q}|_{\bar{A}}^2 dx \right)^{1/2} + C_A \sqrt{\Lambda} 2^{-\alpha k/2} \quad \forall k \in \mathbb{N}.$$

Now if  $\{\theta_k\} \subseteq (1, \infty)$ ,  $\theta = \prod_{k=0}^{\infty} \theta_k < \infty$ ,  $\{\sigma_k\} \subseteq (0, \infty)$ ,  $\sigma = \sum_{k=0}^{\infty} \sigma_k < \infty$ , and  $\{y_k\} \subseteq [0, \infty)$  satisfy  $y_{k+1} \leq \theta_k y_k + \sigma_k$  for each  $k \geq 0$ , then a simple induction argument gives  $y_{k+1} \leq \theta(y_0 + \sigma)$  for each  $k \geq 0$ . As a consequence, if we let

$$y_k = \left( \int_{B_{\rho_k}} |\nabla \bar{Q}|_{\bar{A}}^2 dx \right)^{1/2}, \quad \theta_k = (1 + C_A 2^{-\alpha k/2}), \quad \sigma_k = C_A \sqrt{\Lambda} 2^{-\alpha k/2},$$

then we obtain

$$\left( \int_{B_{\rho_k}} |\nabla \bar{Q}|_{\bar{A}}^2 dx \right)^{1/2} \leq C \left[ \left( \int_{B_{r_1}} |\nabla \bar{Q}|_{\bar{A}}^2 dx \right)^{1/2} + \sqrt{\Lambda} \right] \quad \forall k \in \mathbb{N}, \quad (2.74)$$

for some constant  $C > 0$  depending only on  $A$ ,  $C_*$ ,  $\kappa$ , and  $\alpha$ .

Finally, if  $x_0$  was chosen to be a Lebesgue point of  $|\nabla Q|^2$  (which holds for a.e.  $x_0 \in B_{r_0/2}$  by the Lebesgue differentiation theorem), then 0 is a Lebesgue point for  $|\nabla \bar{Q}|_{\bar{A}}^2$ , and letting  $k \rightarrow \infty$  in (2.74) yields (recall that  $\bar{A}(0) = I$ )

$$|\nabla \bar{Q}(0)|^2 \leq C \left( \int_{B_{r_1}} |\nabla \bar{Q}|_{\bar{A}}^2 dx + \Lambda \right).$$

Changing variables again and using the uniform ellipticity of  $A$ , we deduce from the definition of  $r_1$  that

$$|\nabla Q(x_0)|^2 \leq C' \left( \frac{1}{r_1^3} \int_{B_{r_1/2}(x_0)} |\nabla Q|^2 dx + \Lambda \right) \leq C \left( \frac{1}{r^3} \int_{B_r} |\nabla Q|^2 dx + \Lambda \right),$$

for some constants  $C > 0$  and  $\Lambda > 0$  depending only on  $A$ ,  $C_*$ ,  $\kappa$ , and  $\alpha$  and the conclusion follows.  $\square$

Once Lipschitz continuity is obtained, one can derive higher regularity from linear elliptic theory.

**Corollary 2.19.** *Let  $Q_\lambda \in W^{1,2}(B_r(x_0); \mathbb{S}^4)$  be such that*

$$-\Delta Q_\lambda = |\nabla Q_\lambda|^2 Q_\lambda + \lambda \left( Q_\lambda^2 - \frac{1}{3} I - \text{tr}(Q_\lambda^3) Q_\lambda \right) \quad \text{in } \mathcal{D}'(B_r(x_0)).$$

If  $0 < r < r_{\text{in}}(1 + \lambda)^{-1/2}$  and

$$\sup_{B_\rho(x) \subseteq B_r(x_0)} \frac{1}{\rho} \int_{B_\rho(x)} |\nabla Q_\lambda|^2 dx \leq \varepsilon_{\text{in}},$$

where  $r_{\text{in}}$  and  $\varepsilon_{\text{in}}$  are given by Corollary 2.16, then  $Q_\lambda \in C^\omega(B_{r/4}(x_0))$ . In addition,  $Q_\lambda$  satisfies for each  $k \in \mathbb{N}$ ,

$$\|\nabla^k Q_\lambda\|_{L^\infty(B_{r/8}(x_0))} \leq C_k r^{-k}, \quad (2.75)$$

for a constant  $C_k > 0$  depending only on  $k$ .

*Proof. Step 1.* By Corollary 2.16,  $Q_\lambda \in C^{0,\alpha}(B_{r/2}(x_0))$  with  $[Q_\lambda]_{C^{0,\alpha}(B_{r/2}(x_0))} \leq Cr^{-\alpha}$  for some  $\alpha \in (0, 1)$  and  $C > 0$  independent of  $\lambda$ . Applying Proposition 2.18 with  $A = I$  and

$$G(x, Q, \nabla Q) := |\nabla Q|^2 Q + \lambda(Q^2 - \frac{1}{3}I - \text{tr}(Q^3)Q)$$

(so that  $G$  satisfies (2.62) with  $\Lambda := \lambda + 1$ ) yields  $Q_\lambda \in W^{1,\infty}(B_{r/4}(x_0))$  and

$$\begin{aligned} r^2 \|\nabla Q_\lambda\|_{L^\infty(B_{r/4}(x_0))}^2 &\leq C \left( \frac{1}{r} \int_{B_r(x_0)} |\nabla Q_\lambda|^2 dx + (1 + \lambda)r^2 \right) \\ &\leq C \left( \frac{1}{r} \int_{B_r(x_0)} |\nabla Q_\lambda|^2 dx + 1 \right) \leq C, \end{aligned}$$

for some universal constant  $C > 0$ . As a consequence, we have  $\Delta Q_\lambda \in L^\infty(B_{r/4}(x_0))$ . By linear elliptic regularity theory (see e.g. [24, Theorem 3.13]), it follows that  $Q_\lambda \in C_{\text{loc}}^{1,\alpha}(B_{r/4}(x_0))$  for every  $\alpha \in (0, 1)$ . A classical bootstrap argument based on Schauder estimates then shows that  $Q_\lambda \in C^\infty(B_{r/4}(x_0))$  (see e.g. [22, Chapters 6 & 8]), and standard results in [46, Chapter 6] give analytic regularity.

*Step 2.* In this second step, our aim is to prove the remaining estimate (2.75) for  $k \geq 2$ . Let us fix a point  $y \in B_{r/8}(x_0)$ , and rescale variables setting  $\tilde{Q}(x) := Q_\lambda(y + rx)$ . Then,

$$-\Delta \tilde{Q} = |\nabla \tilde{Q}|^2 \tilde{Q} + \tilde{\lambda} \left( \tilde{Q}^2 - \frac{1}{3}I - \text{tr}(\tilde{Q}^3) \tilde{Q} \right) \quad \text{in } B_{1/8}, \quad (2.76)$$

with  $\tilde{\lambda} := r^2 \lambda \in (0, \mathbf{r}_{\text{in}})$ . Let us fix  $j \in \{1, 2, 3\}$ , and set  $v := \partial_j \tilde{Q}$ . Differentiating (2.76) with respect to the  $j$ -th variable, we obtain that  $v$  satisfies a linear system of the form

$$-\Delta v + b \cdot \nabla v + c \cdot v = d \quad \text{in } B_{1/8},$$

where the coefficients  $b$ ,  $c$ , and  $d$  satisfy

$$\|b\|_{L^\infty(B_{1/8})} + \|c\|_{L^\infty(B_{1/8})} + \|d\|_{L^\infty(B_{1/8})} \leq C$$

since  $|\tilde{Q}| = 1$  and  $\|\nabla \tilde{Q}\|_{L^\infty(B_{1/8})} \leq C$ . By elliptic regularity (see e.g. [22, Chapter 8, Section 8.11]),  $v$  satisfies the estimate

$$\sup_{B_{1/16}} |\nabla v| \leq C (\|v\|_{L^\infty(B_{1/8})} + \|d\|_{L^\infty(B_{1/8})}) \leq C.$$

From the arbitrariness of  $j$ , we conclude that  $\|\nabla^2 \tilde{Q}\|_{L^\infty(B_{1/16})} \leq C$ . Now we can proceed by induction on  $k$  following the same strategy (differentiating  $(k-1)$ -times equation (2.76)) to prove that  $\|\nabla^k \tilde{Q}\|_{L^\infty(B_{2^{-(k+2)}})} \leq C_k$  for a constant  $C_k$  depending only on  $k$ . Scaling variables back, we obtain that  $\|\nabla^k Q_\lambda(y)\| \leq C_k r^{-k}$ , and (2.75) follows from the arbitrariness of  $y$ .  $\square$

A similar argument then yields higher regularity near the boundary when the boundary data are sufficiently regular.

**Corollary 2.20.** *Assume that  $\partial\Omega$  is of class  $C^3$  and  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ . Let  $Q_\lambda \in \mathcal{A}_{Q_b}(\Omega)$  be a critical point of  $\mathcal{E}_\lambda$ ,  $\hat{Q}_\lambda$  its extension to  $\hat{\Omega}$  given by (2.22), and  $B_r(x_0) \subseteq \hat{\Omega}$  with  $x_0 \in \partial\Omega$ . If  $0 < r < \mathbf{r}_{\text{bd}}(1 + \lambda)^{-1/2}$  and*

$$\sup_{B_\rho(x) \subseteq B_r(x_0)} \frac{1}{\rho} \int_{B_\rho(x)} |\nabla \hat{Q}_\lambda|^2 dx \leq \varepsilon_{\text{bd}},$$

where  $\mathbf{r}_{\text{bd}}$  and  $\varepsilon_{\text{bd}}$  are given by Corollary 2.17, then  $\|\nabla \hat{Q}_\lambda\|_{L^\infty(B_{r/4}(x_0))} \leq C_{Q_b} r^{-1}$  for some constant  $C_{Q_b} > 0$  depending only on  $\Omega$  and  $Q_b$ . As a consequence  $Q_\lambda \in C^\omega(B_{r/4}(x_0) \cap \Omega) \cap C_{\text{loc}}^{1,\alpha}(B_{r/4}(x_0) \cap \bar{\Omega})$  for every  $\alpha \in (0, 1)$ .

In addition,

- (i) if  $\partial\Omega$  is of class  $C^{k,\beta}$  and  $Q_b \in C^{k,\beta}(\partial\Omega; \mathbb{S}^4)$  with  $k \geq 2$ , then  $Q_\lambda \in C_{\text{loc}}^{k,\beta}(B_{r/4}(x_0) \cap \bar{\Omega})$ ;
- (ii) if  $\partial\Omega$  is real-analytic and  $Q_b \in C^\omega(\partial\Omega; \mathbb{S}^4)$ , then  $Q_\lambda \in C^\omega(B_{r/4}(x_0) \cap \bar{\Omega})$ .

*Proof.* By Corollary 2.17,  $\hat{Q}_\lambda \in C^{0,\alpha}(B_{r/2}(x_0))$  with  $[\hat{Q}_\lambda]_{C^{0,\alpha}(B_{r/2}(x_0))} \leq C_{Q_b} r^{-\alpha}$  for some exponent  $\alpha \in (0, 1)$  and a constant  $C_{Q_b} > 0$  independent of  $\lambda$ . By Proposition 2.8, we can apply Proposition 2.18 with the matrix field  $A$  given by (2.21), and  $G(x, Q, \nabla Q)$  given by the right-hand side of (2.23) (once again,  $G$  satisfies (2.62) with  $\Lambda := \lambda + 1$ ). It yields  $\hat{Q}_\lambda \in W^{1,\infty}(B_{r/4}(x_0))$

and  $r^2 \|\nabla \widehat{Q}_\lambda\|_{L^\infty(B_{r/4}(x_0))}^2 \leq C_{Q_b}$  (as in the proof of Corollary 2.19, Step 1). From the equation (2.23) satisfied by  $\widehat{Q}_\lambda$ , we deduce that  $\operatorname{div}(A\nabla \widehat{Q}_\lambda) \in L^\infty(B_{r/4}(x_0))$ . By elliptic regularity (see e.g. [24, Theorem 3.13]), it implies that  $\widehat{Q}_\lambda \in C_{\text{loc}}^{1,\alpha}(B_{r/4}(x_0))$  for every  $\alpha \in (0, 1)$ , and consequently  $Q_\lambda \in C_{\text{loc}}^{1,\alpha}(B_{r/4}(x_0) \cap \overline{\Omega})$  for every  $\alpha \in (0, 1)$ . Since  $|\nabla Q_\lambda| \in L^\infty(B_{r/4}(x_0) \cap \Omega)$ , we can argue as in the proof of Corollary 2.19, Step 1, to show that  $Q_\lambda \in C^\omega(B_{r/4}(x_0) \cap \Omega)$ .

Finally, under the assumption that  $\partial\Omega$  is of class  $C^{k,\beta}$  and  $Q_b \in C^{k,\beta}(\partial\Omega; \mathbb{S}^4)$  with  $k \geq 2$ , the fact that  $Q_\lambda \in C_{\text{loc}}^{k,\beta}(B_{r/4}(x_0) \cap \overline{\Omega})$  now follows from equation (2.2) and standard elliptic regularity at the boundary, see e.g. [22, Chapter 6]. The corresponding conclusion within the analytic class follows again from the results in e.g. [46, Chapter 6].  $\square$

**2.5. Bochner inequality and uniform regularity estimates.** In this subsection we refine the previous analysis and clarify the dependence of the regularity estimates for the smooth solutions  $Q_\lambda$  of (1.16) on the parameter  $\lambda$ . The results of this subsection are not used in the present paper but they will be a fundamental tool in the subsequent papers [15, 16] of our series where we will study (axially symmetric) minimizers in the asymptotic limit  $\lambda \rightarrow \infty$ .

**Proposition 2.21.** *Let  $Q_\lambda \in W^{1,2}(B_r; \mathbb{S}^4)$  be a smooth solution of (1.16) in  $B_r$ . There exists a universal constant  $\varepsilon_{\text{reg}} > 0$  such that the condition*

$$\frac{1}{r} \mathcal{E}_\lambda(Q_\lambda, B_r) \leq \varepsilon_{\text{reg}}$$

implies

$$\sup_{B_{r/4}} \left( \frac{1}{2} |\nabla Q_\lambda|^2 + \lambda W(Q_\lambda) \right) \leq Cr^{-2},$$

for a further universal constant  $C > 0$ .

In order to prove Proposition 2.21 we need a couple of auxiliary results.

**Lemma 2.22.** *There exists a universal constant  $\mathbf{c}_\star > 0$  such that for every  $Q \in \mathbb{S}^4$  and  $T \in \mathcal{S}_0$  satisfying  $T : Q = 0$ ,*

$$2 \operatorname{tr}(TQT) \leq \left( \frac{1}{\sqrt{6}} + \mathbf{c}_\star \sqrt{W(Q)} \right) |T|^2.$$

*Proof.* Let  $\mu_3 \leq \mu_2 \leq \mu_1$  be the eigenvalues of  $Q$ . Using that  $\mu_1 + \mu_2 + \mu_3 = \operatorname{tr}(Q) = 0$  and  $\mu_1^2 + \mu_2^2 + \mu_3^2 = |Q|^2 = 1$ , we deduce that  $0 < \mu_1 \leq \frac{2}{\sqrt{6}}$  and  $-\frac{2}{\sqrt{6}} \leq \mu_3 < 0$ . We now consider a matrix  $P \in SO(3)$  such that  $Q = PDP^t$  with  $D = \operatorname{diag}(\mu_1, \mu_2, \mu_3) \in \mathbb{S}^4$ . Setting  $\tilde{T} := P^t T P$ , we observe that  $\tilde{T} : D = T : Q = 0$ ,  $|\tilde{T}| = |T|$ ,  $\operatorname{tr}(\tilde{T} D \tilde{T}) = \operatorname{tr}(TQT)$ , and  $W(Q) = W(D)$ . Hence, it suffices to show that

$$2 \operatorname{tr}(\tilde{T} D \tilde{T}) \leq \left( \frac{1}{\sqrt{6}} + \mathbf{c}_\star \sqrt{W(D)} \right) |\tilde{T}|^2, \quad (2.77)$$

for some universal constant  $\mathbf{c}_\star > 0$ , i.e., that the claim holds when  $Q = D$  is a diagonal matrix. To this purpose, let us first recall that

$$W(D) = 0 \iff \mu_2 = \mu_3 \iff \mu_1 = \frac{2}{\sqrt{6}} \text{ and } \mu_2 = \mu_3 = \frac{-1}{\sqrt{6}}.$$

Let us fix a small constant  $0 < \mathbf{t}_0 < 1$  to be chosen later, and set

$$\ell_0 := \min \left\{ W(\operatorname{diag}(\nu_1, \nu_2, \nu_3)) : \nu_1 \geq \nu_2 \geq \nu_3 + \mathbf{t}_0, \nu_1 + \nu_2 + \nu_3 = 0, \nu_1^2 + \nu_2^2 + \nu_3^2 = 1 \right\} > 0.$$

If  $\mu_2 - \mu_3 \geq \mathbf{t}_0$ , then (2.77) clearly holds for  $\mathbf{c}_\star \geq 2\ell_0^{-1/2}$  since  $|D| = 1$ . Hence it remains to prove the inequality in the case  $\mu_2 - \mu_3 < \mathbf{t}_0$ . To this purpose let us set  $t := \mu_2 - \mu_3 \in [0, \mathbf{t}_0)$ . Choosing  $\mathbf{t}_0$  small enough ensures that  $\mu_2 < 0$ , and direct computations yield

$$\mu_1 = \frac{2}{\sqrt{6}}(1 - t^2/2)^{1/2}, \quad \mu_2 = \frac{t}{2} - \frac{1}{\sqrt{6}}(1 - t^2/2)^{1/2}, \quad \mu_3 = -\frac{t}{2} - \frac{1}{\sqrt{6}}(1 - t^2/2)^{1/2},$$

and, as  $t \rightarrow 0$ ,

$$W(D) = \frac{1 - (1 - t^2/2)^{3/2}}{3\sqrt{6}} + \frac{t^2}{2\sqrt{6}}(1 - t^2/2)^{1/2} = \frac{3}{4\sqrt{6}}t^2 + o(t^2).$$

In particular, if  $t_0$  is sufficiently small, then  $t \in [0, t_0)$  yields

$$\sqrt{W(D)} \geq \frac{t}{4}.$$

Let us now write

$$\tilde{T} = \begin{pmatrix} x_1 & x_4 & x_6 \\ x_4 & x_2 & x_5 \\ x_6 & x_5 & x_3 \end{pmatrix},$$

so that  $|\tilde{T}|^2 = x_1^2 + x_2^2 + x_3^2 + 2x_4^2 + 2x_5^2 + 2x_6^2$ , and

$$2 \operatorname{tr}(\tilde{T}D\tilde{T}) = 2\mu_1 x_1^2 + 2\mu_2 x_2^2 + 2\mu_3 x_3^2 + 2(\mu_1 + \mu_2)x_4^2 + 2(\mu_2 + \mu_3)x_5^2 + 2(\mu_1 + \mu_3)x_6^2.$$

Since  $\mu_1 + \mu_2 + \mu_3 = 0$ ,  $\mu_3 \leq \mu_2 < 0$  and  $\mu_1 \leq \frac{2}{\sqrt{6}}$ , from the previous formulas for the eigenvalues we easily get  $-2\mu_2 \leq \frac{2}{\sqrt{6}}$ ,  $-2\mu_3 \leq t + \frac{2}{\sqrt{6}}$  and

$$\begin{aligned} 2 \operatorname{tr}(\tilde{T}D\tilde{T}) &\leq 2\mu_1 x_1^2 + 2(\mu_1 + \mu_2)x_4^2 + 2(\mu_1 + \mu_3)x_6^2 = 2\mu_1 x_1^2 - 2\mu_3 x_4^2 - 2\mu_2 x_6^2 \\ &\leq \frac{4}{\sqrt{6}} x_1^2 + 2\left(\frac{1}{\sqrt{6}} + 2\sqrt{W(D)}\right)x_4^2 + \frac{2}{\sqrt{6}} x_6^2. \end{aligned} \quad (2.78)$$

On the other hand  $x_1 + x_2 + x_3 = 0$  since  $\operatorname{tr}(\tilde{T}) = 0$ , and  $\mu_1 x_1 + \mu_2 x_2 + \mu_3 x_3 = 0$  since  $\tilde{T} : D = 0$ . It implies that

$$\left(\frac{3}{\sqrt{6}}(1 - t^2/2)^{1/2} - \frac{t}{2}\right)x_1 = tx_3,$$

and consequently,  $x_1^2 \leq t^2 x_3^2 \leq \frac{1}{4}x_3^2$  for  $t_0$  small enough. Back to (2.78), we conclude that

$$2 \operatorname{tr}(\tilde{T}D\tilde{T}) \leq \frac{1}{\sqrt{6}} x_3^2 + 2\left(\frac{1}{\sqrt{6}} + 2\sqrt{W(D)}\right)x_4^2 + \frac{2}{\sqrt{6}} x_6^2 \leq \left(\frac{1}{\sqrt{6}} + 2\sqrt{W(D)}\right)|\tilde{T}|^2,$$

which completes the proof for a (small) universal constant  $t_0 > 0$  and  $\mathbf{c}_* = \max\{2, 2\ell_0^{-1/2}\}$ .  $\square$

**Lemma 2.23** (Bochner inequality). *Let  $Q_\lambda$  be a smooth solution of (1.16) in  $B_r$ . Setting  $e_\lambda := \frac{1}{2}|\nabla Q_\lambda|^2 + \lambda W(Q_\lambda)$ , we have*

$$-\Delta e_\lambda \leq C e_\lambda^2 \quad \text{in } B_r$$

for some universal constant  $C > 0$ .

*Proof.* First compute

$$-\Delta \left(\frac{1}{2}|\nabla Q_\lambda|^2\right) = -|\nabla^2 Q_\lambda|^2 + \nabla Q_\lambda : \nabla(-\Delta Q_\lambda).$$

From (1.16), we derive that

$$\begin{aligned} \partial_k(-\Delta Q_\lambda) &= 2(\nabla Q_\lambda : \nabla(\partial_k Q_\lambda))Q_\lambda + |\nabla Q_\lambda|^2 \partial_k Q_\lambda \\ &\quad + \lambda \left( (\partial_k Q_\lambda)Q_\lambda + Q_\lambda \partial_k Q_\lambda - 3\operatorname{tr}(Q_\lambda^2 \partial_k Q_\lambda)Q_\lambda - \operatorname{tr}(Q_\lambda^3) \partial_k Q_\lambda \right). \end{aligned}$$

Since  $Q_\lambda : \partial_k Q_\lambda = 0$  and  $\operatorname{tr}(Q_\lambda^3) = -3W(Q_\lambda) + 1/\sqrt{6}$ , we obtain

$$-\Delta \left(\frac{1}{2}|\nabla Q_\lambda|^2\right) \leq |\nabla Q_\lambda|^4 + 3\lambda W(Q_\lambda)|\nabla Q_\lambda|^2 + \lambda \sum_{k=1}^3 \left( 2\operatorname{tr}((\partial_k Q_\lambda)Q_\lambda \partial_k Q_\lambda) - \frac{1}{\sqrt{6}}|\partial_k Q_\lambda|^2 \right).$$

It then follows from Lemma 2.22 (applied to  $Q = Q_\lambda$  and  $T = \partial_k Q_\lambda$ ) that

$$-\Delta \left(\frac{1}{2}|\nabla Q_\lambda|^2\right) \leq |\nabla Q_\lambda|^4 + 3\lambda W(Q_\lambda)|\nabla Q_\lambda|^2 + \mathbf{c}_* \lambda \sqrt{W(Q_\lambda)} |\nabla Q_\lambda|^2. \quad (2.79)$$

Next, we compute

$$-\Delta(W(Q_\lambda)) = -\operatorname{tr}(Q_\lambda^2(-\Delta Q_\lambda)) + \sum_{k=1}^3 2\operatorname{tr}((\partial_k Q_\lambda)Q_\lambda \partial_k Q_\lambda),$$

and it follows from (1.16) that

$$-\Delta(W(Q_\lambda)) = -|\nabla Q_\lambda|^2 \operatorname{tr}(Q_\lambda^3) - \lambda \left( \operatorname{tr} Q^4 - \frac{1}{3} - (\operatorname{tr}(Q_\lambda^3))^2 \right) + \sum_{k=1}^3 2\operatorname{tr}((\partial_k Q_\lambda)Q_\lambda \partial_k Q_\lambda).$$

Noticing that  $\operatorname{tr} Q^4 = 1/2$ , we obtain from Lemma 2.22,

$$\begin{aligned} -\Delta(W(Q_\lambda)) &= 3W(Q_\lambda)|\nabla Q_\lambda|^2 + 9\lambda W^2(Q_\lambda) - \lambda\sqrt{6}W(Q_\lambda) + \sum_{k=1}^3 \left( 2\operatorname{tr}((\partial_k Q_\lambda)Q_\lambda\partial_k Q_\lambda) - \frac{1}{\sqrt{6}}|\partial_k Q_\lambda|^2 \right) \\ &\leq 3W(Q_\lambda)|\nabla Q_\lambda|^2 + 9\lambda W^2(Q_\lambda) - \lambda\sqrt{6}W(Q_\lambda) + \mathbf{c}_* \sqrt{W(Q_\lambda)} |\nabla Q_\lambda|^2. \end{aligned} \quad (2.80)$$

Combining (2.79) and (2.80), we are led to

$$\begin{aligned} -\Delta e_\lambda &\leq |\nabla Q_\lambda|^4 + 6\lambda W(Q_\lambda)|\nabla Q_\lambda|^2 + 9\lambda^2 W^2(Q_\lambda) - \lambda^2\sqrt{6}W(Q_\lambda) + 2\mathbf{c}_*\lambda\sqrt{W(Q_\lambda)}|\nabla Q_\lambda|^2 \\ &\leq (1 + \mathbf{c}_*^2/\sqrt{6})|\nabla Q_\lambda|^4 + 6\lambda W(Q_\lambda)|\nabla Q_\lambda|^2 + 9\lambda^2 W^2(Q_\lambda) \\ &\leq Ce_\lambda^2 \end{aligned}$$

for a universal constant  $C > 0$ .  $\square$

**Remark 2.24.** If  $Q_\lambda$  is a smooth solution of (1.16) in  $B_r$ , then  $Q_\lambda$  satisfies the interior monotonicity formula (2.8) in the ball  $B_r$  (see the proof of Proposition 2.4, Step 2, or [58, Chapter 2, Sections 2.2 and 2.4]). As a consequence,  $Q_\lambda$  satisfies

$$\sup_{B_\rho(x) \subseteq B_{r/2}} \frac{1}{\rho} \mathcal{E}_\lambda(Q_\lambda, B_\rho(x)) \leq \frac{2}{r} \mathcal{E}_\lambda(Q_\lambda, B_r),$$

exactly as in Lemma 2.6.

*Proof of Proposition 2.21.* We argue as in [11], where the scaling argument first presented in [54] for harmonic maps is adapted to the harmonic heat flow. Since  $Q_\lambda$  is smooth, we can find  $\sigma_\lambda \in (0, r/2)$  such that

$$\left(\frac{r}{2} - \sigma_\lambda\right)^2 \sup_{B_{\sigma_\lambda}} e_\lambda \geq \frac{1}{2} \sup_{0 < \sigma < r/2} \left(\frac{r}{2} - \sigma\right)^2 \sup_{B_\sigma} e_\lambda.$$

In addition, by continuity we can find  $x_\lambda \in \overline{B_{\sigma_\lambda}}$  such that

$$\sup_{B_{\sigma_\lambda}} e_\lambda = e_\lambda(x_\lambda) := \bar{e}_\lambda.$$

Set  $\rho_\lambda := (r/2 - \sigma_\lambda)/2 > 0$ , and notice that  $B_{\rho_\lambda}(x_\lambda) \subseteq B_{\sigma_\lambda + \rho_\lambda} \subseteq B_{r/2}$ . Since  $\sigma = \rho_\lambda + \sigma_\lambda < r/2$  and  $r/2 - \sigma = \frac{1}{2}(r/2 - \sigma_\lambda)$ , by definition of  $\sigma_\lambda$  we have

$$\sup_{B_{\rho_\lambda}(x_\lambda)} e_\lambda \leq \sup_{B_{\sigma_\lambda + \rho_\lambda}} e_\lambda \leq 8\bar{e}_\lambda.$$

We define  $r_\lambda := \rho_\lambda \sqrt{\bar{e}_\lambda}$ , and, as  $B_{\rho_\lambda}(x_\lambda) \subseteq B_{r/2}$ , we also define

$$\tilde{Q}(x) := Q_\lambda\left(x_\lambda + \frac{x}{\sqrt{\bar{e}_\lambda}}\right) \quad \text{for } x \in B_{r_\lambda}.$$

Then  $\tilde{Q}$  is smooth in  $B_{r_\lambda}$ , and it solves (1.16) in  $B_{r_\lambda}$  with  $\tilde{\lambda} := \lambda/\bar{e}_\lambda$  in place of  $\lambda$ . Setting

$$\tilde{e}_{\tilde{\lambda}} := \frac{1}{2} |\nabla \tilde{Q}|^2 + \tilde{\lambda} W(\tilde{Q}),$$

we infer from our choice of  $\sigma_\lambda$  and  $x_\lambda$  that  $\tilde{e}_{\tilde{\lambda}}(0) = e_\lambda(x_\lambda)/\bar{e}_\lambda = 1$ , and  $\tilde{e}_{\tilde{\lambda}} \leq 8$  in  $B_{r_\lambda}$ . We now claim that  $r_\lambda \leq 1$ . Indeed, assume by contradiction that  $r_\lambda > 1$ . Then we infer from Lemma 2.23 that

$$-\Delta \tilde{e}_{\tilde{\lambda}} \leq C \tilde{e}_{\tilde{\lambda}}^2 \leq 8C \tilde{e}_{\tilde{\lambda}} \quad \text{in } B_1,$$

for a universal constant  $C > 0$ . By Moser's Harnack inequality (see e.g. [24, Theorem 4.1]) and Remark 2.24, we have

$$1 = \tilde{e}_{\tilde{\lambda}}(0) \leq C \int_{B_1} \tilde{e}_{\tilde{\lambda}} dx = C \sqrt{\bar{e}_\lambda} \int_{B_{1/\sqrt{\bar{e}_\lambda}}(x_\lambda)} e_\lambda dx \leq 2C \varepsilon_{\text{reg}},$$

for a universal constant  $C > 0$ . Here we have used that  $B_{1/\sqrt{\bar{e}_\lambda}}(x_\lambda) \subseteq B_{r/2}$  since  $1/\sqrt{\bar{e}_\lambda} < \rho_\lambda$ . Therefore,  $1 \leq 2C \varepsilon_{\text{reg}}$  which is clearly a contradiction if  $\varepsilon_{\text{reg}}$  is small enough.

Knowing that  $r_\lambda \leq 1$ , we may now deduce from our choice of  $\sigma_\lambda$  and the definition of  $\rho_\lambda$  that

$$\sup_{0 < \sigma < r/2} \left(\frac{r}{2} - \sigma\right)^2 \sup_{B_\sigma} e_\lambda \leq 8\rho_\lambda^2 \bar{e}_\lambda = 8r_\lambda^2 \leq 8.$$

Choosing  $\sigma = r/4$  now yields  $e_\lambda \leq 128r^{-2}$  in  $B_{r/4}$ , and the proof is complete.  $\square$

## 3. REGULARITY OF MINIMIZERS UNDER NORM CONSTRAINT

The aim of this section is to prove Theorem 1.2, and the proof is divided according to the following subsections. Recall that in the statement of Theorem 1.2, we assume that the boundary  $\partial\Omega$  is of class  $C^3$  and  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ .

**3.1. Monotonicity formulae.** We start establishing the monotonicity formulae for minimizers of  $\mathcal{E}_\lambda$  over  $\mathcal{A}_{Q_b}(\Omega)$  applying the general principle in Proposition 2.4. First, let us recall that  $\bar{Q}_b \in \mathcal{A}_{Q_b}(\Omega)$  is a given ( $\mathbb{S}^4$ -valued) reference extension to  $\Omega$  of the boundary condition  $Q_b$ .

**Proposition 3.1.** *If  $Q_\lambda$  is a minimizer of  $\mathcal{E}_\lambda$  over  $\mathcal{A}_{Q_b}(\Omega)$ , then  $Q_\lambda$  satisfies the Interior Monotonicity Formula (2.8) and the Boundary Monotonicity Inequality (2.9). Moreover the quantity  $K_\lambda(Q_b, Q_\lambda)$  in (2.9) satisfies*

$$K_\lambda(Q_b, Q_\lambda) \leq C_\Omega \left( \|\nabla_{\tan} Q_b\|_{L^\infty(\partial\Omega)}^2 + \lambda \|W(Q_b)\|_{L^1(\partial\Omega)} + \mathcal{E}_\lambda(\bar{Q}_b) \right). \quad (3.1)$$

*Proof.* We first notice that, due to (1.11) and (1.4), the potential  $W$  is nonnegative for every  $Q \in \mathcal{S}_0$ . Hence, for each  $\varepsilon > 0$  the functional  $\mathcal{G}\mathcal{L}_\varepsilon(Q_\lambda; \cdot)$  defined in (2.6) is well defined and coercive on  $W^{1,2}(\Omega; \mathcal{S}_0)$ . Moreover, using the compact Sobolev embedding  $W^{1,2}(\Omega; \mathcal{S}_0) \hookrightarrow L^4(\Omega)$ , we easily obtain that  $\mathcal{G}\mathcal{L}_\varepsilon(Q_\lambda; \cdot)$  is lower semi-continuous with respect to the weak  $W^{1,2}$ -convergence since all the terms not containing derivatives of  $Q$  are weakly continuous. It then follows from the direct method of calculus of variations that  $\mathcal{G}\mathcal{L}_\varepsilon(Q_\lambda; \cdot)$  admits at least one minimizer  $Q_\varepsilon$  over  $W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$ .

By Proposition 2.4, it now suffices to show that  $Q_\varepsilon$  satisfies (2.7) (with  $Q_\lambda$  in place of  $Q_{\text{ref}}$ ). In addition, observe that (3.1) follows from the minimality of  $Q_\lambda$ . Indeed, since  $\bar{Q}_b \in \mathcal{A}_{Q_b}(\Omega)$  is an admissible competitor, we have  $\|\nabla Q_\lambda\|_{L^2(\Omega)}^2 \leq 2\mathcal{E}_\lambda(Q_\lambda) \leq 2\mathcal{E}_\lambda(\bar{Q}_b)$ .

Now, let us consider an arbitrary sequence  $\varepsilon_n \rightarrow 0$  satisfying  $\varepsilon_n \in (0, \lambda^{-1/2})$ . First, we infer from the minimality of  $Q_{\varepsilon_n}$  that

$$\frac{1}{2} \int_\Omega |\nabla Q_{\varepsilon_n}|^2 + |Q_{\varepsilon_n} - Q_\lambda|^2 dx \leq \mathcal{G}\mathcal{L}_{\varepsilon_n}(Q_\lambda; Q_{\varepsilon_n}) \leq \mathcal{G}\mathcal{L}_{\varepsilon_n}(Q_\lambda; Q_\lambda) = \mathcal{E}_\lambda(Q_\lambda). \quad (3.2)$$

Hence, the sequence  $\{Q_{\varepsilon_n}\}$  is bounded in  $W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$ , and we can extract a (not relabelled) subsequence such that  $Q_{\varepsilon_n} \rightharpoonup Q_*$  weakly in  $W^{1,2}(\Omega)$  for some  $Q_* \in W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$ . Up to a further subsequence, we can assume that  $Q_{\varepsilon_n} \rightarrow Q_*$  strongly in  $L^4(\Omega)$  (and therefore in  $L^2(\Omega)$ ) since the embedding  $W^{1,2}(\Omega) \hookrightarrow L^4(\Omega)$  is compact. As a consequence,  $\int_\Omega W(Q_{\varepsilon_n}) dx \rightarrow \int_\Omega W(Q_*) dx$  which, combined with (3.2), implies that  $\int_\Omega (1 - |Q_{\varepsilon_n}|^2)^2 dx \rightarrow 0$ . Therefore,  $|Q_*| = 1$  a.e. in  $\Omega$ , and thus  $Q_* \in \mathcal{A}_{Q_b}(\Omega)$ . Now we infer from the minimality of  $Q_\lambda$ , the weak lower semicontinuity of  $\mathcal{E}_\lambda$ , the  $L^2$ -convergence and (3.2) that

$$\begin{aligned} \mathcal{E}_\lambda(Q_\lambda) &\leq \mathcal{E}_\lambda(Q_*) + \frac{1}{2} \int_\Omega |Q_* - Q_\lambda|^2 dx \leq \liminf_{n \rightarrow \infty} \left( \mathcal{E}_\lambda(Q_{\varepsilon_n}) + \frac{1}{2} \int_\Omega |Q_{\varepsilon_n} - Q_\lambda|^2 dx \right) \\ &\leq \liminf_{n \rightarrow \infty} \mathcal{G}\mathcal{L}_{\varepsilon_n}(Q_\lambda; Q_{\varepsilon_n}) \leq \limsup_{n \rightarrow \infty} \mathcal{G}\mathcal{L}_{\varepsilon_n}(Q_\lambda; Q_{\varepsilon_n}) \leq \mathcal{E}_\lambda(Q_\lambda). \end{aligned}$$

Consequently,  $Q_* = Q_\lambda$  and  $\lim_n \mathcal{G}\mathcal{L}_{\varepsilon_n}(Q_\lambda; Q_{\varepsilon_n}) = \mathcal{E}_\lambda(Q_\lambda)$ , which completes the proof.  $\square$

**3.2. Compactness of blow-ups and smallness of the scaled energy.** When proving regularity the main issue is to analyse the asymptotic behavior of minimizers at small scales, and the key property is the compactness of rescaled maps. When rescaling around an interior point, we have the following statement.

**Proposition 3.2.** *Let  $Q_\lambda$  be a minimizer of  $\mathcal{E}_\lambda$  over  $\mathcal{A}_{Q_b}(\Omega)$ . Given  $x_0 \in \Omega$  and  $0 < r \leq r_0$  such that  $\overline{B_{r_0}(x_0)} \subseteq \Omega$ , consider the rescaled map  $Q_{\lambda,r} \in W^{1,2}(B_{r_0/r}; \mathbb{S}^4)$  defined by*

$$Q_{\lambda,r}(x) := Q_\lambda(x_0 + rx).$$

*For every sequence  $r_n \rightarrow 0$ , there exist a (not relabeled subsequence) and  $Q_* \in W_{\text{loc}}^{1,2}(\mathbb{R}^3; \mathbb{S}^4)$  such that  $Q_{\lambda,r_n} \rightarrow Q_*$  strongly in  $W_{\text{loc}}^{1,2}(\mathbb{R}^3)$ . In addition,  $Q_*$  is a degree-zero homogeneous energy minimizing harmonic map into  $\mathbb{S}^4$ .*

To prove Proposition 3.2, we need two auxiliary lemmata.

**Lemma 3.3.** *Let  $Q_{\lambda, r_n}$  be as in Proposition 3.2 and  $\rho > 0$ . For each  $n \in \mathbb{N}$  such that  $\rho r_n < r_0$ , let  $v_n \in W^{1,2}(B_\rho; \mathbb{S}^4)$  be such that  $v_n = Q_{\lambda, r_n}$  on  $\partial B_\rho$  in the sense of traces. Then,*

$$\limsup_{n \rightarrow \infty} \int_{B_\rho} |\nabla Q_{\lambda, r_n}|^2 dx \leq \limsup_{n \rightarrow \infty} \int_{B_\rho} |\nabla v_n|^2 dx.$$

*Proof.* By minimality of  $Q_\lambda$  and a change of variables,  $Q_{\lambda, r_n}$  is minimizing  $\mathcal{E}_{\lambda r_n^2}(\cdot, B_\rho)$  among all maps in  $W^{1,2}(B_\rho; \mathbb{S}^4)$  having the same trace  $Q_{\lambda, r_n}$  on  $\partial B_\rho$ . Since  $v_n$  is an admissible competitor and the potential  $W$  is bounded on  $\mathbb{S}^4$ , we have

$$\frac{1}{2} \int_{B_\rho} |\nabla Q_{\lambda, r_n}|^2 dx \leq \mathcal{E}_{\lambda r_n^2}(Q_{\lambda, r_n}, B_\rho) \leq \frac{1}{2} \int_{B_\rho} |\nabla v_n|^2 dx + C\lambda\rho^3 r_n^2,$$

for a constant  $C$  depending only on  $W$ . Then the claim follows letting  $n \rightarrow \infty$ .  $\square$

The following interpolation lemma is due to S. Luckhaus [40].

**Lemma 3.4.** *Let  $u, v \in W^{1,2}(\mathbb{S}^2; \mathbb{S}^4)$ . For each  $\sigma \in (0, 1)$ , there exists  $w \in W^{1,2}(\mathbb{S}^2 \times (1-\sigma, 1); \mathcal{S}_0)$  such that  $w|_{\mathbb{S}^2 \times \{1-\sigma\}} = v$ ,  $w|_{\mathbb{S}^2 \times \{1\}} = u$ ,*

$$\int_{\mathbb{S}^2 \times (1-\sigma, 1)} |\nabla w|^2 dx \leq C\sigma \int_{\mathbb{S}^2} (|\nabla_{\tan} u|^2 + |\nabla_{\tan} v|^2) d\mathcal{H}^2 + C\sigma^{-1} \int_{\mathbb{S}^2} |u - v|^2 d\mathcal{H}^2, \quad (3.3)$$

and

$$\begin{aligned} \text{dist}^2(w(x), \mathbb{S}^4) &\leq C\sigma^{-2} \left( \int_{\mathbb{S}^2} (|\nabla_{\tan} u|^2 + |\nabla_{\tan} v|^2) d\mathcal{H}^2 \right)^{\frac{1}{2}} \left( \int_{\mathbb{S}^2} |u - v|^2 d\mathcal{H}^2 \right)^{\frac{1}{2}} \\ &\quad + C\sigma^{-3} \int_{\mathbb{S}^2} |u - v|^2 d\mathcal{H}^2 \end{aligned} \quad (3.4)$$

for a.e.  $x \in \mathbb{S}^2 \times (1-\sigma, 1)$ , and a universal constant  $C > 0$ .

*Proof of Proposition 3.2.* We essentially follow the proof of [38, Lemma 2.2.13] with minor modifications. By Proposition 3.1,  $Q_\lambda$  satisfies the interior monotonicity formula (2.8). Rescaling this formula yields

$$\frac{1}{R_2} \mathcal{E}_{\lambda r_n^2}(Q_{\lambda, r_n}, B_{R_2}) - \frac{1}{R_1} \mathcal{E}_{\lambda r_n^2}(Q_{\lambda, r_n}, B_{R_1}) \geq \int_{B_{R_2} \setminus B_{R_1}} \frac{1}{|x|} \left| \frac{\partial Q_{\lambda, r_n}}{\partial |x|} \right|^2 dx \quad (3.5)$$

for every  $0 < R_1 < R_2 \leq r_0/r_n$ . As a consequence, for every  $0 < R < r_0/r_n$ , we have

$$\frac{1}{R} \mathcal{E}_{\lambda r_n^2}(Q_{\lambda, r_n}, B_R) \leq \frac{r_n}{r_0} \mathcal{E}_{\lambda r_n^2}(Q_{\lambda, r_n}, B_{r_0/r_n}) = \frac{1}{r_0} \mathcal{E}_\lambda(Q_\lambda, B_{r_0}(x_0)).$$

Consequently, we can find a (not relabeled) subsequence such that  $Q_{\lambda, r_n}$  converges to a map  $Q_*$  weakly in  $W_{\text{loc}}^{1,2}(\mathbb{R}^3)$  and strongly in  $L_{\text{loc}}^2(\mathbb{R}^3)$ . Up to a further subsequence,  $Q_{\lambda, r_n} \rightarrow Q_*$  a.e. in  $\mathbb{R}^3$ , and thus  $Q_* \in W_{\text{loc}}^{1,2}(\mathbb{R}^3; \mathbb{S}^4)$ . By the monotonicity formula (2.8) satisfied by  $Q_\lambda$ , we have

$$\lim_{n \rightarrow \infty} \frac{1}{R} \mathcal{E}_{\lambda r_n^2}(Q_{\lambda, r_n}, B_R) = \lim_{n \rightarrow \infty} \frac{1}{R r_n} \mathcal{E}_\lambda(Q_\lambda, B_{R r_n}(x_0)) = \lim_{r \rightarrow 0} \frac{1}{r} \mathcal{E}_\lambda(Q_\lambda, B_r(x_0))$$

for every  $R > 0$ . Consequently, letting  $n \rightarrow \infty$  in (3.5) yields by  $W^{1,2}$ -weak convergence and lower semicontinuity,

$$\int_{B_{R_2} \setminus B_{R_1}} \frac{1}{|x|} \left| \frac{\partial Q_*}{\partial |x|} \right|^2 dx = 0$$

for every  $0 < R_1 < R_2$ , which shows that  $Q_*$  is 0-homogeneous.

Now we aim to prove that, for every radius  $R > 0$ ,  $Q_{\lambda, r_n} \rightarrow Q_*$  strongly in  $W^{1,2}(B_R)$ , and that

$$\int_{B_R} |\nabla Q_*|^2 dx \leq \int_{B_R} |\nabla \bar{Q}|^2 dx$$

for every competitor  $\bar{Q} \in W^{1,2}(B_R; \mathbb{S}^4)$  such that  $\bar{Q} - Q_*$  is compactly supported in  $B_R$  (i.e.,  $Q_*$  is a minimizing harmonic map into  $\mathbb{S}^4$  on the whole space  $\mathbb{R}^3$  w.r.t. to compactly supported perturbations). By homogeneity of  $Q_*$ , the value of the radius  $R$  does not play a role, and it is enough to show strong  $W^{1,2}$ -convergence and energy minimality in a ball  $B_\rho$  for some radius  $\rho \in (0, 1)$ .

We fix a competitor  $\bar{Q} \in W^{1,2}(B_1; \mathbb{S}^4)$  and  $\delta \in (0, 1)$  such that  $\bar{Q} \equiv Q_*$  a.e. in  $B_1 \setminus B_{1-\delta}$ . Extracting a further subsequence if necessary, by Fatou's lemma and Fubini's theorem, we can select a radius  $\rho \in (1 - \delta, 1)$  and a constant  $C > 0$  such that

$$\lim_{n \rightarrow \infty} \int_{\partial B_\rho} |Q_{\lambda, r_n} - Q_*|^2 d\mathcal{H}^2 = 0 \quad \text{and} \quad \int_{\partial B_\rho} (|\nabla Q_{\lambda, r_n}|^2 + |\nabla Q_*|^2) d\mathcal{H}^2 \leq C. \quad (3.6)$$

We apply Lemma 3.4 with a choice  $\sigma = \sigma_n \in (0, \delta)$ ,  $u(x) = Q_{\lambda, r_n}(\rho x)$  and  $v(x) = Q_*(\rho x)$ ,  $x \in \mathbb{S}^2$ , for a sequence of numbers  $\sigma_n \rightarrow 0$  to interpolate between  $Q_{\lambda, r_n}$  and  $Q_*$ . For  $n$  sufficiently large, we choose  $\sigma_n := \|Q_{\lambda, r_n} - Q_*\|_{L^2(\partial B_\rho)}^{1/3} < \delta$ , and in this way, we obtain  $w_n \in W^{1,2}(B_\rho; \mathbb{S}_0)$  satisfying

$$w_n(x) = \begin{cases} \bar{Q}\left(\frac{x}{1-\sigma_n}\right) & \text{for } |x| \leq \rho(1-\sigma_n), \\ Q_{\lambda, r_n}(x) & \text{for } |x| = \rho, \end{cases}$$

with the estimate

$$\begin{aligned} \int_{B_\rho \setminus B_{\rho(1-\sigma_n)}} |\nabla w_n|^2 dx &\leq C \left( \sigma_n \int_{\partial B_\rho} (|\nabla_{\tan} Q_{\lambda, r_n}|^2 + |\nabla_{\tan} Q_*|^2) d\mathcal{H}^2 \right. \\ &\quad \left. + \frac{1}{\sigma_n} \int_{\partial B_\rho} |Q_{\lambda, r_n} - Q_*|^2 d\mathcal{H}^2 \right) \xrightarrow{n \rightarrow \infty} 0, \end{aligned} \quad (3.7)$$

and  $\text{dist}(w_n, \mathbb{S}^4) = \mathcal{O}(\sigma_n) \rightarrow 0$  uniformly on  $B_\rho \setminus B_{\rho(1-\sigma_n)}$  as  $n \rightarrow \infty$  because of (3.6), (3.4) and our choice of  $\sigma_n$ .

For  $n$  large enough we have  $|w_n| \geq 1/2$  on  $B_\rho$ , hence we can define a sequence of comparison maps  $v_n \in W^{1,2}(B_\rho; \mathbb{S}^4)$ , so that  $v_n = Q_{\lambda, r_n}$  on  $\partial B_\rho$ , by setting

$$v_n(x) := \begin{cases} \bar{Q}\left(\frac{x}{1-\sigma_n}\right) & \text{if } |x| \leq \rho(1-\sigma_n), \\ \frac{w_n(x)}{|w_n(x)|} & \text{if } \rho(1-\sigma_n) \leq |x| \leq \rho. \end{cases} \quad (3.8)$$

Notice that, since  $|w_n| \geq 1/2$ , we have  $|\nabla v_n| \leq C|\nabla w_n|$  a.e. in the annulus  $\{\rho(1-\sigma_n) \leq |x| \leq \rho\}$ . In view of Lemma 3.3, combining (3.7) and (3.8) together with the weak  $W^{1,2}$ -convergence of  $Q_{\lambda, r_n}$  towards  $Q_*$ , we obtain

$$\begin{aligned} \int_{B_\rho} |\nabla Q_*|^2 dx &\leq \liminf_{n \rightarrow \infty} \int_{B_\rho} |\nabla Q_{\lambda, r_n}|^2 dx \leq \limsup_{n \rightarrow \infty} \int_{B_\rho} |\nabla Q_{\lambda, r_n}|^2 dx \\ &\leq \limsup_{n \rightarrow \infty} \int_{B_\rho} |\nabla v_n|^2 dx = \limsup_{n \rightarrow \infty} \left[ (1-\sigma_n) \int_{B_\rho} |\nabla \bar{Q}|^2 dx + \int_{B_\rho \setminus B_{\rho(1-\sigma_n)}} |\nabla v_n|^2 dx \right] \\ &\leq \lim_{n \rightarrow \infty} \left[ (1-\sigma_n) \int_{B_\rho} |\nabla \bar{Q}|^2 dx + C \int_{B_\rho \setminus B_{\rho(1-\sigma_n)}} |\nabla w_n|^2 dx \right] = \int_{B_\rho} |\nabla \bar{Q}|^2 dx. \end{aligned}$$

Since  $\bar{Q}$  and  $\delta$  are arbitrary, this chain of inequalities provides both the strong  $W^{1,2}$ -convergence  $Q_{\lambda, r_n} \rightarrow Q_*$  (using  $\bar{Q} = Q_*$ ) and the energy minimality of  $Q_*$  in the ball  $B_\rho$ .  $\square$

We now aim to perform a similar blow-up analysis around a boundary point. To this purpose, let us recall that  $\partial\Omega$  is assumed to be of class  $C^3$ , and  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ . We consider the enlarged domain  $\hat{\Omega}$  defined in (2.20), and we extend  $Q_b$  to  $\hat{\Omega} \setminus \Omega$  by setting  $\hat{Q}_b(x) := Q_b(\pi_\Omega(x))$  for  $x \in \hat{\Omega} \setminus \Omega$ , where  $\pi_\Omega$  is the nearest point projection on  $\partial\Omega$ . By the regularity assumption on  $\partial\Omega$  and  $Q_b$ , we have  $\hat{Q}_b \in C^{1,1}(\hat{\Omega} \setminus \Omega)$ .

**Proposition 3.5.** *Let  $Q_\lambda$  be a minimizer of  $\mathcal{E}_\lambda$  over  $\mathcal{A}_{Q_b}(\Omega)$ , and denote by  $\hat{Q}_\lambda$  the extension of  $Q_\lambda$  to  $\hat{\Omega}$  given by  $\hat{Q}_\lambda = \hat{Q}_b$  in  $\hat{\Omega} \setminus \Omega$ . Given  $x_0 \in \partial\Omega$  and  $0 < r \leq r_0$  such that  $B_{r_0}(x_0) \subseteq \hat{\Omega}$ , consider the rescaled map  $\hat{Q}_{\lambda, r} \in W^{1,2}(B_{r_0/r}; \mathbb{S}^4)$  defined by*

$$\hat{Q}_{\lambda, r}(x) = \hat{Q}_\lambda(x_0 + rx).$$

*For every sequence  $r_n \rightarrow 0$ , there exist a (not relabeled) subsequence and  $Q_* \in W_{\text{loc}}^{1,2}(\mathbb{R}^3; \mathbb{S}^4)$  such that  $\hat{Q}_{\lambda, r_n} \rightarrow Q_*$  strongly in  $W_{\text{loc}}^{1,2}(\mathbb{R}^3)$ . In addition,  $Q_*$  is homogeneous of degree zero, and up to a rotation of coordinates,  $Q_*$  is a minimizing harmonic map in the upper half space  $\{x_3 > 0\}$  and  $Q_* \equiv Q_b(x_0)$  in  $\{x_3 < 0\}$ .*

*Proof.* Up to a translation and a rotation, we may assume that  $\{x_3 = 0\}$  is the tangent plane to  $\partial\Omega$  at  $x_0$  and the vector  $(0, 0, -1)$  is the outward unit normal. By Proposition 3.1,  $Q_\lambda$  satisfies the Boundary Monotonicity Inequality (2.9), and by rescaling variables,

$$\frac{1}{R_2} \mathcal{E}_{\lambda r_n^2}(\widehat{Q}_{\lambda, r_n}, B_{R_2} \cap \Omega_n) - \frac{1}{R_1} \mathcal{E}_{\lambda r_n^2}(\widehat{Q}_{\lambda, r_n}, B_{R_1} \cap \Omega_n) \geq \int_{(B_{R_2} \setminus B_{R_1}) \cap \Omega_n} \frac{1}{|x|} \left| \frac{\partial \widehat{Q}_{\lambda, r_n}}{\partial |x|} \right|^2 dx - r_n(R_2 - R_1)K_\lambda(Q_b, Q_\lambda) \quad (3.9)$$

for every  $0 < R_1 < R_2 \leq r_0/r_n$ , where we have set  $\Omega_n := r_n^{-1}(\Omega - x_0)$ . As a consequence,

$$\frac{1}{R} \mathcal{E}_{\lambda r_n^2}(\widehat{Q}_{\lambda, r_n}, B_R \cap \Omega_n) \leq \frac{1}{r_0} \mathcal{E}_\lambda(Q_\lambda, B_{r_0}(x_0) \cap \Omega) + r_0 K_\lambda(Q_b, Q_\lambda)$$

for every  $0 < R < r_0/r_n$ . Since  $\widehat{Q}_b \in C^{1,1}(\widehat{\Omega} \setminus \Omega)$  and  $\widehat{Q}_{\lambda, r_n}(x) = \widehat{Q}_b(x_0 + r_n x)$  for  $x \in B_R \setminus \Omega_n$  and  $0 < R < r_0/r_n$ , in view of (3.9) the sequence  $\{\widehat{Q}_{\lambda, r_n}\}$  is bounded in  $W_{\text{loc}}^{1,2}(\mathbb{R}^3)$ . Consequently, there exists a (not relabeled) subsequence such that  $\widehat{Q}_{\lambda, r_n}$  converges to a map  $Q_*$  weakly in  $W_{\text{loc}}^{1,2}(\mathbb{R}^3; \mathbb{S}^4)$  and strongly in  $L_{\text{loc}}^2(\mathbb{R}^3)$ . Up to a further subsequence,  $\widehat{Q}_{\lambda, r_n} \rightarrow Q_*$  a.e. in  $\mathbb{R}^3$ , and thus  $Q_* \in W_{\text{loc}}^{1,2}(\mathbb{R}^3; \mathbb{S}^4)$ . Now observe that  $\Omega_n \rightarrow \{x_3 > 0\}$  locally in the Hausdorff metric. Since  $\widehat{Q}_b$  is continuous at  $x_0$ ,  $\widehat{Q}_{\lambda, r_n} \rightarrow Q_b(x_0)$  locally uniformly in the open half space  $\{x_3 < 0\}$ . Therefore,  $Q_*(x) \equiv Q_b(x_0)$  in  $\{x_3 < 0\}$ , and it has constant trace on the plane  $\{x_3 = 0\}$ . Arguing essentially as in the proof of Proposition 3.2, we can let  $n \rightarrow \infty$  in (3.9) to infer that

$$\int_{(B_{R_2} \setminus B_{R_1}) \cap \{x_3 > 0\}} \frac{1}{|x|} \left| \frac{\partial Q_*}{\partial |x|} \right|^2 dx = 0$$

for every  $0 < R_1 < R_2$ . Since the map  $Q_*$  is constant in  $\{x_3 < 0\}$ , it follows that  $Q_*$  is 0-homogeneous in the whole  $\mathbb{R}^3$ .

Now it remains to show the strong convergence of  $Q_{\lambda, r_n}$  in  $W_{\text{loc}}^{1,2}(\mathbb{R}^3)$ , and the local energy minimality of  $Q_*$  in  $\{x_3 > 0\}$ . As in the proof of Proposition 3.2, by homogeneity, it is enough to show strong  $W^{1,2}$ -convergence in a ball  $B_\rho \subseteq B_1$  (perhaps up to a subsequence), and energy minimality of  $Q_*$  in  $B_\rho \cap \{x_3 > 0\}$ . We first notice that,  $\widehat{Q}_b$  being  $C^{1,1}$  in  $\widehat{\Omega} \setminus \Omega$ , we have

$$\int_{B_\rho \setminus \Omega_n} |\nabla \widehat{Q}_{\lambda, r_n}|^2 dx = \frac{1}{r_n} \int_{B_{\rho r_n}(x_0) \setminus \Omega} |\nabla \widehat{Q}_b|^2 dx \xrightarrow{n \rightarrow \infty} 0 = \int_{B_\rho \cap \{x_3 \leq 0\}} |\nabla Q_*|^2 dx,$$

and we only need to show that

$$\int_{B_\rho \cap \Omega_n} |\nabla \widehat{Q}_{\lambda, r_n}|^2 dx \xrightarrow{n \rightarrow \infty} \int_{B_\rho \cap \{x_3 > 0\}} |\nabla Q_*|^2 dx$$

to establish the strong convergence of  $\widehat{Q}_{\lambda, r_n}$  in  $W^{1,2}(B_\rho)$ . The rest of the proof is quite similar to the one used for the interior case discussed in Proposition 3.2. For this reason; we only sketch few differences in the construction of comparison maps when gluing different maps near the boundary.

The starting point of the construction is to flatten the boundary  $\partial\Omega$  near  $x_0$ . Assuming  $\{r_n\}$  suitably small (depending only on  $x_0$  and the curvature of  $\partial\Omega$  at  $x_0$ ), there exists a sequence of diffeomorphisms  $\{\Phi_n\} \subseteq C^2(\overline{B}_1; \mathbb{R}^3)$  satisfying the following properties:

$$\Omega_n \cap B_r = \Phi_n(B_r^+), \quad \partial\Omega_n \cap B_r = \Phi_n(B_r \cap \{x_3 = 0\}) \quad \forall 0 < r \leq 1, \\ \text{and } \|\Phi_n - \text{id}\|_{C^2(\overline{B}_1)} \xrightarrow{n \rightarrow \infty} 0, \quad (3.10)$$

where we set  $B_r^+ := B_r \cap \{x_3 > 0\}$ ,  $0 < r \leq 1$ . We fix  $0 < \delta < 1/4$  and a competitor  $\bar{Q} \in W_{\text{loc}}^{1,2}(\mathbb{R}^3; \mathbb{S}^4)$  such that  $\bar{Q} = Q_*$  a.e. in  $\mathbb{R}^3 \setminus B_{1-\delta}^+$ . Notice that  $\widehat{Q}_{\lambda, r_n} \circ \Phi_n \rightharpoonup Q_*$  weakly in  $W^{1,2}(B_1^+; \mathbb{S}^4)$  as  $n \rightarrow \infty$ . In addition,  $\widehat{Q}_{\lambda, r_n}(\Phi_n(x)) = Q_b(x_0 + r_n \Phi_n(x))$  and  $\bar{Q}(x) = Q_b(x_0)$  for  $x \in B_1 \cap \{x_3 = 0\}$  because of (3.10). Consequently, since  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$  we get

$$\lim_{n \rightarrow \infty} \int_{B_1 \cap \{x_3 = 0\}} |\widehat{Q}_{\lambda, r_n} \circ \Phi_n - \bar{Q}|^2 d\mathcal{H}^2 = 0 \quad \text{and} \quad \lim_{n \rightarrow \infty} \int_{B_1 \cap \{x_3 = 0\}} |\nabla_{\tan}(\widehat{Q}_{\lambda, r_n} \circ \Phi_n)|^2 d\mathcal{H}^2 = 0.$$

Hence we can argue as in the interior case: by Fatou's lemma and Fubini's theorem, extracting a further subsequence if necessary, we can select  $\rho \in (1 - \delta, 1)$  and a constant  $C > 0$  such that

$$\lim_{n \rightarrow \infty} \int_{\partial B_\rho^+} |\widehat{Q}_{\lambda, r_n} \circ \Phi_n - \bar{Q}|^2 d\mathcal{H}^2 = 0 \quad \text{and} \quad \int_{\partial B_\rho^+} (|\nabla_{\tan}(\widehat{Q}_{\lambda, r_n} \circ \Phi_n)|^2 + |\nabla_{\tan} \bar{Q}|^2) d\mathcal{H}^2 \leq C.$$

We then choose the sequence  $\sigma_n \rightarrow 0$  with  $0 < \sigma_n < \delta$  as  $\sigma_n := \|\widehat{Q}_{\lambda, r_n} \circ \Phi_n - \bar{Q}\|_{L^2(\partial B_\rho^+) }^{1/3}$ .

Before going further, let us notice that we can argue as in Lemma 3.8 (using the weak convergence of  $\widehat{Q}_{\lambda, r_n}$ , its energy minimality on  $\Omega_n \cap B_\rho$ , and (3.10)) to prove the following: for any bounded sequence  $\{v_n\} \subseteq W^{1,2}(B_\rho^+; \mathbb{S}^4)$  such that  $v_n = \widehat{Q}_{\lambda, r_n} \circ \Phi_n$  on  $\partial B_\rho^+$ , we have

$$\begin{aligned} \int_{B_\rho^+} |\nabla Q_*|^2 dx &\leq \liminf_{n \rightarrow \infty} \int_{\Omega_n \cap B_\rho} |\nabla \widehat{Q}_{\lambda, r_n}|^2 dx \leq \limsup_{n \rightarrow \infty} \int_{\Omega_n \cap B_\rho} |\nabla \widehat{Q}_{\lambda, r_n}|^2 dx \\ &\leq \limsup_{n \rightarrow \infty} \mathcal{E}_{\lambda r_n^2}(\widehat{Q}_{\lambda, r_n}, \Omega_n \cap B_\rho) \leq \limsup_{n \rightarrow \infty} \mathcal{E}_{\lambda r_n^2}(v_n \circ \Phi_n^{-1}, \Omega_n \cap B_\rho) \\ &= \limsup_{n \rightarrow \infty} \int_{B_\rho^+} |\nabla v_n|^2 dx, \end{aligned} \quad (3.11)$$

where the last equality follows from a change of variables and (3.10).

Now, to construct an effective sequence of comparison maps, it is convenient to introduce a biLipschitz map  $\Psi: \bar{B}_1 \rightarrow \bar{B}_1^+$ . By means of  $\Psi$ , the comparison maps can be constructed as in the interior case. More precisely, we apply Lemma 3.4 to the pair of maps from the two-sphere  $\mathbb{S}^2$ , namely  $u(\cdot) = \widehat{Q}_{\lambda, r_n} \circ \Phi_n(\rho\Psi(\cdot))$  and  $v(\cdot) = \bar{Q}(\rho\Psi(\cdot))$ . As in the interior case, the lemma produces a sequence  $\{w_n\} \subseteq W^{1,2}(B_1; \mathcal{S}_0)$  satisfying

$$w_n(x) = \begin{cases} \bar{Q}\left(\rho\Psi\left(\frac{x}{1-\sigma_n}\right)\right) & \text{if } |x| \leq 1 - \sigma_n, \\ \widehat{Q}_{\lambda, r_n} \circ \Phi_n(\rho\Psi(x)) & \text{if } |x| = 1, \end{cases}$$

with the estimate

$$\begin{aligned} \int_{B_1 \setminus B_{1-\sigma_n}} |\nabla w_n|^2 dx &\leq C \left( \sigma_n \int_{\partial B_\rho^+} (|\nabla_{\tan}(\widehat{Q}_{\lambda, r_n} \circ \Phi_n)|^2 + |\nabla_{\tan} \bar{Q}|^2) d\mathcal{H}^2 \right. \\ &\quad \left. + \frac{1}{\sigma_n} \int_{\partial B_\rho^+} |\widehat{Q}_{\lambda, r_n} \circ \Phi_n - \bar{Q}|^2 d\mathcal{H}^2 \right) \xrightarrow{n \rightarrow \infty} 0, \end{aligned} \quad (3.12)$$

and  $\text{dist}(w_n, \mathbb{S}^4) \rightarrow 0$  uniformly in  $B_1 \setminus B_{1-\sigma_n}$  as  $n \rightarrow \infty$ .

Since  $|w_n| \geq 1/2$  for  $n$  large enough, we can define a sequence  $\{\bar{v}_n\} \subseteq W^{1,2}(B_1; \mathbb{S}^4)$  by setting

$$\bar{v}_n(x) = \begin{cases} \bar{Q}(\rho\Psi\left(\frac{x}{1-\sigma_n}\right)) & \text{if } |x| \leq 1 - \sigma_n, \\ \frac{w_n(x)}{|w_n(x)|} & \text{if } 1 - \sigma_n \leq |x| \leq 1, \end{cases} \quad (3.13)$$

and it satisfies

$$\int_{B_1 \setminus B_{1-\sigma_n}} |\nabla \bar{v}_n|^2 dx \leq C \int_{B_1 \setminus B_{1-\sigma_n}} |\nabla w_n|^2 dx \xrightarrow{n \rightarrow \infty} 0. \quad (3.14)$$

Now we pull-back  $\bar{v}_n$  on  $B_\rho^+$  by setting  $v_n(x) = \bar{v}_n(\Psi^{-1}(x/\rho))$ , so that  $v_n \in W^{1,2}(B_\rho^+; \mathbb{S}^4)$  and  $v_n = \widehat{Q}_{\lambda, r_n} \circ \Phi_n$  on  $\partial B_\rho^+$  in the sense of traces. Then, a simple computation using the biLipschitz property of  $\Psi$  together with (3.13) and (3.14) yields

$$\begin{aligned} \limsup_{n \rightarrow \infty} \int_{B_\rho^+} |\nabla v_n|^2 dx &\leq \limsup_{n \rightarrow \infty} \int_{B_\rho^+ \setminus (\rho\Psi(B_{1-\sigma_n}))} |\nabla v_n|^2 dx + \limsup_{n \rightarrow \infty} \int_{\rho\Psi(B_{1-\sigma_n})} |\nabla v_n|^2 dx \\ &\leq \limsup_{n \rightarrow \infty} C \int_{B_1 \setminus B_{1-\sigma_n}} |\nabla \bar{v}_n|^2 dx + \limsup_{n \rightarrow \infty} \int_{\rho\Psi(B_{1-\sigma_n})} |\nabla \bar{Q}|^2 dx \leq \int_{B_\rho^+} |\nabla \bar{Q}|^2 dx. \end{aligned} \quad (3.15)$$

Combining (3.11) and (3.15) with  $\bar{Q} \equiv Q_*$ , we infer that  $\int_{\Omega_n \cap B_\rho} |\nabla \widehat{Q}_{\lambda, r_n}|^2 dx \rightarrow \int_{B_\rho^+} |\nabla Q_*|^2 dx$ , while for an arbitrary  $\bar{Q}$ , it yields  $\int_{B_\rho^+} |\nabla Q_*|^2 dx \leq \int_{B_\rho^+} |\nabla \bar{Q}|^2 dx$ . The limiting map  $Q_*$  is thus a minimizing harmonic map in  $B_\rho^+$ , and the proof is complete.  $\square$

All possible limiting maps  $Q_*$  obtained by either Proposition 3.2 or Proposition 3.5 are often referred to as (*minimizing*) *tangent maps* to  $Q_\lambda$  at the given point  $x_0$ . By the monotonicity formulae and the strong compactness of rescaled maps, triviality (i.e., constancy) of all tangent maps implies smallness of the rescaled energy at sufficiently small scale. In our setting, triviality of tangent maps together with smallness of the scaled energy are established in the following propositions.

**Proposition 3.6.** *If  $Q_\lambda$  is a minimizer of  $\mathcal{E}_\lambda$  over  $\mathcal{A}_{Q_b}(\Omega)$ , then*

$$\lim_{r \rightarrow 0} \frac{1}{r} \mathcal{E}_\lambda(Q_\lambda, B_r(x_0)) = 0$$

for every  $x_0 \in \Omega$ .

*Proof.* Let us fix an arbitrary point  $x_0 \in \Omega$  and a sequence  $r_n \rightarrow 0$ . According to Proposition 3.2, up to a subsequence, the rescaled maps satisfy  $Q_{\lambda, r_n} \rightarrow Q_*$  strongly in  $W_{\text{loc}}^{1,2}(\mathbb{R}^3)$  as  $n \rightarrow \infty$  for some  $Q_* \in W_{\text{loc}}^{1,2}(\mathbb{R}^3; \mathbb{S}^4)$ . Moreover,  $Q_*$  is a degree-zero homogeneous energy minimizing harmonic map, so that there exists a smooth harmonic sphere  $\omega : \mathbb{S}^2 \rightarrow \mathbb{S}^4$  such that  $Q_*(x) = \omega(\frac{x}{|x|})$ . On the other hand, according to [57, Theorem 2.7] the map  $Q_*$  is smooth. In particular,  $Q_*$  is smooth at the origin which implies that  $\omega$  must be constant, and thus  $Q_*$  itself is a constant map. Then the interior monotonicity formula (see Proposition 3.1) and the strong  $W^{1,2}$ -convergence yield

$$\lim_{r \rightarrow 0} \frac{1}{r} \mathcal{E}_\lambda(Q_\lambda, B_r(x_0)) = \lim_{n \rightarrow \infty} \mathcal{E}_{\lambda r_n^2}(Q_{\lambda, r_n}, B_1) = \frac{1}{2} \int_{B_1} |\nabla Q_*|^2 dx = 0,$$

which completes the proof.  $\square$

**Proposition 3.7.** *Let  $\Omega \subseteq \mathbb{R}^3$  be a bounded open set with  $\partial\Omega$  of class  $C^3$  and  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ . If  $Q_\lambda$  is a minimizer of  $\mathcal{E}_\lambda$  over  $\mathcal{A}_{Q_b}(\Omega)$  then*

$$\lim_{r \rightarrow 0} \frac{1}{r} \mathcal{E}_\lambda(Q_\lambda, B_r(x_0) \cap \Omega) = 0$$

for every  $x_0 \in \partial\Omega$ .

*Proof.* As in the previous proof, by the strong  $W^{1,2}$ -compactness of rescaled maps, it is enough to prove that any limiting map  $Q_*$  obtained from Proposition 3.5 applied at a point  $x_0 \in \partial\Omega$  is a constant map, i.e.,  $Q_* \equiv Q_b(x_0)$ . Indeed, by the Boundary Monotonicity Inequality (see Proposition 3.1), we have

$$\lim_{r \rightarrow 0} \frac{1}{r} \mathcal{E}_\lambda(Q_\lambda, B_r(x_0) \cap \Omega) = \lim_{n \rightarrow \infty} \mathcal{E}_{\lambda r_n^2}(Q_{\lambda, r_n}, B_1 \cap \Omega_n) = \frac{1}{2} \int_{B_1 \cap \{x_3 > 0\}} |\nabla Q_*|^2 dx = 0,$$

where we have set  $\Omega_n := r_n^{-1}(\Omega - x_0)$ .

Let us now consider a degree zero homogeneous map  $Q_* \in W_{\text{loc}}^{1,2}(\mathbb{R}^3; \mathbb{S}^4)$  which is an energy minimizing harmonic map in  $\{x_3 > 0\}$ , and such that  $Q_* = Q_b(x_0) =: e_0$  in  $\{x_3 < 0\}$ . Setting  $\mathbb{S}_+^2 := \mathbb{S}^2 \cap \{x_3 > 0\}$ , the homogeneity of  $Q_*$  implies that  $Q_*(x) = \omega(\frac{x}{|x|})$  in  $\{x_3 > 0\}$  where  $\omega \in W^{1,2}(\mathbb{S}_+^2; \mathbb{S}^4)$  is a weakly harmonic map on  $\mathbb{S}_+^2$  satisfying  $\omega = e_0$  on  $\partial\mathbb{S}_+^2$  in the sense of traces. It now suffices to show that  $\omega \in C^\infty(\overline{\mathbb{S}_+^2})$ . Indeed, by Lemaire rigidity theorem [36, Theorem 3.2], a smooth harmonic map on the (closed) half 2-sphere which is constant on the boundary has to be constant. In other words  $\omega \equiv e_0$ , whence  $Q_* \equiv e_0$ .

The smoothness of  $\omega$  in the interior  $\mathbb{S}_+^2$  follows from Hélein's theorem [26]. Smoothness up to the boundary  $\partial\mathbb{S}_+^2$  could be asserted directly from [50], but we prefer to give a short argument illustrating in this simple case the reflection principle in Subsection 2.2.

Consider the map  $\widehat{Q}_* \in W_{\text{loc}}^{1,2}(\mathbb{R}^3; \mathbb{S}^4)$  defined by

$$\widehat{Q}_*(x) := \begin{cases} Q_*(x) & \text{if } x_3 > 0, \\ \Sigma Q_*(\bar{x}) & \text{if } x_3 < 0, \end{cases}$$

where  $\bar{x} = (x_1, x_2, -x_3)$  is the reflection of  $x = (x_1, x_2, x_3)$  across the plane  $\{x_3 = 0\}$ , and  $\Sigma := 2e_0 \otimes e_0 - \text{id}$  is the geodesic reflection on  $\mathbb{S}^4$  with respect to the point  $e_0$ . Following the proof of Proposition 2.8 with  $\lambda = 0$  (see also Remark 2.11), we infer that the reflected matrix  $A(x)$  is the identity and  $\widehat{Q}_*$  is weakly harmonic in  $\mathbb{R}^3$ . Since  $\widehat{Q}_*$  clearly inherits homogeneity from  $Q_*$ , we have  $\widehat{Q}_*(x) = \widehat{\omega}(\frac{x}{|x|})$  for a weakly harmonic map  $\widehat{\omega} \in W^{1,2}(\mathbb{S}^2; \mathbb{S}^4)$ . By Hélein's theorem [26],  $\widehat{\omega}$  is smooth on  $\mathbb{S}^2$ , and the conclusion follows since  $\widehat{\omega} = \omega$  in  $\mathbb{S}_+^2$ .  $\square$

**3.3. Full regularity.** Combining the results from the subsections above with the  $\varepsilon$ -regularity theorem and the higher regularity theorem from Section 2.1, we are finally in the position to prove the first regularity result of the paper.

*Proof of Theorem 1.2.* Let  $Q_\lambda$  be a minimizer of  $\mathcal{E}_\lambda$  over  $\mathcal{A}_{Q_b}(\Omega)$ . First, we prove interior regularity of  $Q_\lambda$  by showing smoothness in a neighborhood of an arbitrary point  $x_0 \in \Omega$ . In view of Proposition 3.6, we have  $\frac{1}{r}\mathcal{E}_\lambda(Q_\lambda, B_r(x_0)) \rightarrow 0$  as  $r \rightarrow 0$ . Combining Proposition 3.1 and Lemma 2.6 (with  $Q_{\text{ref}} = Q_\lambda$ ) with Corollary 2.19, we infer that  $Q_\lambda \in C^\omega(B_\rho(x_0))$  for some radius  $\rho > 0$  possibly depending on the point  $x_0$ . Since  $x_0 \in \Omega$  is arbitrary, we conclude that  $Q_\lambda \in C^\omega(\Omega)$ .

To prove boundary regularity, we now fix an arbitrary point  $x_0 \in \partial\Omega$ . By Proposition 3.7, we have  $\frac{1}{r}\mathcal{E}_\lambda(Q_\lambda, B_r(x_0) \cap \Omega) \rightarrow 0$  as  $r \rightarrow 0$ . Then we combine Proposition 3.1 and Lemma 2.10 (with  $Q_{\text{ref}} = Q_\lambda$ ) with Corollary 2.20 to conclude that  $Q_\lambda \in C^{1,\alpha}(B_\rho(x_0) \cap \bar{\Omega})$  for every  $\alpha \in (0, 1)$  and some radius  $\rho > 0$ . Since  $x_0$  is arbitrary, a covering argument yields  $Q_\lambda \in C^{1,\alpha}(\bar{\Omega})$  for every  $\alpha \in (0, 1)$ . Under the further assumption that  $\partial\Omega$  is of class  $C^{k,\beta}$  and  $Q_b \in C^{k,\beta}(\partial\Omega; \mathbb{S}^4)$  for some  $\beta > 0$  and  $k \geq 2$ , then Corollary 2.20 with the same covering argument tells us that  $Q_\lambda \in C^{k,\beta}(\bar{\Omega})$ . Finally, if  $\partial\Omega$  is real-analytic and  $Q_b \in C^\omega(\partial\Omega; \mathbb{S}^4)$ , then Corollary 2.20 again implies that  $Q_\lambda \in C^\omega(\bar{\Omega})$ .  $\square$

#### 4. LDG-MINIMIZERS IN THE LYUKSYUTOV REGIME

The main objective of this section is to prove Theorem 1.3, and in particular to prove that isotropic melting (i.e., presence of the zero phase) is avoided by minimizers of the energy functional  $\mathcal{F}_{\lambda,\mu}$  in (1.10) for values of the parameters in the Lyuksyutov regime  $\mu \rightarrow \infty$ . More precisely, our main goal is to prove that the pointwise norm of any minimizer  $Q_\lambda^\mu$  of  $\mathcal{F}_{\lambda,\mu}$  subject to an  $\mathbb{S}^4$ -valued boundary condition is uniformly bounded from below by a positive constant whenever  $\mu$  is large enough (and  $\lambda$  of order one). As a consequence we deduce that the radial hedgehog (1.20) is not energy minimizing and in Theorem 4.8 below we will show that it is not even a stable critical point of the energy functional  $\mathcal{F}_{\lambda,\mu}$ .

Throughout this section, we assume again that the boundary  $\partial\Omega$  is of class  $C^3$ , and that the boundary condition  $Q_b$  belongs to  $C^{1,1}(\partial\Omega; \mathbb{S}^4)$ . Given  $\lambda > 0$  and  $\mu > 0$ , we shall consider critical point of  $\mathcal{F}_{\lambda,\mu}$  over the class  $W^{1,2}(\Omega; \mathcal{S}_0)$ , including as a particular case solutions of the variational problem

$$\min \left\{ \mathcal{F}_{\lambda,\mu}(Q) : Q \in W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0) \right\}$$

whose resolution follows from the direct method of calculus of variations. We may denote by  $Q_\lambda^\mu$  a critical point of  $\mathcal{F}_{\lambda,\mu}$ , or simply by  $Q^\mu$  (if no confusion arises) hiding the dependence on the fixed parameter  $\lambda$  to simplify the notation. We start with elementary/classical considerations and a priori estimates on  $Q^\mu$ .

**4.1. A priori estimates.** In view of the explicit expression (1.12) of the potential  $W$ , the Euler-Lagrange equation characterizing a critical point  $Q^\mu \in W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$  reads as follows

$$\begin{cases} -\Delta Q^\mu = \lambda \left( (Q^\mu)^2 - \frac{1}{3}|Q^\mu|^2 I - \frac{1}{\sqrt{6}}|Q^\mu|^2 Q^\mu \right) + \mu(1 - |Q^\mu|^2)Q^\mu & \text{in } \Omega, \\ Q^\mu = Q_b & \text{on } \partial\Omega, \end{cases} \quad (4.1)$$

with the term  $\frac{1}{3}|Q^\mu|^2 I$  due to the traceless constraint.

Let us start the analysis by establishing the regularity of critical points.

**Lemma 4.1.** *If  $Q^\mu$  is a critical point of  $\mathcal{F}_{\lambda,\mu}$  over  $W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$ , then  $Q^\mu \in C^\omega(\Omega) \cap C^{1,\alpha}(\bar{\Omega})$  for every  $\alpha \in (0, 1)$ . In addition,*

- (i) *if  $\partial\Omega$  is of class  $C^{k,\beta}$  and  $Q_b \in C^{k,\beta}(\partial\Omega; \mathbb{S}^4)$  for some  $\beta > 0$  and  $k \geq 2$ , then  $Q^\mu \in C^{k,\beta}(\bar{\Omega})$ ;*
- (ii) *if  $\partial\Omega$  is real-analytic and  $Q_b \in C^\omega(\partial\Omega; \mathbb{S}^4)$ , then  $Q^\mu \in C^\omega(\bar{\Omega})$ .*

*Proof.* In view of equation (4.1), the fact that  $Q^\mu \in C^{1,\alpha}(\bar{\Omega})$  for every  $\alpha \in (0, 1)$  follows exactly as in the proof of Proposition 2.4, Step 1. Then, a classical bootstrap argument based on Schauder estimates shows that  $Q^\mu \in C^\infty(\Omega)$  (see e.g. [22, Chapters 6 & 8]), and the standard results in [46, Chapter 6] give interior analytic regularity. Assuming that  $\partial\Omega$  is of class  $C^{k,\beta}$  and  $Q_b \in C^{k,\beta}(\partial\Omega; \mathbb{S}^4)$  with  $k \geq 2$ , we have  $Q_\lambda \in C^{k,\beta}(\bar{\Omega})$  by standard elliptic regularity at the boundary, see e.g. [22, Chapter 6]. The corresponding conclusion within the analytic class follows again from the results in [46, Chapter 6].  $\square$

We now prove an a priori estimate on the modulus and on the gradient of a critical point reminiscent from the Ginzburg-Landau theories.

**Lemma 4.2.** *If  $Q^\mu$  is a critical point point of  $\mathcal{F}_{\lambda,\mu}$  over  $W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$ , then  $|Q^\mu| \leq 1$  in  $\bar{\Omega}$ .*

*Proof.* Consider the scalar function  $u := 1 - |Q^\mu|^2$ . In view of the previous lemma and equation (4.1),  $u$  is continuous in  $\bar{\Omega}$  is a classical solution to

$$-\Delta u + 2\mu|Q^\mu|^2 u \geq \frac{2\lambda}{\sqrt{6}}(|Q^\mu|^4 - \sqrt{6}\text{tr}((Q^\mu)^3)) \quad \text{in } \Omega. \quad (4.2)$$

Let  $x_0 \in \bar{\Omega}$  be a minimum point for  $u$ , and assume by contradiction that  $u(x_0) < 0$ , (in other words,  $|Q^\mu(x_0)| > 1$ ). Since  $u = 1 - |Q_b|^2 \equiv 0$  on  $\partial\Omega$ , we must have  $x_0 \in \Omega$ . Consequently,  $\Delta u(x_0) \geq 0$ , and (4.2) leads to

$$0 > |Q^\mu(x_0)|^4 - \sqrt{6}\text{tr}((Q^\mu)^3)(x_0) \geq |Q^\mu(x_0)|^3 - \sqrt{6}\text{tr}((Q^\mu)^3)(x_0). \quad (4.3)$$

However, (1.4) tells us that the right-hand side of (4.3) is nonnegative, a contradiction.  $\square$

**Lemma 4.3.** *If  $Q^\mu$  is a critical point point of  $\mathcal{F}_{\lambda,\mu}$  over  $W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$ , then*

$$|\nabla Q^\mu| \leq C(\sqrt{\lambda + \mu} + 1) \quad \text{in } \bar{\Omega},$$

for a constant  $C$  depending only on  $\Omega$  and  $Q_b$ .

*Proof.* Consider  $H$  to be the harmonic extension of  $Q_b$  to the domain  $\Omega$ , i.e.,

$$\begin{cases} \Delta H = 0 & \text{in } \Omega, \\ H = Q_b & \text{on } \partial\Omega. \end{cases}$$

By our regularity assumption on  $\partial\Omega$  and  $Q_b$ , we have  $H \in C^{1,\alpha}(\bar{\Omega}) \cap C^2(\Omega)$  for every  $\alpha \in (0, 1)$ . Setting  $U_\mu := Q^\mu - H$ , we deduce from (4.1) and Lemma 4.2 that  $\|\Delta U_\mu\|_{L^\infty(\Omega)} \leq C(\lambda + \mu)$ , and  $U_\mu = 0$  on  $\partial\Omega$ . By interpolation (see e.g. [5, Lemma A.2]) and Lemma 4.2 again, we conclude that

$$\|\nabla U_\mu\|_{L^\infty(\Omega)} \leq C\|\Delta U_\mu\|_{L^\infty(\Omega)}^{1/2}\|U_\mu\|_{L^\infty(\Omega)}^{1/2} \leq C\sqrt{\lambda + \mu},$$

for a constant  $C$  depending only on  $\Omega$  and  $Q_b$ . Since  $\|\nabla Q^\mu\|_{L^\infty(\Omega)} \leq \|\nabla U_\mu\|_{L^\infty(\Omega)} + \|\nabla H\|_{L^\infty(\Omega)}$ , the conclusion follows.  $\square$

The last ingredients we need are the following monotonicity formulae.

**Lemma 4.4.** *If  $Q^\mu$  is a critical point point of  $\mathcal{F}_{\lambda,\mu}$  over  $W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$ , then*

(1) *for every  $x_0 \in \Omega$  and every  $0 < \rho < r < \text{dist}(x_0, \partial\Omega)$ , we have*

$$\frac{1}{\rho}\mathcal{F}_{\lambda,\mu}(Q^\mu, B_\rho(x_0)) \leq \frac{1}{r}\mathcal{F}_{\lambda,\mu}(Q^\mu, B_r(x_0)); \quad (4.4)$$

(2) *there exist a radius  $r_\Omega > 0$  (depending only on  $\Omega$ ) and a constant  $C_{Q_b}^\lambda > 0$  depending only  $\lambda, \Omega, Q_b$ , and on (an upper bound of)  $\|\nabla Q^\mu\|_{L^2(\Omega)}$  but independent of  $\mu$ , such that*

$$\frac{1}{\rho}\mathcal{F}_{\lambda,\mu}(Q^\mu, B_\rho(x_0)) \leq \frac{1}{r}\mathcal{F}_{\lambda,\mu}(Q^\mu, B_r(x_0)) + C_{Q_b}^\lambda(r - \rho) \quad (4.5)$$

for every  $x_0 \in \partial\Omega$  and every  $0 < \rho < r < r_\Omega$ .

The proof of this lemma follows word by word the one in Proposition 2.4 (Step 2 & Step 3), and we shall omit it. We just observe that the constant  $C_{Q_b}^\lambda$  in (4.5) is independent of  $\mu$  because  $Q_b$  has always unit norm on  $\partial\Omega$ .

**4.2. Lyuksyutov regime and absence of isotropic melting.** We now complete the proof of Theorem 1.3 analyzing the asymptotic behavior as  $\mu \rightarrow +\infty$  of minimizers of  $\mathcal{F}_{\lambda,\mu}$  over the class  $W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$ . The heart of the matter is Proposition 4.5 below. We emphasize that Proposition 4.5 does not rely on energy minimality but on the a priori strong convergence towards a smooth limiting map. This allows for more flexibility in its application, see our companion paper [16].

**Proposition 4.5.** *Given a sequence  $\mu_n \rightarrow +\infty$ , consider for each  $\mu_n$  a critical point  $Q_{\lambda}^{\mu_n}$  of  $\mathcal{F}_{\lambda,\mu_n}$  over  $W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$ . Assume that  $Q_{\lambda}^{\mu_n} \rightharpoonup Q_\lambda$  weakly in  $W^{1,2}(\Omega; \mathcal{S}_0)$  as  $n \rightarrow \infty$  for some  $Q_\lambda \in \mathcal{A}_{Q_b}(\Omega) \cap C^1(\bar{\Omega}; \mathbb{S}^4)$ , and that*

$$\lim_{n \rightarrow \infty} \mathcal{F}_{\lambda,\mu_n}(Q_{\lambda}^{\mu_n}) = \mathcal{E}_\lambda(Q_\lambda).$$

Then,

(1)  $Q_{\lambda}^{\mu_n} \rightarrow Q_\lambda$  strongly in  $W^{1,2}(\Omega; \mathcal{S}_0)$ ;

$$(2) \quad \mu_n \int_{\Omega} (1 - |Q_{\lambda}^{\mu_n}|^2)^2 dx \rightarrow 0;$$

$$(3) \quad |Q_{\lambda}^{\mu_n}| \rightarrow 1 \text{ uniformly in } \bar{\Omega}.$$

*Proof. Step 1.* We start proving items (1) and (2). First, notice that  $Q_{\lambda}^{\mu_n} \rightarrow Q_{\lambda}$  strongly in  $L^4(\Omega)$  by the compact embedding  $W^{1,2}(\Omega) \hookrightarrow L^4(\Omega)$ . Hence  $\int_{\Omega} W(Q_{\lambda}^{\mu_n}) dx \rightarrow \int_{\Omega} W(Q_{\lambda}) dx$  and by lower semicontinuity of the Dirichlet integral we get  $\mathcal{E}_{\lambda}(Q_{\lambda}) \leq \liminf_{n \rightarrow \infty} \mathcal{E}_{\lambda}(Q_{\lambda}^{\mu_n})$ .

Hence, we have

$$\mathcal{E}_{\lambda}(Q_{\lambda}) \leq \liminf_{n \rightarrow \infty} \mathcal{E}_{\lambda}(Q_{\lambda}^{\mu_n}) + \limsup_{n \rightarrow \infty} \frac{\mu_n}{4} \int_{\Omega} (1 - |Q_{\lambda}^{\mu_n}|^2)^2 dx \leq \lim_{n \rightarrow \infty} \mathcal{F}_{\lambda, \mu_n}(Q_{\lambda}^{\mu_n}) = \mathcal{E}_{\lambda}(Q_{\lambda}).$$

Therefore  $\mu_n \int_{\Omega} (1 - |Q_{\lambda}^{\mu_n}|^2)^2 dx \rightarrow 0$  and  $\|\nabla Q_{\lambda}^{\mu_n}\|_{L^2(\Omega)}^2 \rightarrow \|\nabla Q_{\lambda}\|_{L^2(\Omega)}^2$ . Combined with the weak  $W^{1,2}$ -convergence, this latter fact implies that  $Q_{\lambda}^{\mu_n} \rightarrow Q_{\lambda}$  strongly in  $W^{1,2}(\Omega)$ .

*Step 2.* It now remains to prove that  $|Q_{\lambda}^{\mu_n}| \rightarrow 1$  uniformly in  $\bar{\Omega}$ . Given  $\delta \in (0, 1)$  arbitrary, we thus have to prove that  $|Q_{\lambda}^{\mu_n}| > \delta$  on  $\bar{\Omega}$  for  $n$  large enough. We argue by contradiction assuming that, along a (not relabeled) subsequence, there exists  $x_n \in \Omega$  such that  $|Q_{\lambda}^{\mu_n}(x_n)| \leq \delta$ . Extracting a further subsequence if necessary, we can assume that  $x_n \rightarrow x_0$  as  $n \rightarrow \infty$  for some  $x_0 \in \bar{\Omega}$ . In view of Lemma 4.3 (and the fact that  $|Q^{\mu}| = 1$  on  $\partial\Omega$ ), we can find a constant  $\kappa \in (0, 1)$  independent of  $n$  such that for  $r_n := \kappa \mu_n^{-1/2} \rightarrow 0$  and for all  $n$  we have

$$B_{r_n}(x_n) \subseteq \Omega \quad \text{and} \quad |Q_{\mu_n}|^2 \leq \frac{1 + \delta^2}{2} \text{ in } B_{r_n}(x_n). \quad (4.6)$$

We now distinguish two cases:

*Case 1:*  $x_0 \in \Omega$ . The limiting map  $Q_{\lambda}$  being of class  $C^1$ , we can find a radius  $r_0 \in (0, \text{dist}(x_0, \partial\Omega))$  such that

$$\frac{1}{r_0} \mathcal{E}_{\lambda}(Q_{\lambda}, B_{r_0}(x_0)) < \frac{\pi \kappa^2 (1 - \delta^2)^2}{24}.$$

From Step 1, we deduce that for  $n$  large enough,

$$\frac{1}{r_0} \mathcal{F}_{\lambda, \mu_n}(Q_{\lambda}^{\mu_n}, B_{r_0}(x_0)) < \frac{\pi \kappa^2 (1 - \delta^2)^2}{24}. \quad (4.7)$$

On the other hand, still for  $n$  large enough, we have  $|x_n - x_0| < r_0/2$  and  $r_n < r_0/2$ . Then we infer from (4.6) and (4.4) that

$$\begin{aligned} \frac{\pi \kappa^2 (1 - \delta^2)^2}{12} &\leq \frac{\mu_n}{4r_n} \int_{B_{r_n}(x_n)} (1 - |Q_{\lambda}^{\mu_n}|^2)^2 dx \leq \frac{1}{r_n} \mathcal{F}_{\lambda, \mu_n}(Q_{\lambda}^{\mu_n}, B_{r_n}(x_n)) \\ &\leq \frac{2}{r_0} \mathcal{F}_{\lambda, \mu_n}(Q_{\lambda}^{\mu_n}, B_{r_0/2}(x_n)) \leq \frac{2}{r_0} \mathcal{F}_{\lambda, \mu_n}(Q_{\lambda}^{\mu_n}, B_{r_0}(x_0)), \end{aligned}$$

which contradicts (4.7).

*Case 2:*  $x_0 \in \partial\Omega$ . Once again, since  $Q_{\lambda} \in C^1(\bar{\Omega})$  and  $\partial\Omega$  is of class  $C^3$ , we can find a small radius  $r_0 \in (0, r_{\Omega})$  where  $r_{\Omega}$  is given by Lemma 4.4 such that the nearest point projection on  $\partial\Omega$  is well defined in the  $r_0$ -tubular neighborhood of  $\partial\Omega$ , and

$$\frac{1}{r_0} \mathcal{E}_{\lambda}(Q_{\lambda}, B_{r_0}(x_0) \cap \Omega) + C_{Q_b}^{\lambda} r_0 < \frac{\pi \kappa^2 (1 - \delta^2)^2}{48},$$

where the constant  $C_{Q_b}^{\lambda}$  is also given by Lemma 4.4 (notice that  $\|\nabla Q_{\lambda}^{\mu_n}\|_{L^2(\Omega)}$  is bounded by Step 1). From Step 1, we deduce that for  $n$  large enough,

$$\frac{1}{r_0} \mathcal{F}_{\lambda, \mu_n}(Q_{\lambda}^{\mu_n}, B_{r_0}(x_0) \cap \Omega) + C_{Q_b}^{\lambda} r_0 < \frac{\pi \kappa^2 (1 - \delta^2)^2}{48}. \quad (4.8)$$

If we denote  $y_n \in \partial\Omega$  the projection of  $x_n$  on  $\partial\Omega$ , we have for  $n$  large enough (by (4.6)),

$$r_n \leq |y_n - x_n| = \text{dist}(x_n, \partial\Omega) \leq |x_n - x_0| < \frac{r_0}{4},$$

so that  $|y_n - x_0| < r_0/2$ . Arguing as in Case 1 and setting  $d_n := |y_n - x_n|$ , we infer from (4.6) and (4.4)-(4.5) that

$$\begin{aligned} \frac{\pi\kappa^2(1-\delta^2)^2}{12} &\leq \frac{1}{r_n} \mathcal{F}_{\lambda, \mu_n}(Q_\lambda^{\mu_n}, B_{r_n}(x_n)) \leq \frac{1}{d_n} \mathcal{F}_{\lambda, \mu_n}(Q_\lambda^{\mu_n}, B_{d_n}(x_n)) \\ &\leq \frac{1}{d_n} \mathcal{F}_{\lambda, \mu_n}(Q_\lambda^{\mu_n}, B_{2d_n}(y_n) \cap \Omega) \leq \frac{4}{r_0} \mathcal{F}_{\lambda, \mu_n}(Q_\lambda^{\mu_n}, B_{r_0/2}(y_n) \cap \Omega) + C_{Q_b}^\lambda r_0 \\ &\leq \frac{4}{r_0} \mathcal{F}_{\lambda, \mu_n}(Q_\lambda^{\mu_n}, B_{r_0}(x_0) \cap \Omega) + C_{Q_b}^\lambda r_0, \end{aligned}$$

which contradicts (4.8).  $\square$

*Proof of Theorem 1.3.* Let us consider an arbitrary sequence  $\mu_n \rightarrow +\infty$  and corresponding  $Q_\lambda^{\mu_n}$  minimizing  $\mathcal{F}_{\lambda, \mu_n}$  over  $W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$ . Since the map  $\bar{Q}_b \in \mathcal{A}_{Q_b}(\Omega)$  is an admissible competitor to the minimality of  $Q_\lambda^{\mu_n}$ , we have

$$\mathcal{F}_{\lambda, \mu_n}(Q_\lambda^{\mu_n}) \leq \mathcal{F}_{\lambda, \mu_n}(\bar{Q}_b) = \mathcal{E}_\lambda(\bar{Q}_b). \quad (4.9)$$

Therefore, the sequence  $\{Q_\lambda^{\mu_n}\}$  is bounded in  $W^{1,2}(\Omega; \mathcal{S}_0)$ , and we can extract a (not relabeled) subsequence such that  $Q_\lambda^{\mu_n} \rightharpoonup Q_\lambda$  weakly in  $W^{1,2}(\Omega)$  for some  $Q_\lambda \in W_{Q_b}^{1,2}(\Omega; \mathcal{S}_0)$ . By the compact embedding  $W^{1,2}(\Omega) \hookrightarrow L^4(\Omega)$ , we have  $\int_\Omega (1 - |Q_\lambda^{\mu_n}|^2)^2 dx \rightarrow \int_\Omega (1 - |Q_\lambda|^2)^2 dx$ , and it follows from (4.9) that

$$\int_\Omega (1 - |Q_\lambda|^2)^2 dx = \lim_{n \rightarrow \infty} \int_\Omega (1 - |Q_\lambda^{\mu_n}|^2)^2 dx \leq \lim_{n \rightarrow \infty} \frac{1}{\mu_n} \mathcal{F}_{\lambda, \mu_n}(Q_\lambda^{\mu_n}) = 0.$$

Hence  $|Q_\lambda| = 1$  a.e. in  $\Omega$ , so that  $Q_\lambda \in \mathcal{A}_{Q_b}(\Omega)$ .

Since any  $Q \in \mathcal{A}_{Q_b}(\Omega)$  is in fact admissible to test the minimality of  $Q_\lambda^{\mu_n}$ , we can proceed as in (4.9) and use the lower semicontinuity of  $\mathcal{E}_\lambda$  to infer that

$$\mathcal{E}_\lambda(Q_\lambda) \leq \liminf_{n \rightarrow \infty} \mathcal{E}_\lambda(Q_\lambda^{\mu_n}) \leq \liminf_{n \rightarrow \infty} \mathcal{F}_{\lambda, \mu_n}(Q_\lambda^{\mu_n}) \leq \mathcal{E}_\lambda(Q) \quad (4.10)$$

for every  $Q \in \mathcal{A}_{Q_b}(\Omega)$ . Hence  $Q_\lambda$  is a minimizer of  $\mathcal{E}_\lambda$  over  $\mathcal{A}_{Q_b}(\Omega)$ , and we deduce from Theorem 1.2 that  $Q_\lambda \in C^{1,\alpha}(\bar{\Omega})$ . In addition, using  $Q = Q_\lambda$  as competitor in (4.10) we obtain that  $\mathcal{F}_{\lambda, \mu_n}(Q_\lambda^{\mu_n}) \rightarrow \mathcal{E}_\lambda(Q_\lambda)$ . The conclusion now follows from Proposition 4.5.  $\square$

**4.3. Instability of the melting hedgehog.** In this subsection we discuss instability of the melting hedgehog  $H_\lambda^\mu$  given in (1.20) in the Lyuksyutov regime  $\mu \rightarrow \infty$ . The conclusion here is similar to the one in [29], where the low-temperature regime  $a^2 \rightarrow \infty$  is considered. However, instead of the careful spectral decomposition considered there, to analyse the linearized operator we will use different and somewhat simpler perturbation arguments. More precisely, the instability property of  $H_\lambda^\mu$  will essentially follow here from the corresponding one for the constant norm hedgehog  $\bar{H}$  seen as a degree-zero homogeneous harmonic map into  $\mathbb{S}^4$ .

First we recall that the constant norm hedgehog

$$\bar{H}(x) = \sqrt{\frac{3}{2}} \left( \frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} I \right)$$

satisfies  $\bar{H} \in W_{\text{loc}}^{1,2}(\mathbb{R}^3; \mathbb{R}P^2) \cap C^\infty(\mathbb{R}^3 \setminus \{0\}; \mathbb{R}P^2)$ . It is a critical point of  $\mathcal{E}_\lambda$  both for  $\lambda = 0$  (i.e., a weakly harmonic map into  $\mathbb{S}^4$ ), and a critical point for  $\lambda > 0$  since  $\nabla_{\text{tan}} W(\bar{H}) \equiv 0$ . In order to discuss its stability properties, we first set for any  $\Phi \in C_c^\infty(B_1; \mathcal{S}_0)$ ,

$$\mathcal{E}_\lambda''(\Phi; \bar{H}) := \left[ \frac{d^2}{dt^2} \mathcal{E}_\lambda \left( \frac{\bar{H} + t\Phi}{|\bar{H} + t\Phi|} \right) \right]_{t=0}.$$

The second variation formula for harmonic maps (see, e.g., [38, Chapter 1]) yields

$$\mathcal{E}_\lambda''(\Phi; \bar{H}) = \int_{B_1} |\nabla \Phi_T|^2 - |\nabla \bar{H}|^2 |\Phi_T|^2 + \lambda D_{\text{tan}}^2 W(\bar{H}) \Phi : \Phi dx, \quad (4.11)$$

where  $\Phi_T := \Phi - \bar{H}(\bar{H} : \Phi)$  is the tangential component of  $\Phi$  along  $\bar{H}$ , and

$$\begin{aligned} D_{\text{tan}}^2 W(\bar{H}) \Phi : \Phi &:= \left[ \frac{d^2}{dt^2} W \left( \frac{\bar{H} + t\Phi}{|\bar{H} + t\Phi|} \right) \right]_{t=0} = D^2 W(\bar{H}) \Phi_T : \Phi_T \\ &= \frac{1}{\sqrt{6}} \left( 2(\bar{H} : \Phi_T)^2 + |\Phi_T|^2 - \sqrt{6} \text{tr}(\bar{H} \Phi_T^2) \right) = \frac{1}{\sqrt{6}} \left( |\Phi_T|^2 - \sqrt{6} \text{tr}(\bar{H} \Phi_T^2) \right). \end{aligned} \quad (4.12)$$

Due to the  $O(3)$ -equivariance of  $\bar{H}$ , the second variation  $\mathcal{E}_0''(\Phi; \bar{H})$  takes a particularly simple form whenever  $\Phi$  is a radial vector field.

**Lemma 4.6.** *For any  $\bar{v} \in \mathbb{S}^4$  and any radial function  $\eta \in C_c^\infty(B_1 \setminus \{0\})$ , we have*

$$\mathcal{E}_0''(\eta\bar{v}; \bar{H}) = \frac{4}{5} \int_{B_1} |\nabla\eta|^2 - \frac{3}{|x|^2} |\eta|^2 dx. \quad (4.13)$$

*Proof.* Let  $\mathbf{i} = (1, 0, 0)^t$ ,  $\mathbf{j} = (0, 1, 0)^t$ ,  $\mathbf{k} = (0, 0, 1)^t$  be the canonical basis of  $\mathbb{R}^3$ . From these vectors, we construct a distinguished orthonormal basis of  $\mathcal{S}_0$  by setting

$$\begin{aligned} e_0 &= \sqrt{\frac{3}{2}} \left( \mathbf{k} \otimes \mathbf{k} - \frac{1}{3} I \right), & e_1 &= \frac{1}{\sqrt{2}} (\mathbf{i} \otimes \mathbf{k} + \mathbf{k} \otimes \mathbf{i}), & e_2 &= \frac{1}{\sqrt{2}} (\mathbf{j} \otimes \mathbf{k} + \mathbf{k} \otimes \mathbf{j}), \\ e_3 &= \frac{1}{\sqrt{2}} (\mathbf{i} \otimes \mathbf{i} - \mathbf{j} \otimes \mathbf{j}), & e_4 &= \frac{1}{\sqrt{2}} (\mathbf{i} \otimes \mathbf{j} + \mathbf{j} \otimes \mathbf{i}). \end{aligned}$$

In terms of the latitude  $\theta \in [0, \pi]$  and of the colatitude  $\phi \in [0, 2\pi)$  on  $\mathbb{S}^2$ , the components of  $\bar{H}$  with respect to this basis are easily seen to be

$$\begin{aligned} \bar{H} : e_0 &= \frac{3}{2} \left( \cos^2 \theta - \frac{1}{3} \right), & \bar{H} : e_1 &= \frac{\sqrt{3}}{2} \sin 2\theta \cos \phi, & \bar{H} : e_2 &= \frac{\sqrt{3}}{2} \sin 2\theta \sin \phi, \\ \bar{H} : e_3 &= \frac{\sqrt{3}}{2} \sin^2 \theta \cos 2\phi, & \bar{H} : e_4 &= \frac{\sqrt{3}}{2} \sin^2 \theta \sin 2\phi. \end{aligned}$$

Therefore a straightforward calculation gives

$$\int_{\mathbb{S}^2} (\bar{H} : e_i)(\bar{H} : e_j) d\text{vol}_{\mathbb{S}^2} = \frac{4\pi}{5} \delta_{ij} \quad (4.14)$$

for any  $i, j = 0, \dots, 4$ . As a consequence, if we write  $\bar{v} = \sum_i \bar{v}_i e_i$  with  $|\bar{v}|^2 = \sum_i \bar{v}_i^2 = 1$ , then  $\bar{h} := \bar{H} : \bar{v}$  satisfies

$$\int_{\mathbb{S}^2} \bar{h}^2 d\text{vol}_{\mathbb{S}^2} = \sum_{i,j=0}^4 \int_{\mathbb{S}^2} (\bar{H} : e_i)(\bar{H} : e_j) \bar{v}_i \bar{v}_j d\text{vol}_{\mathbb{S}^2} = \sum_{i,j=0}^4 \frac{4\pi}{5} \delta_{ij} \bar{v}_i \bar{v}_j = \frac{4\pi}{5}. \quad (4.15)$$

Next, we notice that  $\bar{H}$  is a degree-zero homogeneous harmonic map and  $|\nabla \bar{H}|^2 = |\nabla_{\tan} \bar{H}|^2 = \frac{6}{|x|^2}$ , hence

$$\Delta_{\mathbb{S}^2} \bar{h} = -|\nabla_{\tan} \bar{H}|^2 \bar{h} = -6\bar{h},$$

and in view of (4.15) we obtain

$$\int_{\mathbb{S}^2} \bar{h}^2 |\nabla_{\tan} \bar{H}|^2 d\text{vol}_{\mathbb{S}^2} = \int_{\mathbb{S}^2} |\nabla \bar{h}|^2 d\text{vol}_{\mathbb{S}^2} = 6 \int_{\mathbb{S}^2} \bar{h}^2 d\text{vol}_{\mathbb{S}^2} = \frac{6}{5} \cdot 4\pi. \quad (4.16)$$

Finally, evaluating  $\mathcal{E}_0''$  in (4.11) for  $\Phi = \eta\bar{v}$  and integrating by parts, since  $\eta$  is radial and (4.16) holds, we conclude that

$$\begin{aligned} \mathcal{E}_0''(\eta\bar{v}; \bar{H}) &= \int_{B_1} (1 - \bar{h}^2) |\nabla\eta|^2 + \frac{\eta^2}{|x|^2} \left( 2|\nabla\bar{h}|^2 - (1 - \bar{h}^2) |\nabla_{\tan} \bar{H}|^2 \right) dx \\ &= \left( \int_{\mathbb{S}^2} (1 - \bar{h}^2) d\text{vol}_{\mathbb{S}^2} \right) \int_0^1 (\eta')^2 r^2 dr + \left( \int_{\mathbb{S}^2} 2|\nabla\bar{h}|^2 - (1 - \bar{h}^2) |\nabla_{\tan} \bar{H}|^2 d\text{vol}_{\mathbb{S}^2} \right) \int_0^1 \eta^2 dr \\ &= \frac{4}{5} \cdot 4\pi \int_0^1 (\eta')^2 r^2 dr - \frac{12}{5} \cdot 4\pi \int_0^1 \eta^2 dr = \frac{4}{5} \int_{B_1} |\nabla\eta|^2 - \frac{3}{|x|^2} |\eta|^2 dx, \end{aligned}$$

and the proof is complete.  $\square$

The instability property of  $\bar{H}$  for the Dirichlet energy  $\mathcal{E}_0$  along some vector field can be derived from the general instability result for harmonic tangent maps from  $\mathbb{R}^3$  in to  $\mathbb{S}^4$  proved in [57] and [37]. Here, exploiting the  $O(3)$ -equivariance of  $\bar{H}$  and using Lemma 4.6, we obtain a stronger and more explicit instability result for  $\bar{H}$  as a common critical point of all the functionals  $\mathcal{E}_\lambda$ .

**Proposition 4.7.** *Let  $\bar{H}$  be the constant norm hedgehog. There exists a radial function  $\xi \in C_c^\infty(B_1 \setminus \{0\})$  such that for any vector  $\bar{v} \in \mathbb{S}^4$ ,  $\bar{H}$  is a critical point of  $\mathcal{E}_0$  which is unstable along the vector field  $\Phi := \xi\bar{v}$ , i.e.,  $\mathcal{E}_0''(\Phi; \bar{H}) < 0$ .*

*As a consequence, for each  $\lambda > 0$  there exists a radial function  $\xi_\lambda \in C_c^\infty(B_1 \setminus \{0\})$  such that for any vector  $\bar{v} \in \mathbb{S}^4$ ,  $\bar{H}$  is a critical point of  $\mathcal{E}_\lambda$  which is unstable along the vector field  $\Phi_\lambda := \xi_\lambda \bar{v}$ , i.e.,  $\mathcal{E}_\lambda''(\Phi_\lambda; \bar{H}) < 0$ .*

*Proof.* As already proved in Lemma 4.6 above, we have

$$\mathcal{E}_0''(\eta\bar{v}; \bar{H}) = \frac{4}{5} \int_{B_1} |\nabla\eta|^2 - \frac{3}{|x|^2} |\eta|^2 dx$$

for any radial function  $\eta \in C_c^\infty(B_1 \setminus \{0\})$ . In view of the standard Hardy inequality in  $\mathbb{R}^3$ , the quadratic form is not bounded from below and there exists a radial function  $\eta \in C_0^\infty(B_1 \setminus \{0\})$  such that  $\mathcal{E}_0''(\eta\bar{v}; \bar{H}) < 0$ . Indeed, setting  $\eta_n(x) := [\min\{n|x|, |x|^{-1/2}\} - 2]_+$ , we have a sequence of radial functions  $\eta_n \in \text{Lip}(B_1)$  compactly supported in  $B_1 \setminus \{0\}$  satisfying

$$\int_{B_1} |\nabla\eta_n|^2 dx = \frac{1}{4} \int_{\frac{1}{n^{2/3}} < |x| < \frac{1}{4}} \frac{dx}{|x|^3} + \mathcal{O}(1) = \frac{1}{4} \int_{B_1} \frac{\eta_n^2}{|x|^2} dx + \mathcal{O}(1) \quad \text{as } n \rightarrow \infty,$$

whence  $\mathcal{E}_0''(\eta_n\bar{v}; \bar{H}) \rightarrow -\infty$  as  $n \rightarrow \infty$ . In particular,  $\mathcal{E}_0''(\eta_n\bar{v}; \bar{H}) < 0$  for  $n$  large enough. Finally, as  $\eta_n \equiv 0$  for  $|x| < 1/n$  and  $|x| > 1/4$ , taking  $\xi = \eta_n * \rho_\varepsilon$  a regularization by convolution with  $\varepsilon < 1/n$  and  $\{\rho_\varepsilon\}$  a family of radial mollifiers, we have a (family of) radial function  $\xi \in C_c^\infty(B_1 \setminus \{0\})$  satisfying  $\mathcal{E}_0''(\xi\bar{v}; \bar{H}) < 0$  for  $\varepsilon > 0$  small enough, which proves the first claim of the theorem.

In order to discuss the case  $\lambda > 0$ , we rescale the radial function  $\xi$  above setting  $\xi_\delta(x) := \xi(x/\delta)$  for  $0 < \delta < 1$  to be chosen later. Computing the second variation of  $\mathcal{E}_\lambda$  along the vector field  $\Phi^\delta := \xi_\delta\bar{v} \in C_c^\infty(B_1; \mathcal{S}_0)$ , equation (4.11) with  $\Phi_T^\delta = \Phi^\delta - \bar{H}(\bar{H} : \Phi^\delta)$  (the tangential component of  $\Phi^\delta$  along  $\bar{H}$ ) yields

$$\mathcal{E}_\lambda''(\Phi^\delta; \bar{H}) = \mathcal{E}_0''(\Phi^\delta; \bar{H}) + \lambda \int_{B_1} D_{\text{tan}}^2 W(\bar{H}) \Phi^\delta : \Phi^\delta dx.$$

As  $\bar{H}$  is degree-zero homogeneous, a simple rescaling gives

$$\begin{aligned} \mathcal{E}_\lambda''(\Phi^\delta; \bar{H}) &= \int_{B_1} |\nabla\Phi_T^\delta|^2 - |\nabla\bar{H}|^2 |\Phi_T^\delta|^2 + D^2 W(\bar{H}) \Phi_T^\delta : \Phi_T^\delta dx \\ &= \delta \left( \mathcal{E}_0''(\Phi; \bar{H}) + \lambda \delta^2 \int_{B_1} D^2 W(\bar{H}) \Phi_T : \Phi_T dx \right). \end{aligned}$$

Since by construction  $\mathcal{E}_0''(\Phi; \bar{H}) < 0$ , the conclusion follows for  $\delta > 0$  small enough.  $\square$

Finally we consider the radial hedgehog  $H_\lambda^\mu$  as the uniaxial critical point of the functional  $\mathcal{F}_{\lambda,\mu}$  of the form (1.20) discussed in the introduction. Recall that such critical point is the unique minimizer of  $\mathcal{F}_{\lambda,\mu}$  in the class of  $O(3)$ -equivariant maps in  $W^{1,2}(B_1; \mathcal{S}_0)$  which agree with  $\bar{H}$  on the boundary (see [30, Theorem 1.4]). Moreover, arguing as in the proof of Theorem 1.3 above, it is not difficult to show that  $H_\lambda^\mu \rightarrow \bar{H}$  strongly in  $W^{1,2}$  as  $\mu \rightarrow \infty$  (convergence of minimizers in the class of  $O(3)$ -equivariant maps). In addition, the convergence is locally uniform away from the origin because  $|H_\lambda^\mu| = \sqrt{2/3} s_\lambda^\mu \rightarrow 1$  locally uniformly away from the origin as  $\mu \rightarrow \infty$ .

Exploiting the aforementioned convergence of  $H_\lambda^\mu$  to its constant norm counterpart, we are going to infer the instability property of  $H_\lambda^\mu$  from the corresponding one for  $\bar{H}$  passing to the limit in the second variations of the energies  $\mathcal{F}_{\lambda,\mu}$ , and using Proposition 4.7. With this respect, we first set for any  $\Psi \in C_c^\infty(B_1; \mathcal{S}_0)$ ,

$$\mathcal{F}'_{\lambda,\mu}(\Psi; H_\lambda^\mu) := \left[ \frac{d}{dt} \mathcal{F}_{\lambda,\mu}(H_\lambda^\mu + t\Psi) \right]_{t=0}, \quad \mathcal{F}''_{\lambda,\mu}(\Psi; H_\lambda^\mu) := \left[ \frac{d^2}{dt^2} \mathcal{F}_{\lambda,\mu}(H_\lambda^\mu + t\Psi) \right]_{t=0}.$$

Simple calculations based on (1.10) now yield

$$\mathcal{F}'_{\lambda,\mu}(\Psi; H_\lambda^\mu) = \int_{B_1} \nabla H_\lambda^\mu : \nabla\Psi + \lambda \nabla W(H_\lambda^\mu) : \Psi + \mu (|H_\lambda^\mu|^2 - 1) H_\lambda^\mu : \Psi dx, \quad (4.17)$$

and

$$\mathcal{F}''_{\lambda,\mu}(\Psi; H_\lambda^\mu) = \int_{B_1} |\nabla\Psi|^2 + \lambda D^2 W(H_\lambda^\mu) \Psi : \Psi + \mu (2(H_\lambda^\mu : \Psi)^2 + (|H_\lambda^\mu|^2 - 1)|\Psi|^2) dx. \quad (4.18)$$

We have the following instability result for the radial hedgehog in the Lyuksyutov regime.

**Theorem 4.8.** *Let  $\lambda > 0$  be fixed and for each  $\mu > 0$ , let  $H^\mu := H_\lambda^\mu$  be the radial hedgehog. There exists a radial function  $\xi \in C_c^\infty(B_1 \setminus \{0\})$  such that the following holds. Given a vector  $\bar{v} \in \mathbb{S}^4$ , if  $\Phi_T$  denotes the tangential part along  $\bar{H}$  of the vector field  $\Phi = \xi\bar{v} \in C_c^\infty(B_1 \setminus \{0\}; \mathcal{S}_0)$ , then  $\Phi_T \in C_c^\infty(B_1 \setminus \{0\}; \mathcal{S}_0)$  and  $\mathcal{F}''_{\lambda,\mu}(\Phi_T; H_\lambda^\mu) < 0$  for all  $\mu$  large enough. As a consequence, the radial hedgehog  $H_\lambda^\mu$  is an unstable critical point of  $\mathcal{F}_{\lambda,\mu}$  for all  $\mu$  sufficiently large.*

*Proof.* Given  $\lambda > 0$  and  $\bar{v} \in \mathbb{S}^4$ , we fix the radial function  $\xi \in C_c^\infty(B_1 \setminus \{0\})$  as constructed in Proposition 4.7 (which depends on  $\lambda$ , but not on  $\bar{v}$ ). Then we introduce the vector fields  $\Phi := \xi \bar{v}$  and  $\Phi_T := \Phi - \bar{H}(\bar{H} : \Phi)$ . Since  $\Phi_T \in C_c^\infty(B_1 \setminus \{0\}; \mathcal{S}_0)$ , it is admissible for the second variation formula (4.18).

Since by construction  $H_\lambda^\mu : \Phi_T \equiv 0$ , we obtain

$$\mathcal{F}_{\lambda,\mu}''(\Phi_T; H_\lambda^\mu) = \int_{B_1} |\nabla \Phi_T|^2 + \lambda D^2 W(H_\lambda^\mu) \Phi_T : \Phi_T + \mu(|H_\lambda^\mu|^2 - 1)|\Phi_T|^2 dx. \quad (4.19)$$

Recall that  $H_\lambda^\mu \rightarrow \bar{H}$  strongly in  $W^{1,2}(B_1; \mathcal{S}_0)$  and locally uniformly away from the origin as  $\mu \rightarrow \infty$ . As a consequence, the dominated convergence theorem yields

$$\lim_{\mu \rightarrow \infty} \int_{B_1} |\nabla \Phi_T|^2 + \lambda D^2 W(H_\lambda^\mu) \Phi_T : \Phi_T dx = \int_{B_1} |\nabla \Phi_T|^2 + \lambda D^2 W(\bar{H}) \Phi_T : \Phi_T dx. \quad (4.20)$$

On the other hand, since  $H_\lambda^\mu$  is a critical point of  $\mathcal{F}_{\lambda,\mu}$ , computing (4.17) with the vector field  $\Psi := \frac{|\Phi_T|^2}{|H_\lambda^\mu|^2} H_\lambda^\mu \in C_c^\infty(B_1 \setminus \{0\}; \mathcal{S}_0)$  yields

$$0 = \mathcal{F}'_{\lambda,\mu}(\Psi; H_\lambda^\mu) = \int_{B_1} \nabla H_\lambda^\mu : \nabla \left( \frac{|\Phi_T|^2}{|H_\lambda^\mu|^2} H_\lambda^\mu \right) + \lambda \frac{|\Phi_T|^2}{|H_\lambda^\mu|^2} \nabla W(H_\lambda^\mu) : H_\lambda^\mu + \mu(|H_\lambda^\mu|^2 - 1)|\Phi_T|^2 dx,$$

whence

$$\begin{aligned} \int_{B_1} \mu(|H_\lambda^\mu|^2 - 1)|\Phi_T|^2 dx &= - \int_{B_1} |\nabla H_\lambda^\mu|^2 \frac{|\Phi_T|^2}{|H_\lambda^\mu|^2} dx \\ &\quad - \int_{B_1} \nabla H_\lambda^\mu : H_\lambda^\mu \nabla \frac{|\Phi_T|^2}{|H_\lambda^\mu|^2} + \lambda \frac{|\Phi_T|^2}{|H_\lambda^\mu|^2} \nabla W(H_\lambda^\mu) : H_\lambda^\mu dx. \end{aligned}$$

Since  $\nabla \bar{H} : \bar{H} \equiv 0$ ,  $\nabla W(\bar{H}) : \bar{H} = (1 - \tilde{\beta}(\bar{H}))/\sqrt{6} \equiv 0$ ,  $H_\lambda^\mu \rightarrow \bar{H}$  strongly in  $W^{1,2}(B_1; \mathcal{S}_0)$  and uniformly on the support of  $\xi$ , letting  $\mu \rightarrow \infty$  in the previous formula leads to

$$\lim_{\mu \rightarrow \infty} \int_{B_1} \mu(|H_\lambda^\mu|^2 - 1)|\Phi_T|^2 dx = - \int_{B_1} |\nabla \bar{H}|^2 |\Phi_T|^2 dx. \quad (4.21)$$

Combining (4.19) with (4.20)-(4.21) and taking into account (4.11) and (4.12), we infer that

$$\lim_{\mu \rightarrow \infty} \mathcal{F}_{\lambda,\mu}''(\Phi_T; H_\lambda^\mu) = \mathcal{E}_\lambda''(\Phi; \bar{H}),$$

and the conclusion follows, since the right hand side is negative by construction of  $\xi$  and  $\Phi$ .  $\square$

**Remark 4.9.** As  $H_\lambda^\mu$  is  $O(3)$ -equivariant, it is also  $\mathbb{S}^1$ -equivariant in the sense of condition (1.24). Hence, if we choose  $\bar{v} \in \mathbb{S}^4$  such that  $R^t \bar{v} R = \bar{v}$  for any  $R \in \mathbb{S}^1$ , then each map  $H_\lambda^\mu + t \xi \bar{v}$  is  $\mathbb{S}^1$ -equivariant for any  $t \in \mathbb{R}$ . As a consequence, according to Theorem 4.8 the radial hedgehog is an unstable critical point of  $\mathcal{F}_{\lambda,\mu}$  also in the restricted class of  $\mathbb{S}^1$ -equivariant maps (a similar conclusion is valid for  $\bar{H}$  as critical point of  $\mathcal{E}_\lambda$  in view of Proposition 4.7).

In the next remark we discuss the role of the biaxial phase in the instability results.

**Remark 4.10.** Let  $\Phi \in C_0^\infty(B_1; \mathcal{S}_0)$  be fixed and  $\Phi_T$  its tangential part along  $\bar{H}$ . Simple calculations using (1.4), (1.15), (4.12), and Lemma 2.22, give

$$\left. \frac{d^2}{dt^2} \tilde{\beta} \left( \frac{\bar{H} + t\Phi}{|\bar{H} + t\Phi|} \right) \right|_{t=0} = -3\sqrt{6} \left. \frac{d^2}{dt^2} W \left( \frac{\bar{H} + t\Phi}{|\bar{H} + t\Phi|} \right) \right|_{t=0} = -3 \left( |\Phi_T|^2 - \sqrt{6} \operatorname{tr}(\bar{H} \Phi_T^2) \right) \leq -\frac{3}{2} |\Phi_T|^2,$$

and in turn

$$\left. \frac{d^2}{dt^2} \tilde{\beta} (H_\lambda^\mu + t\Phi) \right|_{t=0} = \left. \frac{d^2}{dt^2} \tilde{\beta} \left( \frac{\bar{H} + t \frac{\Phi}{|H_\lambda^\mu|}}{|\bar{H} + t \frac{\Phi}{|H_\lambda^\mu|}|} \right) \right|_{t=0} \leq -\frac{3}{2} \frac{|\Phi_T|^2}{|H_\lambda^\mu|^2}.$$

Expanding around the value  $t = 0$  and using stationarity of  $\bar{H}$  and  $H_\lambda^\mu$  both for  $\tilde{\beta}$  and for the energy functionals, as  $t \rightarrow 0$  we infer

$$\tilde{\beta} \left( \frac{\bar{H} + t\Phi}{|\bar{H} + t\Phi|} \right) \leq 1 - \frac{3}{4} |\Phi_T|^2 t^2 + o(t^2), \quad \mathcal{E}_\lambda \left( \frac{\bar{H} + t\Phi}{|\bar{H} + t\Phi|} \right) = \mathcal{E}_\lambda(\bar{H}) + \mathcal{E}_\lambda''(\Phi; \bar{H}) \frac{t^2}{2} + o(t^2), \quad (4.22)$$

together with

$$\tilde{\beta} (H_\lambda^\mu + t\Phi) \leq 1 - \frac{3}{4} \frac{|\Phi_T|^2}{|H_\lambda^\mu|^2} t^2 + o(t^2), \quad \mathcal{F}_{\lambda,\mu} (H_\lambda^\mu + t\Phi) = \mathcal{F}_{\lambda,\mu} (H_\lambda^\mu) + \mathcal{F}_{\lambda,\mu}''(\Phi_T; H_\lambda^\mu) \frac{t^2}{2} + o(t^2). \quad (4.23)$$

As a consequence of (4.22) and (4.23), we see that for  $t$  sufficiently small *biaxial escape* occurs for the perturbed maps in the set where  $\Phi_T \neq 0$ . Moreover, if  $\Phi = \xi\bar{v}$  with  $\bar{v} \in \mathbb{S}^4$  and  $\mu$  is large enough, then Proposition 4.7 and Theorem 4.8 show that this escape is energetically more favourable because the second variations of the energy functionals in (4.22) and (4.23) are negative.

As a final remark in this section, we further comment on the actual range of validity of our results in the Lyuksyutov regime (1.18).

**Remark 4.11.** When studying asymptotic limits from a physical perspective, it is important that all quantities to be compared have the same physical dimensions. Experts often rescale the energy in such a way to recast it in a new fully adimensional form (see, e.g., [18]). Our energy (1.10) is only partially non-dimensionalized, because the terms under integral sign are not pure numbers but they all have the same physical dimension. In fact, the parameters  $\lambda$  and  $\mu$  in the energy density of  $\mathcal{F}_{\lambda,\mu}$  have the dimension of the inverse of a length squared ( $Q$ -tensors are adimensional by definition), so the resulting value of the energy  $\mathcal{F}_{\lambda,\mu}$  has the physical dimension of a length; in addition, the ratio  $\mu/\lambda$  is adimensional and we are allowed to compare them in a physically meaningful way, considering in particular the case  $\mu \gg \lambda$ . Thus, in the Lyuksyutov regime (1.18) we are requiring that on a fixed domain  $\Omega$  the parameter  $\lambda$  is constant, hence of the same order of  $(\text{diam } \Omega)^{-2}$ , whereas  $\mu$  is much larger.

On the other hand, we could obtain a fully non-dimensionalized energy functional by first choosing a reference length and then rescaling the domain with respect to it. In the present situation there are at least three natural choices of length, namely,  $\frac{1}{\sqrt{\lambda}}$ ,  $\frac{1}{\sqrt{\mu}}$ , and  $\text{diam } \Omega$ , where the first two choices, up to an harmless numerical factor, correspond to the *biaxial coherence length* and the *nematic-isotropic correlation length* respectively, see [49, 32, 18]. Calling  $\ell$  the chosen reference length, the original energy functional  $\tilde{\mathcal{F}}_{LG}(\mathbf{Q}, \Omega)$  under the further rescaling  $\mathbf{x} = \ell x$  turns into the non-dimensionalized functional  $\mathcal{F}_{\tilde{\lambda}, \tilde{\mu}}(Q, \Omega)$  as in (1.10), where  $\Omega = \ell\Omega$  and the new parameters are given by  $\tilde{\lambda} = \ell^2\lambda$ ,  $\tilde{\mu} = \ell^2\mu$ , with  $\lambda$  and  $\mu$  as in (1.18). Thus, the adimensional energy  $\mathcal{F}_{\tilde{\lambda}, \tilde{\mu}}$  is formally identical to  $\mathcal{F}_{\lambda,\mu}$ , and our results continue to hold without any change in the regime  $\tilde{\lambda} \sim 1$  and  $\tilde{\mu} \gg 1$  on a fixed reference domain  $\Omega$ . It turns out that the second choice,  $\ell = 1/\sqrt{\mu}$ , amounts to  $\mu \sim \lambda$  and  $\tilde{\mu} = 1$ , so it is not covered by our results. However, the first and the third choices both correspond to  $\text{diam } \Omega \sim 1/\sqrt{\lambda}$  and  $\tilde{\mu} \sim \mu/\lambda \gg 1$ , i.e., to the following generalization of (1.18) to domains of unconstrained size, namely

$$\text{diam } \Omega \sim \frac{1}{\sqrt{\lambda}} = \sqrt{\frac{L}{b^2 s_+}}, \quad \frac{1}{\sqrt{\lambda}} \cdot \left(\frac{1}{\sqrt{\mu}}\right)^{-1} = \sqrt{\frac{a^2}{b^2 s_+}} \gg 1. \quad (4.24)$$

As a consequence, we see that the diameter  $\text{diam } \Omega$  must be comparable to the the biaxial coherence length, while the nematic correlation length must be negligible with respect to them. Finally, notice that the second condition in (4.24) holds in particular in the *low temperature* limit  $a^2 \rightarrow \infty$  but in domains  $\Omega$  of smaller and smaller size because of (1.6), or, alternatively, in the limit  $b \rightarrow 0$  but on domains  $\Omega$  with suitably expanding diameter. For a more detailed discussion of this non-dimensionalization procedure and related issues, the interested reader is referred to [18] and the references therein.

## 5. TOPOLOGY OF MINIMIZERS

In this section, we discuss topological properties of field configurations  $Q$  satisfying assumptions  $(HP_0) - (HP_3)$ , and restricting to energy minimizing configurations, we will obtain in particular the proof of Theorem 1.6.

In connection with assumption  $(HP_2)$ , we start recalling the following auxiliary result which characterizes simple connectivity of any smooth bounded domain  $\Omega \subseteq \mathbb{R}^3$ .

**Lemma 5.1.** [4, Thm.3.2 and Corollary 3.5] *Let  $\Omega \subseteq \mathbb{R}^3$  be a bounded connected open set with boundary of class  $C^1$ . Then  $\Omega$  is simply connected if and only if its boundary can be written as  $\partial\Omega = \cup_{i=1}^N S_i$  and each surface  $S_i$  is diffeomorphic to the standard sphere  $\mathbb{S}^2 \subseteq \mathbb{R}^3$ .*

As already mentioned in the Introduction, by assumption  $(HP_1)$  the maximal eigenvalue  $\lambda_{\max}(x)$  of the matrix  $Q(x)$  is simple for every  $x \in \partial\Omega$ , and there is a well defined smooth eigenspace map  $V_{\max}: \partial\Omega \rightarrow \mathbb{R}P^2$ . In addition, as  $\Omega$  is simply connected and in view of Lemma 5.1, there exists a smooth lifting  $v_{\max} \in C^1(\partial\Omega; \mathbb{S}^2)$  such that, under the inclusion  $\mathbb{R}P^2 \subseteq \mathbb{S}^4$ , we have  $V_{\max}(x) = \sqrt{3/2}(v_{\max}(x) \otimes v_{\max}(x) - \frac{1}{3}I)$  for all  $x \in \partial\Omega$ .

Notice that as in (1.21), the case  $\bar{\beta} = 1$  in (HP1) corresponds to  $Q/|Q|: \partial\Omega \rightarrow \mathbb{R}P^2 \subseteq \mathbb{S}^4$ . In this case we have  $\lambda_{\max} \equiv \sqrt{\frac{2}{3}}|Q|$  on  $\partial\Omega$ . Still in view of (HP2) there exists a map  $v' \in C^1(\partial\Omega; \mathbb{S}^2)$  such that  $Q = |Q|\sqrt{3/2}(v' \otimes v' - \frac{1}{3}I)$  on  $\partial\Omega$  (under the inclusion  $\mathbb{R}P^2 \subseteq \mathbb{S}^4$ ). Hence, under the assumption  $\bar{\beta} = 1$ , one has  $Q \equiv |Q|V_{\max}$  on  $\partial\Omega$ .

Recall also that assumption (HP3) on the lifting  $v_{\max}$  of the map  $V_{\max}: \partial\Omega \rightarrow \mathbb{R}P^2$ , namely that the total degree  $\deg(v_{\max}, \partial\Omega) = \sum_{i=1}^N \deg(v_{\max}, S_i)$  is odd, does not depend on the chosen lifting. Indeed, since on each spherical component  $S_i$  of  $\partial\Omega$  the lifting exists by simple connectivity of  $S_i$ , and it is unique up a sign, each  $\deg(v_{\max}, S_i)$  may only change by a sign when passing to a different lifting.

Now we discuss properties of the biaxiality regions defined in (1.23). The first result below shows that the biaxial escape observed in the introduction is indeed topological in nature, and that every possible value of the biaxiality is attained.

**Lemma 5.2.** *Let  $\Omega \subseteq \mathbb{R}^3$  be a bounded open set with boundary of class  $C^1$ , and  $Q: \bar{\Omega} \rightarrow \mathcal{S}_0$ . If  $\Omega$  and  $Q$  satisfy (HP0) – (HP3), then the subset  $\{\beta = -1\} \subseteq \bar{\Omega}$  is not empty. As a consequence,  $\{\beta = t\} \subseteq \bar{\Omega}$  is not empty for every  $t \in [-1, \beta_0]$ , where  $\beta_0 := \max_{\partial\Omega} \beta$ . In particular, if  $\bar{\beta} = 1$ , then the range of  $\beta$  is  $[-1, 1]$ .*

*Proof.* The consequence follows trivially from the definition of  $\beta_0$ , as the set  $\Omega$  (hence  $\bar{\Omega}$ ) is connected, and furthermore  $\beta_0 = 1$  whenever  $\bar{\beta} = 1$ .

To prove the first statement, we argue by contradiction assuming that  $\min_{\bar{\Omega}} \beta > -1$ . Then the maximal eigenvalue  $\lambda_{\max}(x)$  of  $Q(x)$  is always simple for every  $x \in \bar{\Omega}$ , hence of class  $C^1$ , and there is a well defined eigenspace map  $\tilde{V} \in C^1(\bar{\Omega}; \mathbb{R}P^2)$  which extends  $V_{\max}$  from the boundary of  $\Omega$  to its interior. Since  $\bar{\Omega}$  is simply connected this map can be lifted to  $\tilde{v} \in C^1(\bar{\Omega}; \mathbb{S}^2)$  which has to satisfy  $\deg(\tilde{v}, \partial\Omega) = 0$  by Stokes's theorem. On the other hand, as both  $v_{\max}$  and  $\tilde{v}$  are liftings of the same map  $V_{\max}$  at the boundary, we have  $v_{\max} = \pm\tilde{v}$  on each  $S_i$ , whence  $\deg(v_{\max}, S_i) = \pm \deg(\tilde{v}, S_i)$  for all  $i = 1, \dots, N$ . Summing up over  $i$  and passing to *mod* 2, we have

$$\deg(v_{\max}, \partial\Omega) = \sum_{i=1}^N \deg(v_{\max}, S_i) = \sum_{i=1}^N \deg(\tilde{v}, S_i) = 0 \pmod{2},$$

which contradicts (HP3).  $\square$

We now further investigate properties of the biaxiality regions  $\{\beta \leq t\}$ ,  $\{\beta \geq t\}$ . The following lemma and its corollary below represents the key points where the analyticity assumption is used.

**Lemma 5.3.** *Let  $\Omega \subseteq \mathbb{R}^3$  be a bounded open set with boundary of class  $C^1$ , and  $Q: \bar{\Omega} \rightarrow \mathcal{S}_0$ . If  $\Omega$  and  $Q$  satisfy (HP0) – (HP3), then the set of singular (critical) value of  $\beta = \tilde{\beta} \circ Q$  in  $(-1, \bar{\beta})$  is at most countable and can accumulate only at  $\bar{\beta}$ . As a consequence,*

- 1) *for any  $t \in (-1, \bar{\beta})$  there exists a regular value  $t' \in (-1, t)$  such that  $\{\beta \geq t\} \subseteq \bar{\Omega}$  is a deformation retract of  $\{\beta \geq t'\}$ ;*
- 2) *for any  $t \in [-1, \bar{\beta})$  there exists a regular value  $t' \in (t, \bar{\beta})$  such that  $\{\beta \leq t\} \subseteq \Omega$  is a deformation retract of  $\{\beta \leq t'\}$ .*

*Proof.* Since  $\beta = \tilde{\beta} \circ Q \in C^\omega(\Omega)$ , by Sard's theorem for analytic functions (see [59]) the set of singular value is finite on each compact set  $K \subseteq \Omega$ , hence all but countably many  $t \in (-1, \bar{\beta})$  are regular for  $\beta$  in  $\Omega$ . For such  $t$ , the level set  $\{\beta = t\}$  is contained in  $\Omega$  by definition of  $\bar{\beta}$  and it is a finite union of analytic, connected, orientable and boundaryless surfaces. However, since the singular values are finite on compact sets and in view of the definition of  $\bar{\beta}$ , the only accumulation point for the singular values can be  $\bar{\beta}$ . Indeed, otherwise there would be a countably many distinct singular value  $\beta_n \rightarrow \beta_* \in [-1, \bar{\beta})$  and corresponding distinct critical points  $x_n \in \{\beta = \beta_n\} \subseteq \Omega$  such that up to subsequences  $x_n \rightarrow x_* \in \{\beta = \beta_*\}$ . Notice that  $x_* \in \partial\Omega$ , otherwise  $x_*$  would be a critical point as well and  $\beta_*$  would be a singular value, with countably many singular values attained in a neighborhood of  $x_*$ , which contradicts Sard's Theorem. Thus  $x_* \in \{\beta = \beta_*\} \cap \partial\Omega$ , which is however impossible by definition of  $\bar{\beta}$ . To conclude the proof, we observe that the set of regular value is open. Then, given a regular value  $t$ , choosing  $t'$  sufficiently close to  $t$ , the conclusion 1) (resp. 2)) follows by a standard retraction following the gradient (resp. negative gradient) flow associated to  $\beta$  in  $\Omega$  in a neighborhood of  $\{\beta = t\} \subseteq \Omega$ . Actually the same argument applies for any singular value  $t$ , such value being isolated by the discussion above, and the conclusion follows from real analyticity and the retraction theorem of Łojasiewicz (see [39, Theorem 5]).  $\square$

**Corollary 5.4.** *Let  $\Omega \subseteq \mathbb{R}^3$  be a bounded open set with boundary of class  $C^1$ , and  $Q : \bar{\Omega} \rightarrow \mathcal{S}_0$ . If  $\Omega$  and  $Q$  satisfy  $(HP_0) - (HP_3)$  with  $\bar{\beta} = 1$  and  $Q \in C^\omega(\bar{\Omega}; \mathcal{S}_0)$ , then the set of singular (critical) value of  $\beta$  in  $(-1, 1)$  is finite, and there exists a regular value  $t' \in (-1, 1)$  such that  $\{\beta = 1\} \subseteq \bar{\Omega}$  is a deformation retract of  $\{\beta \geq t'\} \subseteq \bar{\Omega}$ .*

*Proof.* The proof is similar to the one of Lemma 5.3, so it will be just sketched. In view of the analytic regularity up to the boundary, the tensor  $Q$  has an analytic extension  $\widehat{Q}$  (simply by power series) to a larger open set  $\widehat{\Omega} \supseteq \bar{\Omega}$ . Then the function  $\widehat{\beta} := \bar{\beta} \circ \widehat{Q}$  is analytic in  $\widehat{\Omega}$  with finitely many critical values in  $\bar{\Omega}$  again by Sard's theorem. Clearly 1 is a critical value (maximum) of  $\widehat{\beta}$ . Hence, choosing a slightly smaller regular value  $t'$ , the conclusion still follows from [39] retracting the set  $\{\beta \geq t'\} \subseteq \bar{\Omega}$  onto  $\{\beta = 1\}$  by the gradient flow of  $\widehat{\beta}$  in  $\Omega$ .  $\square$

The first information on the topology of the biaxiality regions is contained in the following result.

**Proposition 5.5.** *Let  $\Omega \subseteq \mathbb{R}^3$  be a bounded open set with boundary of class  $C^1$ , and  $Q : \bar{\Omega} \rightarrow \mathcal{S}_0$ . If  $\Omega$  and  $Q$  satisfy  $(HP_0) - (HP_3)$ , then the biaxiality regions satisfy*

- 1)  $\{\beta \geq t\}$  is not simply connected for any  $t \in (-1, \bar{\beta})$ ;
- 2)  $\{\beta \leq t\}$  is not simply connected for any  $t \in (-1, \bar{\beta})$ ;
- 3) the negative uniaxial set  $\{\beta = -1\}$  is not simply connected;
- 4)  $\{\beta = t\}$  contains a surface of positive genus for any regular value  $t \in (-1, \bar{\beta})$  of the function  $\beta$ ;
- 5) if in addition  $\bar{\beta} = 1$  and  $Q \in C^\omega(\bar{\Omega}; \mathcal{S}_0)$ , then the set  $\{\beta = 1\} \subseteq \bar{\Omega}$  is not simply connected.

*Proof.* In view of Lemma 5.3 it is enough to prove claim 1) and 2) for a regular value  $t \in (-1, \bar{\beta})$  since (non)simple connectivity passes to deformation retracts. A similar argument applies to claim 3). Indeed,  $t = -1$  is a singular value (minimum), and it is isolated by Lemma 5.3. Hence, combining claim 2) for regular values  $t'$  close to  $-1$ , the set  $\{\beta \leq t'\}$  is not simply connected, and thus its deformation retract  $\{\beta = -1\}$  is also nonsimply connected.

Let us now prove claims 1) and 4). We assume that  $t \in (-1, \bar{\beta})$  is a fixed regular value of  $\beta \in C^\omega(\Omega)$ . Then the set  $\{\beta \geq t\}$  is the closure of the open set  $\Omega \cap \{\beta > t\}$  which is bounded with smooth boundary. In addition,  $\{\beta \geq t\}$  and  $\Omega \cap \{\beta > t\}$  are homotopically equivalent (by inward-retracting both sets along the normal direction in a small neighborhood of the boundary). So it is enough to show that  $\widetilde{\Omega} := \Omega \cap \{\beta > t\}$  is not simply connected. Observe that in view of the regularity of  $t$  and the smoothness of the boundary, we can write  $\partial\widetilde{\Omega}$  as a disjoint union

$$\partial\widetilde{\Omega} = \partial\Omega \cup \{\beta = t\} = (\cup_{i=1}^N S_i) \cup (\cup_{j=1}^M \widetilde{S}_j),$$

where each  $S_i$  is diffeomorphic to  $\mathbb{S}^2$  and each  $\widetilde{S}_j$  is compact, analytic, connected, orientable and boundaryless surface because  $\{\beta = t\} \subseteq \Omega$ . Now we claim that there exists an index  $j_*$  such that the surface  $\widetilde{S}_{j_*}$  has positive genus. In other words, claim 4) holds and the open set  $\widetilde{\Omega}$  is not simply connected in view of Lemma 5.1, i.e., claim 1) also holds.

To prove the existence of the distinguished surface  $\widetilde{S}_{j_*}$ , we argue by contradiction assuming that the genus  $g(\widetilde{S}_j) = 0$  for each  $j = 1, \dots, M$ . Hence the Euler characteristic  $\chi(\widetilde{S}_j) = 2 - 2g(\widetilde{S}_j) = 2$  for each  $j = 1, \dots, M$ , and we shall derive a contradiction from this fact. Indeed, notice first that the maximal eigenvalue  $\lambda_{\max}(Q(x))$  is simple for every  $x \in \{\beta \geq t\} \subseteq \bar{\Omega}$ . Therefore, there is a well defined smooth eigenspace map  $\widetilde{V} : \{\beta \geq t\} \rightarrow \mathbb{R}P^2$ ,  $\widetilde{V}(x) = \text{Ker}(Q(x) - \lambda_{\max}(Q(x))I)$ . Since each  $\widetilde{S}_j$  are assumed to be of zero genus, both  $\widetilde{\Omega}$  and  $\{\beta \geq t\}$  are simply connected by Lemma 5.1. Therefore the map  $\widetilde{V} \in C^1(\{\beta \geq t\}; \mathbb{R}P^2)$  has a lifting  $\widetilde{v} \in C^1(\{\beta \geq t\}; \mathbb{S}^2)$  as in the proof of Lemma 5.2. From Stokes' theorem we infer that

$$\deg(\widetilde{v}, \partial\widetilde{\Omega}) = \sum_{i=1}^N \deg(\widetilde{v}, S_i) + \sum_{j=1}^M \deg(\widetilde{v}, \widetilde{S}_j) = 0.$$

Then assumption  $(HP_3)$  yields  $\sum_{j=1}^M \deg(\widetilde{v}, \widetilde{S}_j) \neq 0$ , so that there exists  $1 \leq j_* \leq M$  such that  $\deg(\widetilde{v}, \widetilde{S}_{j_*}) \neq 0$ .

Now consider  $F = T\mathbb{S}^2 \rightarrow \mathbb{S}^2$  the (real, oriented, rank-two) tangent bundle of  $\mathbb{S}^2$  with its Euler class  $e(F) \in H^2(\mathbb{S}^2; \mathbb{Z})$ . With respect to a normalized volume form on  $\mathbb{S}^2$ , we can write  $e(F) = 2d\text{vol}_{\mathbb{S}^2} \in H_{dR}^2(\mathbb{S}^2; \mathbb{R})$ , and its Euler number (i.e., Euler characteristic) is  $\chi(\mathbb{S}^2) = \int_{\mathbb{S}^2} e(F) = 2$ .

Using the map  $\tilde{v}$  we can consider the pull-back bundle  $\tilde{v}^*F \rightarrow \tilde{S}_{j_*}$  which is a smooth real oriented rank-two vector bundle over  $\tilde{S}_{j_*}$ . By functoriality of the Euler class (see e.g. [6]), we have

$$\int_{\tilde{S}_{j_*}} e(\tilde{v}^*F) = \int_{\tilde{S}_{j_*}} \tilde{v}^*e(F) = 2 \int_{\tilde{S}_{j_*}} \tilde{v}^*d\text{vol}_{\mathbb{S}^2} = 2 \deg(\tilde{v}, \tilde{S}_{j_*}) \neq 0,$$

hence the pull-back bundle  $\tilde{v}^*F \rightarrow \tilde{S}_{j_*}$  is nontrivial. On the other hand, since  $\tilde{S}_{j_*} \subseteq \{\beta = t\}$  and  $t \in (-1, 1)$  is a regular value, each eigenvalue  $\lambda \in \sigma(Q(x)) = \{\lambda_{\max}(x), \lambda_{\text{mid}}(x), \lambda_{\min}(x)\}$  is simple for every  $x \in \tilde{S}_{j_*}$ . Therefore there are well defined eigenspace maps  $\tilde{V}_{\text{mid}}, \tilde{V}_{\min} \in C^1(\tilde{S}_{j_*}; \mathbb{R}P^2)$  and corresponding liftings  $\tilde{v}_{\text{mid}}, \tilde{v}_{\min} \in C^1(\tilde{S}_{j_*}; \mathbb{S}^2)$  (since  $\tilde{S}_{j_*}$  simply connected, i.e.,  $g(\tilde{S}_{j_*}) = 0$ ). By the spectral theorem we have  $F_{\tilde{v}(x)} = T_{\tilde{v}(x)}\mathbb{S}^2 = \{\tilde{v}(x)\}^\perp = \mathbb{R}\tilde{v}_{\text{mid}}(x) \oplus \mathbb{R}\tilde{v}_{\min}(x)$  for every  $x \in \tilde{S}_{j_*}$ . Hence the bundle  $\tilde{v}^*F \rightarrow \tilde{S}_{j_*}$  is trivial and  $\tilde{v}_{\text{mid}}, \tilde{v}_{\min} \in C^1(\tilde{S}_{j_*}; F)$  provides a trivializing frame (up to orientation), a contradiction.

To prove claim 2) we fix a regular value  $t \in (-1, \bar{\beta})$ , and we recall that  $\partial\{\beta \leq t\} = \{\beta = t\} \subseteq \Omega$  is a finite union of surfaces of class  $C^1$  (in fact analytic) which are disjoint, embedded, connected and boundaryless. Notice that  $\partial\{\beta \geq t\} = \partial\Omega \cup \{\beta = t\}$  is also a finite union of  $C^1$ -surfaces which are disjoint, embedded, connected and boundaryless. Moreover, since  $\Omega$  is simply connected and  $\{\beta \geq t\}$  is not (because of claim 1)), one of the component of  $\{\beta = t\}$  has positive genus by Lemma 5.1. Applying again Lemma 5.1 to  $\{\beta < t\} \subseteq \Omega$ , we infer that  $\{\beta < t\}$  is not simply connected because the total genus of its boundary is positive. Hence  $\{\beta \leq t\}$  is also not simply connected since the two sets are homotopically equivalent.

Finally, the proof of claim 5) follows from claim 1) for regular values  $t \in (-1, 1)$  combined with the homotopic equivalence property stated in Corollary 5.4.  $\square$

As a direct consequence of the previous proposition, we have the linking property between biaxiality sets.

**Proposition 5.6.** *Let  $\Omega \subseteq \mathbb{R}^3$  be a bounded open set with boundary of class  $C^1$ , and  $Q : \bar{\Omega} \rightarrow \mathcal{S}_0$ . Assume that  $\Omega$  and  $Q$  satisfy (HP<sub>0</sub>) – (HP<sub>3</sub>). If  $[t_1, t_2] \subseteq [-1, \bar{\beta}]$  is such that  $(t_1, t_2)$  contains no singular value of  $\beta = \bar{\beta} \circ Q$ , then  $\{\beta \leq t_1\} \subseteq \Omega$  and  $\{\beta \geq t_2\} \subseteq \bar{\Omega}$  are nonempty compact and disjoint subset of  $\bar{\Omega}$ , and they are mutually linked.*

*Proof.* In view of Lemma 5.2 the sets  $\{\beta \leq t_1\} \subseteq \Omega$  and  $\{\beta \geq t_2\} \subseteq \bar{\Omega}$  are nonempty compact and disjoint subset of  $\bar{\Omega}$ . Since  $[t_1, t_2] \subseteq [-1, \bar{\beta}]$  we clearly have  $\{\beta \leq t_1\} \subseteq \bar{\Omega} \setminus \{\beta \geq t_2\} = \{\beta < t_2\}$  and  $\{\beta \geq t_2\} \subseteq \bar{\Omega} \setminus \{\beta \leq t_1\} = \{\beta > t_1\}$ . As  $(t_1, t_2)$  contains no singular value, these two sets are homotopically equivalent to  $\{\beta \leq t_1\}$  and  $\{\beta \geq t_2\}$ . Indeed, the gradient flow of  $\pm\beta$  gives a deformation retract of each larger set onto the corresponding smaller one (this is standard if  $t_1$  and  $t_2$  are regular values, and otherwise, it follows from [39, Theorem 5] as in Lemma 5.3 thanks to real analyticity). Thus  $\{\beta \leq t_1\}$  is contractible in  $\bar{\Omega} \setminus \{\beta \geq t_2\}$  if and only if it is contractible, and  $\{\beta \geq t_2\}$  is contractible in  $\bar{\Omega} \setminus \{\beta \leq t_1\}$  if and only if it is contractible. On the other hand, the sets  $\{\beta \leq t_1\}$  and  $\{\beta \geq t_2\}$  are not simply connected by Proposition 5.5. Hence both of them are not contractible and therefore mutually linked.  $\square$

In the final result of this section, which contains Theorem 1.6 as a particular case, we summarize the topological information obtained as a straightforward combination of Lemma 5.2, Lemma 5.3, Corollary 5.4, Proposition 5.5 and Proposition 5.6.

**Theorem 5.7.** *Let  $\Omega \subseteq \mathbb{R}^3$  be a bounded open set with boundary of class at least  $C^1$ , and  $Q : \bar{\Omega} \rightarrow \mathcal{S}_0$ . Assume that  $\Omega$  and  $Q$  satisfy (HP<sub>0</sub>) – (HP<sub>3</sub>) (e.g., suppose  $\partial\Omega$  has an odd number of connected components and that  $Q(x) = \sqrt{3/2}(\vec{n}(x) \otimes \vec{n}(x) - \frac{1}{3}I)$  on  $\partial\Omega$ , so that  $\bar{\beta} = 1$ ). Then the biaxiality sets satisfy:*

- 1) *the set of singular values of  $\beta$  in  $[-1, \bar{\beta}]$  is at most countable and can accumulate only at  $\bar{\beta}$ ; moreover, for any regular value  $-1 < t < \bar{\beta}$ , the set  $\{\beta = t\} \subseteq \Omega$  is a smooth surface with a connected component of positive genus;*
- 2) *for any  $-1 \leq t_1 < t_2 < \bar{\beta}$ , the sets  $\{\beta \leq t_1\} \subseteq \Omega$  and  $\{\beta \geq t_2\} \subseteq \bar{\Omega}$  are nonempty, compact, and not simply connected;*
- 3) *if in addition  $Q \in C^\omega(\bar{\Omega})$  and  $\bar{\beta} = 1$ , then  $\{\beta = 1\} \subseteq \bar{\Omega}$  is also nonempty, compact, and not simply connected; in particular  $\{\beta = 1\} \cap \Omega$  is not empty;*
- 4) *for any  $-1 \leq t_1 < t_2 < \bar{\beta}$  such that  $(t_1, t_2)$  contains no singular value, the sets  $\{\beta \leq t_1\}$  and  $\{\beta \geq t_2\}$  are mutually linked.*

## REFERENCES

- [1] F.J. ALMGREN, E.H. LIEB : Singularities of energy minimizing maps from the ball to the sphere: examples, counterexamples, and bounds, *Ann. of Math.* **128** (1988), 483–530.
- [2] J. BALL : *Liquid crystals and their defects*. Mathematical thermodynamics of complex fluids, 1–46, Lecture Notes in Math., **2200**, Fond. CIME/CIME Found. Subser., Springer, Cham, 2017.
- [3] J. BALL, A. ZARNESCU : *Orientability and energy minimization in liquid crystal models*. Arch. Ration. Mech. Anal. **202** (2011), 493–535.
- [4] R. BENEDETTI, R. FRIGERIO, R.GHILONI : *The topology of Helmholtz domains*. Expo. Math. **30** (2012), 319–375.
- [5] F. BETHUEL, H. BREZIS, F. HÉLEIN : *Asymptotics for the minimization of a Ginzburg-Landau functional*. Calc. Var. Partial Differential Equations **1** (1993), 123–148.
- [6] R. BOTT, L. TU : *Differential forms in algebraic topology*. Graduate Texts in Mathematics, **82**. Springer-Verlag, New York-Berlin, 1982.
- [7] A. BRAIDES :  *$\Gamma$ -convergence for beginners*. Oxford Lecture Series in Mathematics and its Applications, **22**. Oxford University Press, Oxford, 2002.
- [8] H. BREZIS, J. M. CORON, E. H. LIEB : *Harmonic maps with defects*. Comm. Math. Phys. **107** (1986), 649–705.
- [9] G. CANEVARI : *Biaxiality in the asymptotic analysis of a 2D Landau-de Gennes model for liquid crystals*. ESAIM Control Optim. Calc. Var. **21** (2015), 101–137.
- [10] S.Y. CHANG, L. WANG, P. YANG : *Regularity of harmonic maps*. Comm. Pure Appl. Math. **52** (1999), 1099–1111.
- [11] Y.M. CHEN, M. STRUWE : *Existence and partial regularity results for the heat flow for harmonic maps*. Math. Z. **201** (1989), 83–103.
- [12] A. CONTRERAS, X.LAMY : *Biaxial escape in nematics at low temperature*. J. Funct. Anal. **272** (2017), 3987–3997.
- [13] P. G. DE GENNES, J. PROST : *The Physics of Liquid Crystals*. International Series of Monographs on Physics, **83**. Clarendon Press, 1993.
- [14] G. DE LUCA, A.D.REY : *Point and ring defects in nematics under capillary confinement* J. Chem. Phys. **127** (2007), 104902.
- [15] F. DIPASQUALE, V.MILLOT, A.PISANTE : *Torus-like solutions for the Landau- De Gennes model. Part II: Topology of  $S^1$ -equivariant minimizers*. In preparation.
- [16] F. DIPASQUALE, V.MILLOT, A.PISANTE : *Torus-like solutions for the Landau- De Gennes model. Part III: torus solutions vs split solutions*. In preparation.
- [17] L. C EVANS : *Partial regularity for stationary harmonic maps into spheres*. Arch. Rat. Mech. Anal. **116** (1991), 101–113.
- [18] E.C. JR. GARTLAND : *Scaling and limits of Landau-de Gennes models for liquid crystals: a comment on some recent analytical papers*. Math. Model. Anal. **23** (2018) 414-432.
- [19] E.C. JR. GARTLAND, S. MKADDEM : *Fine structure of defects in radial nematic droplets*. Phys. Rev. E **62** (2000), 6694–6705.
- [20] E.C. JR. GARTLAND, S. MKADDEM : *Instability of radial hedgehog configurations in nematic liquid crystals under Landau-de Gennes free-energy models*. Phys. Rev. E **59** (1999), 563–567.
- [21] M. GIAQUINTA, L. MARTINAZZI : *An introduction to the regularity theory for elliptic systems harmonic maps and minimal graphs*. Lecture Notes. Scuola Normale Superiore di Pisa (New Series) **11**, Edizioni della Normale, Pisa (2012).
- [22] D. GILBARG, N.S. TRUDINGER : *Elliptic Partial Differential Equations of Second Order*. Classics in Mathematics, Springer-Verlag, Berlin (2001).
- [23] E. GIUSTI : *Direct methods in the calculus of variations*. World Scientific Publishing Co., Inc., River Edge, NJ, (2003).
- [24] Q. HAN, F.H. LIN : *Elliptic partial differential equations*. Courant Lecture Notes in Mathematics **1**, American Mathematical Society (1997).
- [25] J. HEINONEN, T. KILPELÄINEN, O. MARTIO : *Nonlinear potential theory of degenerate elliptic equations*. Unabridged republication of the 1993 original. Dover Publications, Inc., Mineola, NY, 2006.
- [26] F. HÉLEIN : *Régularité des applications faiblement harmoniques entre une surface et une variété riemannienne*. C. R. Acad. Sci. Paris Sér. I Math. **312**, (1991) 591–596.
- [27] D. HENAO, A. MAJUMDAR, A. PISANTE : *Uniaxial versus biaxial character of nematic equilibria in three dimensions*. Calc. Var. Partial Differential Equations **56** (2017), 22 pp.
- [28] R. HARDT, F.H. LIN : *Mappings minimizing the  $L^p$  norm of the gradient*. Comm. Pure Appl. Math. **40** (1987), 555–588.
- [29] R. IGNAT, L. NGUYEN, V. SLASTIKOV, A. ZARNESCU: *Stability of the melting hedgehog in the Landau-de Gennes theory of nematic liquid crystals*. Arch. Ration. Mech. Anal. **215** (2015), 633–673.
- [30] R. IGNAT, L. NGUYEN, V. SLASTIKOV, A. ZARNESCU: *Uniqueness results for an ODE related to a generalized Ginzburg-Landau model for liquid crystals*. SIAM J. Math. Anal. **46** (2014), 3390–3425.
- [31] M. KLEMAN : *Defects in liquid crystals*. Reports on Progress in Physics **52** (1989).
- [32] S. KRALJ, E. G. VIRGA, S. ZUMER : *Biaxial torus around nematic point defects*. Phys. Rev. E **60** (1999), 1858–1866.
- [33] S. KRALJ , E.G. VIRGA : *Universal fine structure of nematic hedgehogs*. J. Phys. A **34** (2001), 829–838.
- [34] X. LAMY : *Uniaxial symmetry in nematic liquid crystals*. Ann. Inst. H. Poincaré Anal. Non Linéaire **32** (2015), 1125–1144.

- [35] O. LAVRENTOVICH, P. PASINI, C. ZANNONI, S. ZUMER (EDS.) : *Defects in Liquid Crystals: Computer Simulations, Theory and Experiments*. Nato Science Series II. Proceedings of the Nato advanced research workshop, Erice 19-23 september 2000. Springer, 2012.
- [36] L. LEMAIRE : *Applications harmoniques de surfaces Riemanniennes*. J. Differential Geometry **13** (1978), 51–78.
- [37] F.H. LIN, C.Y. WANG: *Stable Stationary Harmonic Maps to Spheres*. Acta Math. Sin. (Engl. Ser.) **22** (2006), 319–330.
- [38] F.H. LIN, C.Y. WANG: *The analysis of harmonic maps and their heat flows*. World Scientific, 2008.
- [39] S. LOJASIEWICZ : *Une propriété topologique des sous-ensembles analytiques réels*. Les Équations aux Dérivées Partielles (Paris, 1962), pp. 87–89, Éditions du Centre National de la Recherche Scientifique, Paris, 1963.
- [40] S. LUCKHAUS : *Partial Hölder Continuity for Minima of Certain Energies among Maps into a Riemannian Manifold*. Indiana Univ. Math. J. **37** (1988), 349–367.
- [41] I.F. LYUKSYUTOV : *Topological instability of singularities at small distances in nematics*. Zh. Eksp. Teor. Fiz **75** (1978), 358–360.
- [42] F. MAGGI : *Sets of finite perimeter and geometric variational problems, An introduction to Geometric Measure Theory*. Cambridge Studies in Advanced Mathematics **135**, Cambridge University Press, 2012.
- [43] A. MAJUMDAR: *The radial-hedgehog solution in Landau-de Gennes theory for nematic liquid crystals*. European J. Appl. Math. **23** (2012), 61–97.
- [44] A. MAJUMDAR, A. ZARNESCU : *Landau - De Gennes Theory of Nematic Liquid Crystals: the Oseen-Frank Limit and Beyond*. Arch. Rational Mech. Anal. **196** (2010), 227-280.
- [45] N.J. MOTTRAM, C.J.P. NEWTON : *Introduction to Q-tensor theory*. <https://arxiv.org/pdf/1409.3542.pdf>
- [46] C. B. MORREY, JR. : *Multiple integrals in the calculus of variations*. Springer Science & Business Media, 1966.
- [47] R. MOSER : *Partial Regularity for Harmonic Maps and Related Problems*. World Scientific, 2005.
- [48] G. PANATI, A. PISANTE : *Bloch Bundles, Marzari-Vanderbilt Functional and Maximally Localized Wannier Functions*. Comm. Math. Phys. **322** (2013), 835–875.
- [49] E. PENZENSTADLER, H.-R. TREBIN : *Fine structure of point defects and soliton decay in nematic liquid crystals* J. Phys. France **50**, (1989), 1027–1040
- [50] J. QING : *Boundary regularity of weakly harmonic maps from surfaces*. J. Funct. Anal. **114** (1993), 458–466.
- [51] T. RIVIÈRE : *Everywhere discontinuous harmonic maps into spheres*. Acta Math. **175** (1995), 197–226.
- [52] T. RIVIÈRE, M. STRUWE : *Partial regularity for harmonic maps and related problems*. Comm. Pure Appl. Math. **61** (2008), 451–463.
- [53] C. SCHEVEN : *Variational harmonic maps with general boundary conditions: Boundary regularity*. Calc. Var. Partial Differential Equations **4** (2006), 409–429.
- [54] R. SCHOEN : *Analytic aspects of the harmonic map problem*. Seminar on nonlinear partial differential equations (Berkeley, Calif., 1983), 321–358, Math. Sci. Res. Inst. Publ., **2**, Springer, New York, 1984.
- [55] R. SCHOEN, K. UHLENBECK : *A regularity theory for harmonic maps*. J. Diff. Geom. **17** (1982), 307–335.
- [56] R. SCHOEN, K. UHLENBECK : *Boundary regularity and the Dirichlet problem for harmonic maps*. J. Diff. Geom. **18** (1983), 253–268.
- [57] R. SCHOEN, K. UHLENBECK : *Regularity of minimizing harmonic maps into the sphere*. Invent. Math. **78** (1984), 89–100.
- [58] L. SIMON : *Theorems on Regularity and Singularity of Energy Minimizing Maps*. Lectures in Mathematics: ETH Zürich. Birkhäuser Basel, 2012.
- [59] J. SOUCEK, V. SOUCEK : *Morse-Sard theorem for real-analytic functions*. Comment. Math. Univ. Carolin., **13** (1972), 45–51
- [60] S. G. STAPLES : *Lp-averaging domains and the Poincaré inequality*. Ann. Acad. Sci. Fenn. Ser. A I Math. **14** (1989), 103–127.
- [61] E. G. VIRGA. : *Variational theories for liquid crystals*. Vol. **8**. CRC Press, 1995.

DIPARTIMENTO DI MATEMATICA, SAPIENZA UNIVERSITÀ DI ROMA, P.LE ALDO MORO 5, 00185 ROMA, ITALY  
*E-mail address:* `dipasquale@mat.uniroma1.it`

LAMA, UNIV PARIS EST CRETEIL, UNIV GUSTAVE EIFFEL, UPEM, CNRS, F-94010, CRÉTEIL, FRANCE  
*E-mail address:* `vincent.millot@u-pec.fr`

DIPARTIMENTO DI MATEMATICA, SAPIENZA UNIVERSITÀ DI ROMA, P.LE ALDO MORO 5, 00185 ROMA, ITALY  
*E-mail address:* `pisante@mat.uniroma1.it`