# ANNALES DE LA FACULTÉ DES SCIENCES TOULOUSE Mathématiques

# ADRIANO PISANTE Torus-like solutions for the Landau–De Gennes model.

Tome XXX, nº 2 (2021), p. 301–326.

https://doi.org/10.5802/afst.1676

© Université Paul Sabatier, Toulouse, 2021.

L'accès aux articles de la revue « Annales de la faculté des sciences de Toulouse Mathématiques » (http://afst.centre-mersenne.org/) implique l'accord avec les conditions générales d'utilisation (http://afst.centre-mersenne.org/legal/). Les articles sont publiés sous la license CC-BY 4.0.





Publication membre du centre Mersenne pour l'édition scientifique ouverte http://www.centre-mersenne.org/

# Torus-like solutions for the Landau–De Gennes model.

Adriano Pisante<sup>(1)</sup>

**ABSTRACT.** — In this note we report on some recent progress [10, 11, 12] about the study of global minimizers of a continuum Landau–De Gennes energy functional for nematic liquid crystals in three-dimensional domains. First, we discuss absence of singularities for minimizing configurations under norm constraint, as well as absence of the isotropic phase for the unconstrained minimizers, together with the related biaxial escape phenomenon. Then, under suitable assumptions on the topology of the domain and on the Dirichlet boundary condition, we show that smoothness of energy minimizing configurations yields the emergence of nontrivial topological structure in their biaxiality level sets. Then, we discuss the previous properties under both the norm constraint and an axial symmetry constraint, showing that in this case only partial regularity is available, away from a finite set located on the symmetry axis. In addition, we show that singularities may appear due to energy efficiency and we describe precisely the asymptotic profile around singular points. Finally, in an appropriate class of domains and boundary data we obtain qualitative properties of the biaxial surfaces, showing that smooth minimizers exibit torus structure, as predicted in [16, 24, 25, 39].

**RÉSUMÉ.** — Dans cette note, nous présentons des avancées récentes [10, 11, 12] sur l'étude des minimiseurs globaux d'une énergie continue de Landau-De Gennes dans des domaines 3D utilisée dans la modélisation des cristaux liquides nématiques.Dans un premier temps, nous décrivons l'absence de singularités des configurations minimisantes sous contrainte de norme, ainsi que l'absence de phase isotrope pour les minimiseurs non contraints, et le phénomène de fuite biaxiale en résultant. Sous certaines hypothèses sur la topologie du domaine et la condition de Dirichlet au bord, nous montrons ensuite comment la régularité / absence de phase isotrope des configurations minimisantes permet de déduire une structure topologique non triviale des ensembles de niveau de la biaxialité. Enfin, nous discutons ces mêmes proprietés pour des minimiseurs sous contrainte de symétrie axiale et sous contrainte de norme. Dans ce dernier cas, nous montrons que les minimiseurs ne satisfont qu'une régularité partielle, à savoir la régularité en dehors d'un ensemble fini situé sur l'axe de symétrie. De plus, nous démontrons que ces singularités ponctuelles peuvent en effet exister pour des raisons énergétiques, et nous décrivons en détails le comportement asymptotique des minimiseurs près de ces points singuliers. Pour terminer, nous donnons quelques propriétés qualitatives des surfaces de biaxialité pour une classe de domaines et de données au bord montrant que les minimiseurs réguliers présentent une structure en tore biaxial comme celle prédite dans [16, 24, 25, 39].

Keywords: Liquid crystals; axisymmetric torus solutions; harmonic maps.

<sup>&</sup>lt;sup>(1)</sup> Dipartimento di Matematica, Sapienza Università di Roma, P.le Aldo Moro 5, 00185 Roma, Italy — pisante@mat.uniroma1.it

# 1. Introduction

Nematic liquid crystals are mesophases of matter intermediate between crystalline solids and isotropic fluids (see [17]). Nematic molecules typically have elongated shape, approximately rod-like, and the interaction between them yields a local (mean) orientational order. These molecules also exhibit high responsivity to external stimuli (e.g., electromagnetic fields) so to affect the local orientation, which is the fundamental reason for their ubiquitous use in contemporary technological devices.

For a nematic liquid crystal filling a region  $\Omega \subseteq \mathbb{R}^3$  the key feature of a (mean) orientational order can be modeled in different ways, depending on the choice of parameters. Among different possibilities (see [3, 46]) we mention, in decreasing order of complexity, the following ones:

- Onsager-type theories: the description of the mean orientation is encoded in a family of probability measures  $\Omega \ni x \to \mu_x \in \mathcal{P}(\mathbb{S}^2)$ subject to the balancing condition  $\mu_x(B) = \mu_x(-B)$  for any  $x \in \Omega$ and any  $B \subseteq \mathbb{S}^2$  (head-to-tail symmetry of the molecules).
- Landau–De Gennes theory: local orientation is described by the socalled Q-tensor, i.e., a family of symmetric traceless matrices  $\Omega \ni x \to Q(x) \in S_0 \approx \mathbb{R}^5$ , with

$$\mathcal{S}_0 := \left\{ Q = (Q_{ij}) \in \mathscr{M}_{3 \times 3}(\mathbb{R}) : Q = Q^{\mathsf{t}}, \ \mathrm{tr}(Q) = 0 \right\}.$$
(1.1)

- Ericksen theory: local orientation is described by a vector field together with a scalar (the *degree of orientation*), i.e.,  $\Omega \ni x \to (s(x), n(x)) \in \mathbb{R} \times S^2$ , corresponding to special (*uniaxial*) *Q*-tensors of the form  $Q = s (n \otimes n - \frac{1}{3}I)$ .
- Oseen–Frank theory: mean orientation is encoded in a family of vectors  $\Omega \ni x \to n(x) \in S^2$  (with constant degree of orientation), taking possibly into account the *head-to-tail* symmetry by identifying opposite vectors to get a map into the projective plane  $\mathbb{R}P^2$  of the form  $\Omega \ni x \to (n(x) \otimes n(x) \frac{1}{3}I) \in \mathbb{R}P^2$ .

The first description, though closer to the statistical mechanics interpretation of the local orientation of nematic molecules, is notoriously awkward, since the state space  $\mathcal{P}(\mathbb{S}^2)$  is infinite dimensional. In the present note we will follow the second approach, using the description of nematics in terms of *Q*-tensors (see [38] for an introduction), which seems to give the most convincing description of the experimentally observed optical defects [23, 27]. Note that this second possibility can be regarded as a five-dimensional approximation of the first one in view of the formula

$$Q(x) = \int_{\mathbb{S}^2} \left( p \otimes p - \frac{1}{3}I \right) \mathrm{d}\mu_x(p) \,,$$

although we will drop for simplicity the resulting constraint  $Q(x) \ge -\frac{1}{3}I$ given in terms of the identity tensor. The Ericksen and the Oseen–Frank theory can be regarded as special cases of de Landau–de Gennes theory of Q-tensor. However, we will not discuss this connection here and for mathematical results on these two simpler models we refer the interested reader, e.g., to [1, 5, 18, 30].

According to the (LdG) theory, we consider  $S_0$  as in (1.1), endowed with the Hilbertian structure given by the usual (Frobenius) inner product and the induced norm,

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

Upon the choice of an orthonormal basis  $\{E_j\}_{j=0,\ldots,4}$ , the space  $\mathcal{S}_0$  can be identified with the Euclidean space  $\mathbb{R}^5$ . In particular,

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

As anticipated above, a liquid crystal configuration in an occupied region  $\Omega \subseteq \mathbb{R}^3$  (bounded, with smooth boundary) will be described through a map  $\Omega \ni x \to Q(x) \in S_0$ , so that at each point  $x \in \Omega$  the corresponding spectrum of Q(x) will be  $\sigma(Q(x)) = \{\lambda_1(x), \lambda_2(x), \lambda_3(x)\} \subseteq \mathbb{R}$ , where the three eigenvalues are ordered increasingly and satisfy the constraint  $\sum_{j=1}^3 \lambda_j(x) \equiv 0$ .

In order to discuss the properties of liquid crystal configurations (such as isotropic/nematic phase transition, biaxial escape), following [12] we find convenient to modify the usual definition of the biaxiality parameter as follows.

DEFINITION 1.1. — For any  $Q \in S_0 \setminus \{0\}$ , we define the signed biaxiality parameter of Q as

$$\widetilde{\beta}(Q) := \sqrt{6} \frac{\operatorname{tr}(Q^3)}{|Q|^3} \in [-1, 1].$$
 (1.2)

Observe that under the previous convention on the eigenvalues,  $\tilde{\beta}(Q) = \pm 1$  iff the minimal/maximal eigenvalue of Q 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). Note that in the uniaxial region, i.e. the regions { $\tilde{\beta} \circ Q(\cdot) = \pm 1$ }  $\subseteq \Omega$ , the tensors are those admissible in the Ericksen theory. Thus, the main feature of

the Landau–De Gennes model will be the presence in the energy minimizing configuration of biaxial phase  $\{\tilde{\beta} \circ Q(\cdot) \neq \pm 1\} \neq \emptyset$  (*biaxial escape*). The goal here is to account on some results from [10, 11, 12] on the regularity of minimizers and the emergence of topological structure in the corresponding *biaxial surfaces*  $\{\tilde{\beta} \circ Q(\cdot) = t\}, t \in (-1, 1)$ , which in the model case of a nematic droplet are expected to be of torus type [16, 24, 25, 39].

# 2. Energy functionals and Lyuksyutov constraint

Let  $\Omega \subseteq \mathbb{R}^3$  a bounded domain with (at least)  $C^1$ -smooth boundary, and  $\mathbf{Q}: \Omega \to S_0$  a configuration in the Sobolev space  $W^{1,2}(\Omega; S_0)$ . We consider the Landau–De Gennes energy functional of the form

$$\mathcal{F}_{\mathrm{LG}}(\mathbf{Q}) = \int_{\Omega} \frac{L}{2} |\nabla \mathbf{Q}|^2 + F_B(\mathbf{Q}) \,\mathrm{d}x\,, \qquad (2.1)$$

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

$$F_B(\mathbf{Q}) := -\frac{a^2}{2} \operatorname{tr}(\mathbf{Q}^2) - \frac{b^2}{3} \operatorname{tr}(\mathbf{Q}^3) + \frac{c^2}{4} \left( \operatorname{tr}(\mathbf{Q}^2) \right)^2, \qquad (2.2)$$

where a, b and c are material-dependent strictly positive constants. Critical points  $\mathbf{Q} \in W^{1,2}(\Omega; \mathcal{S}_0)$  of the energy functional  $\mathcal{F}_{\mathrm{LG}}$  under smooth and compactly supported perturbations are weak solutions to the following semilinear elliptic system of Euler–Lagrange equations

$$-L\Delta \mathbf{Q} + \frac{\partial F_B}{\partial \mathbf{Q}} - \frac{1}{3} \left( \operatorname{tr} \frac{\partial F_B}{\partial \mathbf{Q}} \right) I = 0,$$

where the last term in the equation is present in view of the trace constraint.

Under sufficiently nice Dirichlet boundary condition (strong anchoring) on  $\partial\Omega$ , e.g.,  $\mathbf{Q} = \mathbf{Q}_b \in \operatorname{Lip}(\partial\Omega; S_0)$ , it is routine to prove existence of energy minimizing configurations  $\mathbf{Q} \in W^{1,2}(\Omega; S_0)$  by the direct method in the Calculus of Variations. In addition, elliptic regularity theory yields Holder continuity up to the boundary together with  $\mathbf{Q} \in C^{\omega}(\Omega; S_0)$ , i.e., real-analyticity in the interior.

In order to single-out relevant Dirichlet boundary conditions and exploit the presence of topological defects in the energy minimizing configurations, it is fundamental to discuss qualitative properties of the potential energy  $F_B(Q)$ . It turns out that the potential is minimal when the signed biaxiality is maximal, and  $F_B(Q) = 0$  iff  $Q \in Q_{\min}$ , i.e., if Q is in the vacuum-manifold of positive uniaxial matrices

$$\mathcal{Q}_{\min} := \left\{ Q \in \mathcal{S}_0 : \quad Q = s_+ \left( n \otimes n - \frac{1}{3}I \right) , \quad n \in \mathbb{S}^2 \right\} , \qquad (2.3)$$

where

$$s_{+} := \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2} \tag{2.4}$$

is the positive root of the characteristic equation

$$2c^2t^2 - b^2t - 3a^2 = 0. (2.5)$$

Notice that, up to a multiplicative constant,  $\mathcal{Q}_{\min} \sim \mathbb{R}P^2 \subseteq \mathbb{S}^4$ , therefore  $\mathcal{Q}_{\min}$  has nontrivial topology. In particular, there are nontrivial homotopy groups  $\pi_2(\mathcal{Q}_{\min}) = \mathbb{Z}$  and  $\pi_1(\mathcal{Q}_{\min}) = \mathbb{Z}_2$ . The choice of boundary data with zero potential energy which explore this nontrivial topology is the key ingredient leading to the presence of topological defects and to the *biaxial escape* phenomenon.

To simplify the presentation we mainly focus in this note on the model case of a nematic droplet, i.e., when  $\Omega = \{|x| < 1\}$  is the unit ball (possibly up to diffeomorphism). 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

$$\mathbf{Q}_{\mathrm{b}}(x) = s_{+} \left( \vec{n}(x) \otimes \vec{n}(x) - \frac{1}{3}I \right) \,. \tag{2.6}$$

Thus, the energy functional  $\mathcal{F}_{LG}$  has an O(3)-equivariant (radial) critical point usually known as the *melting hedgehog* 

$$H(x) := s(|x|) \left( \frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}I \right), \quad 0 < |x| < 1.$$
(2.7)

This solution is obtained from a unique function s(|x|) increasing from 0 to  $s_+$  solving an ODE with the prescribed values at |x| = 0 and |x| = 1, see e.g. [21, 35] and the references therein. It turns out to be the unique uniaxial critical point of  $\mathcal{F}_{\lambda,\mu}$  w.r.t. arbitrary (not necessarily uniaxial) perturbations, see [26]. Moreover, the origin is an isotropic point. Stability/instability of the melting hedgehog as well as its energy minimality property depends in a crucial way on the choice of the parameters  $a^2, b^2, c^2$ , and L. In particular, instability of (2.7) in the *low-temperature limit* (essentially  $a^2 \to \infty$ ) was proved in [22] (see also [15, 35]) and the explicit form of the destabilizing perturbation shows an (infinitesimal) biaxial escape phenomenon and rules out its energy minimality.

Without altering any of the previous considerations, it is convenient to subtract-off an additive constant and introduce

$$\widetilde{F}_B(\mathbf{Q}) := F_B(\mathbf{Q}) - \min_{\mathcal{S}_0} F_B \,, \tag{2.8}$$

– 305 –

so that the potential becomes nonnegative. The corresponding energy functional is

$$\widetilde{\mathcal{F}}_{LG}(\mathbf{Q}) := \int_{\Omega} \frac{L}{2} |\nabla \mathbf{Q}|^2 + \widetilde{F}_B(\mathbf{Q}) \,\mathrm{d}x\,, \qquad (2.9)$$

which is the sum of two nonnegative terms, penalizing respectively spatial variations and deviations from the vacuum manifold  $Q_{\min}$ .

As in [12], we rescale a tensor by setting

$$\mathbf{Q} \coloneqq s_+ \sqrt{\frac{2}{3}} Q \,.$$

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 (2.3), i.e., through the so-called *Veronese immersion*. Thus, we can rewrite the energy functional (2.9) as

$$\widetilde{\mathcal{F}}_{LG}(\mathbf{Q}) = \frac{2}{3} s_+^2 L \, \mathcal{F}_{\lambda,\mu}(Q) \,, \qquad (2.10)$$

with

$$\mathcal{F}_{\lambda,\mu}(Q) := \int_{\Omega} \frac{1}{2} |\nabla Q|^2 + \lambda W(Q) + \frac{\mu}{4} (1 - |Q|^2)^2 \,\mathrm{d}x \,. \tag{2.11}$$

Here the reduced parameters  $\lambda$  and  $\mu$  are given by

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

where  $\frac{1}{\sqrt{\lambda}}$  and  $\frac{1}{\sqrt{\mu}}$  are, up to an harmless numerical factor, the *biaxial* coherence length and the nematic-isotropic correlation length respectively, see [14, 25, 39].

On the other hand, the reduced smooth potential  $W: S_0 \to \mathbb{R}$  is nonnegative, vanishes exactly on  $\mathbb{R}P^2$  and in view of (2.4)–(2.5) it is given by the equivalent formulas

$$W(Q) = \frac{1}{3\sqrt{6}} \left( |Q|^3 - \sqrt{6} \operatorname{tr}(Q^3) \right) + \frac{1}{12\sqrt{6}} \left( 3|Q|^2 + 2|Q| + 1 \right) \left( |Q| - 1 \right)^2, \quad (2.12)$$

or

$$W(Q) = \frac{1}{4\sqrt{6}}|Q|^4 - \frac{1}{3}\operatorname{tr}(Q^3) + \frac{1}{12\sqrt{6}}.$$
 (2.13)

The structure relations (2.11) and (2.12) suggests that, in a regime where  $\lambda$  is fixed and  $\mu$  is large, the energy  $\mathcal{F}_{\lambda,\mu}$  favours minimizing configurations of approximatively unit norm. More precisely, as introduced and rigorously discussed in [11, 12], this phenomenon happens in the *Lyuksyutov regime*, which is defined by the relations

diam 
$$\Omega \sim \frac{1}{\sqrt{\lambda}} = \sqrt{\frac{L}{b^2 s_+}}, \qquad \frac{1}{\sqrt{\lambda}} \cdot \left(\frac{1}{\sqrt{\mu}}\right)^{-1} = \sqrt{\frac{a^2}{b^2 s_+}} \gg 1.$$
 (2.14)

In particular, as detailed in [12], such restriction on the parameters yields absence of the isotropic phase in any energy minimizers (see also the next section) and in the special case of a nematic droplet the instability of the melting hedgehog in a broader range of parameters.

To simplify the presentation and in view of the previous considerations, in this note we make the fundamental assumption that the norm of any admissible configuration is given by the constant value proper of the vacuum manifold [34], i.e.,

$$|\mathbf{Q}(x)| \equiv \sqrt{\frac{2}{3}} s_+$$
 (Lyuksyutov constraint). (2.15)

Under the Lyuksyutov constraint, the energy functional takes the form

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

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

$$\mathcal{E}_{\lambda}(Q) := \int_{\Omega} \frac{1}{2} |\nabla Q|^2 + \lambda W(Q) \,\mathrm{d}x \,. \tag{2.16}$$

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

$$W(Q) = \frac{1}{3\sqrt{6}} \left( 1 - \widetilde{\beta}(Q) \right) \qquad \forall Q \in \mathbb{S}^4,$$
(2.17)

it 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 (2.16) reduces to the Dirichlet integral for maps into  $\mathbb{R}P^2$ , 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, 5], whereas connections between the two models are not discussed here but can be found, e.g., in [36] for  $\mathcal{F}_{\lambda,\mu}$  and in [11] for  $\mathcal{E}_{\lambda}$ , in the regimes  $L \to 0$  and  $\lambda \to +\infty$  respectively.

# 3. Regularity of energy minimizing configurations

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 following elliptic system of Euler–Lagrange equations

$$\Delta Q_{\lambda} + |\nabla Q_{\lambda}|^2 Q_{\lambda} = \lambda \nabla_{\tan} W(Q_{\lambda}), \qquad (3.1)$$

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

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

Observe that the left hand side of (3.1) is the so-called *tension field* of Q, a tangent field along Q in  $\mathbb{S}^4$ , and equation (3.1) 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. Since everywhere discontinuous weakly harmonic maps among maps in  $W^{1,2}$  do exist, we expect smoothness of solutions to (3.1) to fail in general because in the left hand side of (3.1) the quadratic term in the gradient is critical, having the same scaling property of the Laplace operator, while the right hand side should be of lower order perturbation. As a consequence, under the constraint (2.15) we will restrict to weak solution to (3.1) which are energy minimizers, possibly in some restricted class of symmetric maps, exploiting energy minimality to obtain regularity properties.

In this section we first consider the minimization of the energy functional  $\mathcal{E}_{\lambda}$  among Sobolev maps in the space  $W^{1,2}(\Omega; \mathbb{S}^4)$  satisfying a Dirichlet boundary condition. We fix a Lipschitz boundary datum  $Q_{\rm b} \in \operatorname{Lip}(\partial\Omega; \mathbb{S}^4)$ , and we consider the set of admissible configurations

$$\mathcal{A}_{Q_{\mathrm{b}}}(\Omega) := \left\{ Q \in W^{1,2}(\Omega; \mathcal{S}_{0}) : Q_{|\partial\Omega} = Q_{\mathrm{b}}, \ |Q| = 1 \text{ a.e. in } \Omega \right\}$$
$$\subseteq W^{1,2}(\Omega; \mathbb{S}^{4}), \quad (3.2)$$

which is always nonempty by standard theory of Sobolev maps between manifolds. Indeed, since  $\mathbb{S}^4$  is simply connected and  $\pi_2(\mathbb{S}^4) = 0$ , one has strong density of maps which are continuous up to the boundary and smooth in the interior.

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  $\mathcal{E}_{\lambda}$ . Under more regularity of the boundary map  $Q_{b}$  in [12] the following result is proved.

THEOREM 3.1. — 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  $Q_\lambda \in C^{\omega}(\Omega) \cap C^{1,\alpha}(\overline{\Omega})$ for every  $\alpha \in (0, 1)$ . If in addition  $\Omega$  is a domain with analytic boundary and  $Q_b \in C^{\omega}(\partial\Omega; \mathbb{S}^4)$ , then  $Q_\lambda \in C^{\omega}(\overline{\Omega}; \mathbb{S}^4)$ .

Since the energy functional  $\mathcal{E}_{\lambda}$  in (2.9) is a perturbation of the Dirichlet energy for maps in the space  $W^{1,2}(\Omega; \mathbb{S}^4)$ , the proof of this theorem relies in an essential way on ideas and techniques from the regularity theory of harmonic maps, starting from the pioneering papers [42, 43, 44], as summarized, e.g., in the books [31, 45]. The regularity properties claimed in the theorem could be obtained combining the results in [42, 43, 44]. However, as commented below, the proof in [12] is somewhat different and it is organized so that the argument also covers the case of minimization in a symmetric class of maps, as considered in [10, 11], with only minor modifications. The argument requires two steps:

- (A) Hölder-continuity of minimizers of the functional (2.9) (difficult).
- (B) Real-analyticity of Hölder continuous solutions to (3.1) (easy).

(B). — The second step is much simpler than the first one, as it essentially follows from classical (interior and boundary) regularity theory for elliptic systems according to the following implications:

$$Q \in W^{1,2} \cap C^{0,\alpha} \Longrightarrow Q \in C^{0,1} \Longrightarrow Q \in C^{k,\alpha} \Longrightarrow Q \in C^{\omega} .$$

The crucial point is to get Lipschitz continuity, which is obtained using the harmonic approximation technique, adapting the argument of [41] for harmonic maps. Then, higher order regularity follows from standard Calderon–Zygmund and Schauder theories and the analyticity results in [37].

(A). — The first step is much more difficult and it is where energy minimality comes into play. The main goal is to show that the  $L^2$ -deviation of Q from its average  $\oint Q$  has a power-like decay at small scales, i.e.,

$$f_B \left| Q - f_B Q \right|^2 \leqslant C |B|^{2\alpha/3}, \qquad (3.3)$$

for some absolute constant C > 0 and  $\alpha > 0$  and for any sufficiently small ball B, a property which is known to be equivalent to the fact that  $Q \in C^{0,\alpha}$ . To do this a useful ingredient is the Poincarè inequality

$$\int_{B} \left| Q - \int_{B} Q \right|^{2} \leqslant C |B|^{2/3} \int_{B} |\nabla Q|^{2} , \qquad (3.4)$$

for an absolute constant C > 0 and any ball B, which allows to bound the left hand side of (3.3) when the right hand side of (3.4) is bounded and in turn to show that the former has even a power-type decay when the latter is sufficiently small. More precisely, following [12], both in the interior and at the boundary Hölder continuity is obtained combining the following four steps:

Step (A1): Interior and boundary monotonicity formulae. — These are derived in form of identities, as opposed to those in [42, 43] which are just in form of inequalities obtained by comparison maps using energy minimality. As a consequence, both boundedness and asymptotic monotonicity for the function giving the scaled energy on balls of small radii  $0 < r \ll 1$ , i.e.

$$g(r) = \frac{1}{r} \mathcal{E}_{\lambda}(Q; B_r \cap \Omega) , \qquad (3.5)$$

are obtained. In particular, the right hand side in (3.4) is bounded. Note that the monotonicity formulae are not obtained by inner variations, as in [45] for the interior case, but instead by a penalty approximation, passing to

the limit in monotonicity formulae for smooth solutions of approximated problems. This approach is more flexible, as it applies also on the boundary and it is of use even in the symmetric case considered in [10, 11], where inner variations no longer give admissible deformations.

Step (A2): Strong compactness of blow-ups. — When analyzing Q at small scales around a given point  $\bar{x}$  one considers  $Q_r(x) = Q(\bar{x} + rx)$  to zoom Q into possible singularities; the previous step guarantees that the scaled maps are locally bounded in  $W^{1,2}$ , so one can pass to subsequences and study weak blow-up limits  $Q_* \in W^{1,2}_{loc}(\mathbb{R}^3; \mathbb{S}^4)$ . Strong compactness of blowups relies on energy minimality; it is obtained by construction of comparison maps using the Luckhaus interpolation lemma [33], arguing as in [45] for harmonic maps again both in the interior and near the boundary. As a consequence minimality is preserved under blow-up and any  $Q_*$  is locally minimizing the Dirichlet integral.

Step (A3): Constancy of blow-up limits (Liouville property). — As a consequence of the previous steps, when rescaling around an interior point strong limits of rescaled maps are degree-zero homogeneous and minimizing harmonic maps from  $\mathbb{R}^3$  into  $\mathbb{S}^4$ , hence  $Q_*(x) = \omega(x/|x|)$  for some harmonic sphere  $\omega: \mathbb{S}^2 \to \mathbb{S}^4$  and  $Q_*$  is stable under compactly supported perturbations. Then, following [44], for the 1-parameter family of maps

$$Q_*^t(x) = \frac{Q_*(x) + t\Phi(x)}{|Q_*(x) + t\Phi(x)|}, \qquad \Phi \in C_0^{\infty}(\mathbb{R}^3; \mathcal{S}_0),$$

one has a stability inequality from the second variation formula at t = 0 for the Dirichlet energy  $\mathcal{E}_0$ , i.e.,

$$\mathcal{E}_{0}^{''}(\Phi;Q_{*}) = \int_{B_{1}} |\nabla \Phi_{T}|^{2} - |\nabla Q_{*}|^{2} |\Phi_{T}|^{2} \,\mathrm{d}x \ge 0 \,,$$

where  $\Phi_T := \Phi - Q_*(Q_* : \Phi)$  is the tangential component of  $\Phi$  along  $Q_*$ . Then, averaging over (localized) conformal vector fields  $\Phi_j = \varphi E_j, \varphi \in C_0^{\infty}(\mathbb{R}^3)$  and  $\{E_j\} \subseteq S_0$  o.n.b., by the Bochner's method one finally gets  $\int_{\mathbb{S}^2} |\nabla_T \omega|^4 = 0$  and constancy follows. At a boundary point, strong limits of rescaled maps are of the form  $Q_*(x) = \omega^+(x/|x|)$  with  $x_3 > 0$  (up to rotations in the domain), for some harmonic half-sphere  $\omega^+ : \mathbb{S}^2_+ \to \mathbb{S}^4$  with constant trace on  $\partial \mathbb{S}^2_+$ . Then a somewhat different argument from [29], this time using Pohozaev identity and unique continuation, gives constancy also in this case.

Step (A4): Continuity under smallness of the scaled energy ( $\varepsilon$ -regularity). As a consequence of the previous steps one clearly has smallness of the scaled energy around any point for sufficiently small scales, because  $\frac{1}{r}\mathcal{E}_{\lambda}(Q; B_r \cap \Omega) \to 0$  as  $r \to 0$ , the limit being the energy of any constant blow-up  $Q_*$ . The approach in [12] to  $\varepsilon$ -reguarity is a purely PDEs argument and it treats in a unified way the interior and the boundary case, adapting for the latter the clever nonlinear reflection trick introduced in [40] for harmonic maps. On the contrary, the argument in [42, 43] is essentially variational, constructing comparison maps and exploiting energy minimality to show that the right hand side in (3.4) has power-type decay, whence Hölder-continuity follows from Morrey's growth lemma.

To obtain Hölder-continuity of solutions to (3.1) under monotonicity and smallness of the scaled energy the method is not indirect, as the compactness argument using the Hardy-BMO duality presented in [13]. The approach in [12] follows the elementary iteration via harmonic replacement introduced in [7] for harmonic maps, based on the divergence structure of the quadratic gradient term in (3.1). As a consequence one obtains the power decay with respect to the radius for the BMO seminorm on balls, or the family of quantities equivalent to it,

$$\|u\|_{\mathrm{BMO}(B)}^{p} \sim \sup_{\overline{B}_{\rho}(y) \subseteq B} \oint_{B_{\rho}(y)} \left| u - \oint_{B_{\rho}(y)} u \right|^{p} \mathrm{d}x \,,$$

associated to the left hand side of (3.3) and in turn Hölder continuity of Q.

Relying on Theorem 3.1, we can relax the norm constraint (2.15) and discuss briefly the full energy functional (2.11). One minimizes  $\mathcal{F}_{\lambda,\mu}$  over maps in  $W^{1,2}(\Omega; \mathcal{S}_0)$  still satisfying a Dirichlet boundary condition given by  $Q_{\rm b} \in \operatorname{Lip}(\partial\Omega; \mathcal{S}_0)$ . Existence and regularity for such problem have been already recalled above, hence minimizers  $Q_{\lambda}^{\mu} \in W^{1,2}(\Omega; \mathcal{S}_0)$  actually satisfy  $Q_{\lambda}^{\mu} \in C^{\alpha}(\overline{\Omega}; \mathcal{S}_0) \cap C^{\omega}(\Omega; \mathcal{S}_0)$  for some  $\alpha \in (0, 1)$ .

On a fixed domain  $\Omega$  the Lyuksyutov regime (2.14) corresponds to

$$\lambda = \sqrt{\frac{2}{3}} \frac{b^2 s_+}{L} \equiv \text{const}, \qquad \mu = \frac{a^2}{L} \to +\infty, \qquad (3.6)$$

particular cases being  $a^2 \to \infty$ ,  $b^2 \sim |a|^{-1}$  or  $L \to 0$ ,  $b^2 \sim L$ .

Under these restrictions on the parameters, since the last term in  $\mathcal{F}_{\lambda,\mu}$ acts as a penalty approximation of the norm constraint (2.15), one can prove convergence of the family  $\{\mathcal{F}_{\lambda,\mu}\}_{\mu}$  to the functional  $\mathcal{E}_{\lambda}$  (in the sense of  $\Gamma$ convergence), and in particular that minimizers of  $\mathcal{F}_{\lambda,\mu}$  converge to minimizers of  $\mathcal{E}_{\lambda}$ . The following result is taken from [12].

THEOREM 3.2. — As  $\mu \to \infty$  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  $\mathcal{A}_{Q_{\mathrm{b}}}(\Omega)$ such that, up to a subsequence,  $Q_{\lambda}^{\mu} \to Q_{\lambda}$  strongly in  $W^{1,2}(\Omega; \mathcal{S}_0)$ ;
- (2)  $\mathcal{F}_{\lambda,\mu}(Q^{\mu}_{\lambda}) \to \mathcal{E}_{\lambda}(Q_{\lambda}) \text{ and } |Q^{\mu}_{\lambda}| \to 1 \text{ uniformly in } \overline{\Omega};$

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

The last claim of the theorem above is by far the most interesting as it guarantees that the isotropic phase is avoided by energy minimizing configurations  $Q^{\mu}_{\lambda}$  in the Lyuksyutov regime, as already proved [8, 20] in 3D domains in the low-temperature limit  $a^2 \to \infty$ . The proof of this property is based in a crucial way on the regularity of minimizers from Theorem 3.1. Indeed, smoothness of the limiting minimizer  $Q_{\lambda}$  and the strong  $W^{1,2}$ -convergence yield smallness of the scaled energy of  $Q^{\mu}_{\lambda}$  in (3.5) at a sufficiently small scale. Combining monotonicity formulae with elliptic regularity in a way similar to [36], it is then possible to show that  $|Q^{\mu}_{\lambda}|$  has to converge to one uniformly as  $\mu \to \infty$  since the potential energy must become uniformly small in a pointwise sense.

There is a clear interpretation of the previous results in the model case of a nematic droplet discussed above. Indeed, the radial hedgehog described in (2.7) is a critical point of  $\mathcal{F}_{\lambda,\mu}$  with an isotropic point at the origin. As a consequence of Theorem 3.2 we see that it does not minimize  $\mathcal{F}_{\lambda,\mu}$  in the class  $W_{Q_{\rm b}}^{1,2}(\Omega; \mathcal{S}_0)$ , at least for  $\mu$  large enough. Thus, biaxial escape must occur for minimizers. In addition, some more work in [12] on the second variations  $\mathcal{F}_{\lambda,\mu}''$  shows even its energy instability w.r.t. biaxial perturbations for  $\mu$  large enough.

# 4. Topology of minimizing configurations

In the previous section we have seen that the minimizers  $Q_{\lambda}$  of the energy  $\mathcal{E}_{\lambda}$  have constant norm and they are smooth. Similarly, at least in the Lyuksyutov regime (3.6), minimizers  $Q_{\lambda}^{\mu}$  of the energy  $\mathcal{F}_{\lambda,\mu}$  are smooth and with empty isotropic phase. Here we want to 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  $\mathcal{Q}_{\min} \sim \mathbb{R}P^2$ .

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

DEFINITION 4.1. — For a configuration  $Q \in C^1(\overline{\Omega}; S_0 \setminus \{0\})$  we define its biaxiality function  $\beta := \widetilde{\beta} \circ Q$  and for each  $t \in [-1, 1]$  the associated biaxiality regions as the closed subsets of  $\overline{\Omega}$  given by

$$\{\beta \leqslant t\} := \{x \in \overline{\Omega} : \widehat{\beta} \circ Q(x) \leqslant t\}$$
  
and 
$$\{\beta \geqslant t\} := \{x \in \overline{\Omega} : \widetilde{\beta} \circ Q(x) \geqslant t\},$$

$$(4.1)$$

where  $\tilde{\beta}$  is the signed biaxiality parameter (1.2). The corresponding biaxial surfaces are defined as

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

Observe that if  $t \in (-1, 1)$  is a regular value of  $\beta$ , then biaxial surfaces are smooth surfaces inside  $\overline{\Omega}$ , possibly with boundary which is anyway smooth and contained in  $\partial\Omega$ .

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

DEFINITION 4.2. — Let  $A, B \subseteq \overline{\Omega}$  be two compact subset. The sets Aand B are said to be mutually linked<sup>(1)</sup> if A is not contractible in  $\overline{\Omega} \setminus B$  and B is not contractible in  $\overline{\Omega} \setminus A$ .

To gain more insight in the previous definitions, it is convenient to focus on the case of a nematic droplet. If  $\Omega$  is the unit ball and  $Q_{\rm b}$  is the radial boundary datum (2.6), then the energy minimizer cannot inherit O(3)-symmetry of the boundary datum because of the instability of O(3)equivariant critical point, both for  $\mathcal{E}_{\lambda}$  and for  $\mathcal{F}_{\lambda,\mu}$ , therefore symmetry breaking occurs. Thus, it is natural to expect the minimizers  $Q_{\lambda}$  or  $Q_{\lambda}^{\mu}$ to be axially symmetric around a fixed axis (in a sense made precise in the next section). In particular, the corresponding biaxiality regions (4.1) should 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  $t = \pm 1$ , the set  $\{\beta = -1\}$  should be a circle with axial symmetry, and  $\{\beta = 1\}$  the sphere  $\partial \Omega$  with a diameter lying on the symmetry axis added. Clearly sub and superlevel of the biaxiality function should be mutually linked in the sense of Definition 4.2 above. There is a wide numerical evidence for these symmetry properties and indeed this conjectural picture has been already investigated in [16, 24, 25, 39], where authors refer to such an equilibrium configuration as the "torus solution" of the Landau-De Gennes model. The situation here clearly reminds the one corresponding to the Hopf fibration

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

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

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).

In the paper [12] a class of domains  $\Omega \subseteq \mathbb{R}^3$  and configurations Q is singled-out that includes energy minimizers  $Q_{\lambda}$  and  $Q_{\lambda}^{\mu}$  on a nematic droplet under radial anchoring. The class is defined by the following assumptions:

- (HP1)  $Q \in C^1(\overline{\Omega}; \mathcal{S}_0 \setminus \{0\}) \cap C^{\omega}(\Omega; \mathcal{S}_0).$
- $(\mathrm{HP2}) \ \overline{\beta} := \min_{x \in \partial \Omega} \widetilde{\beta} \circ Q(x) > -1 \, .$
- (HP3)  $\Omega$  is smooth, connected and simply connected.
- (HP4) For  $x \in \partial\Omega$  the maximal eigenvalue  $\lambda_{\max}(x)$  admits a smooth choice of eigenvectors  $v_{\max} \in C^1(\partial\Omega; \mathbb{S}^2)$  with total degree which is odd.

Roughly speaking, the idea is to restrict the attention to smooth configurations without isotropic phase by (HP1), such that the maximal eigenvalue is simple at the boundary in view of (HP2), on connected domains with only spherical boundary components because of (HP3). Then the corresponding eigenspace map  $V_{\max} \in C^1(\partial\Omega; \mathbb{R}P^2)$  has an orientation  $v_{\max} \in C^1(\partial\Omega; \mathbb{S}^2)$ with total degree which is odd due to (HP4). These conditions are satisfied, e.g., if the domain  $\Omega$  is topologically a ball possibly with an even number of disjoint closed balls removed from its interior and the boundary condition is the radial anchoring, so that  $Q_b \in C^1(\partial\Omega; \mathbb{R}P^2)$ . Several interesting cases are left out, e.g., the case of nematic shells and the case of toroidal domains.

Note that under the previous assumptions, if in particular the trace of Q at the boundary satifies  $Q_b \in C^1(\partial\Omega; \mathbb{R}P^2)$ , then it has a lifting by (HP2), i.e.,  $Q_b$  is of the form (2.6), up to a constant factor, with  $v_{\max}(x)$  instead of the outer normal. Moreover, any lifting  $v \in C^1(\partial\Omega; \mathbb{S}^2)$  of  $Q_b$  admits a finite energy extension  $\overline{v} \in W^{1,2}(\Omega; \mathbb{S}^2)$  but no continuous extension because of assumption (HP3). As a consequence,  $Q_b$  admits an extension  $\overline{Q} \in W^{1,2}(\Omega; \mathbb{R}P^2)$  of the form

$$\overline{Q}(x) = \sqrt{\frac{3}{2}} \left( \overline{v}(x) \otimes \overline{v}(x) - \frac{1}{3}I \right) \,. \tag{4.2}$$

In view of [4] and (HP3), any extension  $\overline{Q} \in W^{1,2}(\Omega; \mathbb{R}P^2)$  of  $Q_{\rm b}$  is in fact of the form (4.2) for a suitable (necessarily) discontinuous map  $\overline{v} \in$  $W^{1,2}(\Omega; \mathbb{S}^2)$ . The configuration Q being smooth and without isotropic phase by assumption (HP1), it cannot be purely uniaxial (i.e.,  $\mathbb{R}P^2$ -valued) and *biaxial escape* must occur for purely topological reasons.

A weak counterpart of the conjectural picture described in the example above with a foliation of the domain by axially symmetric tori is the main topological result in [12] and we refer to solutions of (3.1) satisfying the conclusion of the theorem below on a general domain as "torus-like solutions".

THEOREM 4.3. — If assumptions (HP1)–(HP4) hold (e.g., if  $\Omega$  is smooth, connected and simply connected,  $\partial\Omega$  has an odd number of connected components, and that  $Q_{\rm b}(x) = \sqrt{3/2}(\vec{n}(x) \otimes \vec{n}(x) - \frac{1}{3}I)$  is the radial anchoring), then the biaxiality regions associated to the configuration Qsatisfy:

- the set of singular values of β = β̃ ∘ Q in [-1, β̄] is at most countable, and it can accumulate only at β̄; moreover, for any regular value -1 < t < β̄ of β the set {β = t} ⊆ Ω is a smooth surface with a connected component of positive genus;
- (2) for any  $-1 \leq t_1 < t_2 < \overline{\beta}$ , the sets  $\{\beta \leq t_1\} \subseteq \Omega$  and  $\{\beta \geq t_2\} \subseteq \overline{\Omega}$  are nonempty, compact, and not simply connected;
- (3) if in addition  $Q \in C^{\omega}(\overline{\Omega})$  and  $\overline{\beta} = 1$ , then the set of critical values is finite and  $\{\beta = 1\} \subseteq \overline{\Omega}$  is nonempty, compact, and not simply connected; in particular  $\{\beta = 1\} \cap \Omega$  is not empty;
- (4) for any  $-1 \leq t_1 < t_2 < \overline{\beta}$ , 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. The rest of the claim together with claim (2) is proved by contradiction, supposing is that each component of a biaxial surface  $\{\beta = t\}$  is spherical and using a degree-counting argument based on (HP3) to reach a contradiction. The argument for (2) and (3) above applies for regular values  $t \in (-1, \overline{\beta})$ , and the extension to arbitrary values is based on the analytic regularity of Q and the Łojasiewicz retraction theorem [32]. 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  $t \in (\overline{\beta}, 1)$ , but this range seems to be more difficult to analyze, since the biaxial surfaces meet the boundary  $\partial\Omega$  and the degree-counting argument mentioned above should take these boundary components into account.

## 5. Axially symmetric minimizing configurations

From now on we consider the energy functional (2.9) restricted to a class of  $\mathbb{S}^1$ -equivariant configurations. Let us now first make the concept of  $\mathbb{S}^1$ equivariance precise. We consider  $\mathbb{R}^3$  with the standard basis  $\{e_1, e_2, e_3\}$ , and

we identify the group  $\mathbb{S}^1$  with the subgroup of SO(3) of rotations around the vertical axis  $\mathbb{R}e_3 \subseteq \mathbb{R}^3$ , so that in the standard basis a matrix  $R \in \mathcal{M}_{3\times 3}(\mathbb{R})$  represents a rotation of angle  $\alpha$  around the vertical axis iff it can be written in the form

$$R = \begin{pmatrix} \widetilde{R} & 0\\ 0 & 1 \end{pmatrix} \quad \text{with} \quad \widetilde{R} := \begin{pmatrix} \cos \alpha & -\sin \alpha\\ \sin \alpha & \cos \alpha \end{pmatrix}.$$
(5.1)

In particular, under the previous identification we will also use the complex notation  $R = e^{i\alpha} \in \mathbb{S}^1$  for both the complex number, the rotation in  $\mathbb{R}^2$  (or  $\mathbb{C}$ ), and, possibly, the corresponding rotation around the vertical axis in  $\mathbb{R}^3$ , so that for  $x = (x', x_3) \in \mathbb{R}^3$  we have  $R \cdot x = (e^{i\alpha}x', x_3)$ .

The  $\mathbb{S}^1$ -action by rotation on  $\mathbb{R}^3$  yields an induced action on  $\mathcal{S}_0$  given by  $\mathcal{S}_0 \ni Q \mapsto R \cdot Q := R Q R^t \in \mathcal{S}_0$ . For elements in  $\mathcal{S}_0$ , let us use the notation

$$Q =: \begin{pmatrix} \widetilde{Q} - \frac{q_0}{2}I & \mathbf{q} \\ \mathbf{q}^{\mathsf{t}} & q_0 \end{pmatrix},$$

where  $q_0 \in \mathbb{R}$ ,  $\mathbf{q} \in \mathscr{M}_{2 \times 1}(\mathbb{R}) \simeq \mathbb{R}^2$ , and  $\widetilde{Q} = \widetilde{Q}^t \in \mathscr{M}_{2 \times 2}(\mathbb{R})$  satisfies  $\operatorname{tr}(\widetilde{Q}) = 0$ . In this way, for a rotation around the  $x_3$ -axis  $R \in \mathbb{S}^1$ , and  $\widetilde{R} \in SO(2)$  the corresponding rotation in the  $(x_1, x_2)$ -plane, we have

$$R \cdot Q = RQR^{\mathsf{t}} = \begin{pmatrix} \widetilde{R}\widetilde{Q}\widetilde{R}^{\mathsf{t}} - \frac{q_0}{2}I & \widetilde{R}\mathbf{q} \\ (\widetilde{R}\mathbf{q})^{\mathsf{t}} & q_0 \end{pmatrix}.$$
 (5.2)

We assume that the open set  $\Omega \subseteq \mathbb{R}^3$  is bounded, smooth and  $\mathbb{S}^1$ -invariant or axisymmetric/rotationally symmetric, i.e.,  $R\Omega = \Omega$  for any  $R \in \mathbb{S}^1$ , and we restrict ourselves to maps  $Q: \Omega \to S_0$  which are  $\mathbb{S}^1$ -equivariant, i.e., such that

$$Q(Rx) = RQ(x)R^{\mathsf{t}}, \quad \text{a.e. } x \in \Omega, \quad \forall R \in \mathbb{S}^{1},$$
(5.3)

with the obvious analogue definition for the boundary conditions  $Q_{\rm b}: \partial\Omega \to S_0$ .

Thus, we may consider continuous, Lipschitz or  $W^{1,2}$  configuration just adding the constraint (5.3) of being equivariant. In particular, if  $\Omega$  is rotationally symmetric around the  $x_3$ -axis and  $Q_b$  is  $\mathbb{S}^1$ -equivariant and Lipschitz continuous, we set

$$\mathcal{A}_{Q_{\mathrm{b}}}^{\mathrm{sym}}(\Omega) := \left\{ Q \in W^{1,2}(\Omega; \mathbb{S}^{4}) : Q_{|\partial\Omega} = Q_{\mathrm{b}} \text{ and } Q \text{ is } \mathbb{S}^{1}\text{-equivariant} \right\}$$
$$\subsetneq \mathcal{A}_{Q_{\mathrm{b}}}(\Omega) . \quad (5.4)$$

It is not difficult to see that for  $Q_{\rm b}$  as above the set  $\mathcal{A}_{Q_{\rm b}}^{\rm sym}(\Omega)$  is always not empty. In addition, any element  $Q \in \mathcal{A}_{Q_{\rm b}}^{\rm sym}(\Omega)$  has a well defined trace on the symmetry axis and (5.3) together with the norm constraint implies that a.e. on  $\{x_1^2 + x_2^2 = 0\} \cap \Omega$  one has  $Q(0, 0, x_3) = \pm E_0$ , the unique norm-one matrices in  $\mathcal{S}_0$  which are fixed by the  $\mathbb{S}^1$ -action on  $\mathcal{S}_0$ ,

$$E_0 := \sqrt{\frac{3}{2}} \left( e_3 \otimes e_3 - \frac{1}{3}I \right) = \frac{1}{\sqrt{6}} \begin{pmatrix} -1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 2 \end{pmatrix}$$

The same restriction occurs on  $\{x_1^2 + x_2^2 = 0\} \cap \partial \Omega$  for the boundary datum  $Q_b$ . In particular, if  $\Omega$  is the unit ball and  $Q_b$  satisfies  $Q_b(0, 0, \pm 1) = \pm E_0$ , then the class  $\mathcal{A}_{Q_b}^{\text{sym}}(\Omega)$  contains no map which is continuous up to the boundary, because  $x_3 \to Q(0, 0, x_3) : E_0$  should be constant.

As a consequence, we can minimize the energy functional (2.9) in the class  $\mathcal{A}_{Q_{\rm b}}^{\rm sym}(\Omega)$  of equivariant configurations and the direct method in the Calculus of Variations easily applies as the constraint (5.4) is weakly closed in  $W^{1,2}$ , but energy minimizers could have singularities, sometimes just for trivial topological reasons as in the example suggested above.

Indeed, the following partial regularity result holds.

THEOREM 5.1. — Let  $\Omega \subseteq \mathbb{R}^3$  be a rotationally symmetric Lipschitz domain, let  $\overline{Q}_b \in W^{1,2}(\Omega; \mathbb{S}^4)$  be an  $\mathbb{S}^1$ -equivariant map in the sense of (5.3) and let  $Q_\lambda \in W^{1,2}(\Omega; \mathbb{S}^4)$  be a minimizer of  $\mathcal{E}_\lambda$  in the class  $\mathcal{A}_{Q_b}^{\text{sym}}(\Omega)$ . Then  $Q_\lambda \in C^{\omega}(\Omega \setminus \text{Sing } Q_\lambda; \mathbb{S}^4)$ , where Sing  $Q_\lambda \subseteq \Omega$  is a locally finite subset of the  $x_3$ -axis or empty.

Moreover the following holds:

- (1) If in addition  $\partial\Omega$  is  $C^3$  and  $Q_b \in C^{1,1}(\partial\Omega; \mathbb{S}^4)$ , then  $Q_\lambda \in C^{1,\alpha}(\overline{\partial\Omega}_{\rho}; \mathbb{S}^4)$  for any  $\alpha \in (0, 1)$ , where  $\partial\Omega_{\rho} \subseteq \Omega$  is a tubular neighbourhood of the boundary, and Sing  $Q_\lambda$  is finite or empty. Finally, if  $\Omega$  is a domain with analytic boundary and  $Q_b \in C^{\omega}(\partial\Omega; \mathbb{S}^4)$  then  $Q_\lambda \in C^{\omega}(\overline{\partial\Omega_{\rho}}; \mathbb{S}^4)$ .
- (2) For any  $\bar{x} \in \text{Sing } Q_{\lambda}$  there exists  $s \in \mathbb{R}$  such that if  $Q^{(s)}(x)$  is the corresponding stable homogeneous equivariant blow-up as in (6.7) below, then there exists  $\nu > 0$  such that

$$\|Q_{\lambda}(\overline{x}+rx)-Q^{(s)}(x)\|_{C^2(\mathbb{S}^2;\mathbb{S}^4)}=\mathcal{O}(r^{\nu})\quad asr\to 0.$$

To compare the previous regularity result with the one in the nonsymmetric case we first observe that minimizers of (2.9) in the symmetric class  $\mathcal{A}_{Q_{\rm b}}^{\rm sym}(\Omega)$  essentially satisfy Palais' Symmetric Criticality Principle (although neither the functional is  $C^1$ -differentiable, nor the space  $W^{1,2}(\Omega; \mathbb{S}^4)$  has a Banach manifold structure), therefore they are true critical point of (2.9), i.e., they are weak solution of (3.1). One can try to discuss (partial) regularity along the lines on Section 3 an indeed both step (B) and Step (A4)

discussed there apply to the present case without any modification. On the other hand, these critical points satisfy an energy minimality property only in the restricted class  $\mathcal{A}_{Q_{\rm b}}^{\rm sym}(\Omega)$  of equivariant configurations, so the arguments to obtain (A1)–(A3) here are similar in the spirit but actually deviate from those mentioned in Section 3 and even the conclusion are different, because in the present context singularities on the symmetry axis are allowed.

More precisely, smallness of the scaled energy both in interior or at boundary points  $x = (x', x_3) \in \overline{\Omega}$  automatically holds out of the symmetry axis, i.e.,

$$x' \neq 0 \implies \frac{1}{r} \mathcal{E}_{\lambda}(Q; B_r(x) \cap \Omega) \stackrel{r \to 0}{\longrightarrow} 0,$$

in view of a classical capacity argument (as nontrivial  $\mathbb{S}^1$ -orbits have positive  $\mathcal{H}^1$ -measure), therefore the singular set is confined to the symmetry axis. Around points on the symmetry axis we wish to apply Steps (A1)-(A3) as in the nonsymmetric case. Here monotonicity formulas are obtained by adapting the same penalization trick from [12] to the  $S^1$ -equivariant case. Compactness of blow-ups centered on the symmetry axis are discussed following the same strategy as in the general case, but constructing suitable  $\mathbb{S}^1$ -equivariant comparison maps. The Liouville property at the boundary is obtained in a way similar to the nonsymmetric case, hence boundary regularity also follows in the present case. The crucial difference for the proof of Theorem 5.1 is the Liouville property in the interior since in the nonsymmetric case any locally minimizing harmonic tangent map into  $\mathbb{S}^4$  is constant by [44]. On the contrary, as shown in [10] and reviewed in the next section, there exists a one-parameter family of nonconstant degree-zero homogeneous  $\mathbb{S}^1$ -equivariant harmonic tangent maps  $\{Q^{(s)}\}_{s\in\mathbb{R}}$  which are smooth out of the origin and locally minimizing the Dirichlet energy among compactly supported axisymmetric perturbations. As a consequence, singularities of minimizers to (2.9) may occurr, but they form a locally finite set (actually finite when boundary regularity holds).

As for harmonic maps near isolated singularities [45], rescaling around any point  $\bar{x} \in \text{Sing } Q_{\lambda}$ , the maps  $Q_{\lambda}(\bar{x}+rx)$  have a unique asymptotic limit in  $C^2_{\text{loc}}$ -topology away from the origin which is an element of the family of degree-zero homogeneous maps  $\{Q^{(s)}\}_{s\in\mathbb{R}}$  mentioned above. The key point is that is that by homogeneity

$$Q^{(s)}(x) = \omega_\eta \left(\frac{x}{|x|}\right), \qquad \eta = e^{is}, \quad s \in \mathbb{R},$$

where the harmonic spheres  $\{\omega_{\eta}\}_{\eta\in\mathbb{S}^1} \subseteq C^3(\mathbb{S}^2;\mathbb{S}^4)$  all satisfy  $\mathcal{E}_0(\omega_{\eta}) \equiv 4\pi$  as reviewed in the next section. Since all these possible tangent maps belong

to the manifold of  $4\pi$ -energy harmonic spheres into  $\mathbb{S}^4$ , i.e.,

 $\left(\operatorname{Conf}^+(\mathbb{S}^2;\mathbb{S}^4)\times\operatorname{Isom}(\mathbb{S}^2;\mathbb{S}^4)\right)/SO(3)\subseteq C^3(\mathbb{S}^2;\mathbb{S}^4)\,,$ 

one can apply the Simon–Łojasiewicz inequality with optimal exponent for the Dirichlet energy  $\mathcal{E}_0$  on  $C^3(\mathbb{S}^2; \mathbb{S}^4)$ , namely

$$|\mathcal{E}_0(u) - \mathcal{E}_0(\omega_\eta)| \leqslant C |\nabla \mathcal{E}(u)|_{L^2}^2, \qquad \|u - \omega_\eta\|_{C^3} \ll 1, \qquad (5.5)$$

and following [45] obtain the unique asymptotic limit together with the power-type decay.

In the final part of this section we present the topological counterpart of the previous regularity result. Still in the simple case of axisymmetric domain equivalent the a ball we have the following result from [10].

THEOREM 5.2. — Let  $\Omega \subseteq \mathbb{R}^3$  be a rotationally symmetric domain with  $C^3$ boundary diffeomorphic to the unit ball and suppose that  $Q_b \in C^2(\partial\Omega; \mathbb{R}P^2)$ is the ( $\mathbb{S}^1$ -equivariant) radial anchoring as in (2.6). Let  $Q_\lambda \in W^{1,2}(\Omega; \mathbb{S}^4)$  be a minimizer of  $\mathcal{E}_\lambda$  in the class  $\mathcal{A}_{Q_b}^{\text{sym}}(\Omega)$  and  $\Sigma \subseteq \Omega \cap \{x'=0\}$  the (possibly empy) subset of its singularities. Then the following holds.

- (1) If  $\Sigma = \emptyset$  then  $Q_{\lambda}$  is a torus-like solution; moreover, for any regular value  $t \in (-1, 1)$  the biaxial surface  $\{\beta = t\}$  is a finite union of axially symmetric tori.
- (2) If  $\Sigma \neq \emptyset$  then  $Q_{\lambda}$  is a split solution; the set  $\Sigma$  contains 2m > 0points and for any regular value  $t \in (-1,1)$  (for  $Q_{\lambda}$  in  $\overline{\Omega} \setminus \Sigma$ ) the biaxial surface  $\{\beta = t\}$  contains m > 0 disjoint axially symmetric spheres each touching  $\{x' = 0\}$  at a pair of singular points (i.e.,  $\overline{\{\beta = t\}} \cap \{x' = 0\} = \Sigma$ ).

As we will see in the final section, both the cases in the two theorems above are indeed possible, depending on the geometry of the domain  $\Omega$ . However, in case of smooth (torus-like) solution, the S<sup>1</sup>-symmetry simplifies the possible topology in the smooth configurations and only tori are possible as connected component in any regular biaxial surface. On the other hand, when singularities are present, the biaxial surfaces must contain spheres, pairwise connecting these singularities, and, possibly, extra smooth tori. In the latter case numerical simulations suggest in case of a nematic droplet that the level sets { $\beta = t$ } as  $t \in (-1, 1)$  varies, should give a foliation of the domain (minus the symmetry axis) by spheres and no extra tori should appear.

## 6. Asymptotic behaviour at axially symmetric singularities

According to Theorem 5.1, it is possible to describe the behaviour of axially symmetric energy minimizing configurations  $Q_{\lambda}$  in terms of suitable equivariant degree-zero homogeneous harmonic maps (*tangent maps*) into  $\mathbb{S}^4$ , which are locally minimizing the Dirichlet integral with respect to compactly supported axially symmetric perturbations. Recall that such maps appear as degree-zero homogeneous extension of harmonic spheres, i.e., maps  $\omega \in C^{\infty}(\mathbb{S}^2; \mathbb{S}^4)$  which are critical points of the Dirichlet integral.

In order to describe these equivariant maps and to discuss their stability/instability properties, starting from (5.2) it is convenient to decompose  $S_0$  into invariant subspaces  $\{L_i\}_{i=0,1,2}$ , so that

$$\mathcal{S}_0 = L_0 \oplus L_1 \oplus L_2 \approx \mathbb{R} \oplus \mathbb{C} \oplus \mathbb{C}$$
.

The previous identification allows to rewrite the  $\mathbb{S}^1$ -action (5.2) in terms of complex numbers, so that for any  $w = (w_0, \mathbf{w}_1, \mathbf{w}_2) \in \mathcal{S}_0$  and  $R = e^{i\alpha} \in \mathbb{S}^1$  we have

$$R \cdot (w_0, \mathbf{w}_1, \mathbf{w}_2) = (w_0, e^{i\alpha} \mathbf{w}_1, e^{i2\alpha} \mathbf{w}_2).$$

$$(6.1)$$

Note that if  $\omega$  is an equivariant map then  $V = span_{\mathbb{R}}\omega(\mathbb{S}^2) \subseteq S_0$  is an invariant subspace. Combining this observation with [6], we deduce that  $\mathbb{S}^4$ -valued equivariant harmonic spheres are either linearly degenerate, i.e.,

$$\omega^{(1)}(x) = (w_0(x), \mathbf{w}_1(x), 0), \quad \text{or} \quad \omega^{(2)}(x) = (w_0(x), 0, \mathbf{w}_2(x)),$$

hence  $S^2$ -valued, or *linearly full*, i.e., dimV = 5 otherwise. In the linearly degenerate case it is not difficult to show that, up to a possible application of the antipodal map  $a : S^4 \to S^4$ , for k = 1, 2 we have

$$\omega^{(k)}(x) = \sigma^{-1} \left( \mu_k \left( \sigma(x) \right)^k \right), \quad \mu_k \in \mathbb{C}^*,$$
(6.2)

where  $\sigma \colon \mathbb{S}^2 \to \mathbb{C} \cup \{\infty\}$  is the stereographic projection from the south pole.

In order to describe linearly full harmonic spheres  $\omega$  into  $\mathbb{S}^4$ , following [6] (see also, e.g., [2, 28] for more details) it is convenient to identify  $\mathbb{S}^2$  with  $\mathbb{C}P^1$  and to study their canonical (or twistor) lift  $\tilde{\omega}$  to  $\mathbb{C}P^3$ , the twistor space of  $\mathbb{S}^4$ . As detailed, e.g., in [2, Chapter 7], the twistor space of  $\mathbb{S}^4$ , i.e., the space of orthogonal complex structures on  $\mathbb{S}^4$ , is  $\mathrm{SO}(5)/U(2)$ ; however, it is elementary but not obvious to identify it with complex projective 3-space  $\mathbb{C}P^3$ . Thus,  $\mathbb{C}P^3$  has a natural structure of fibre bundle over  $\mathbb{S}^4$ with fiber  $\mathrm{SO}(4)/U(2) = \mathbb{S}^2$ . In addition, for any  $x \in \mathbb{S}^2$  the corresponding  $\tilde{\omega}(x)$  is the natural orthogonal complex structure on  $T_{\omega(x)}\mathbb{S}^4$  for which the oriented subspaces  $V = Im d\omega_x$  and  $V^{\perp}$  are complex lines. Notice that  $\mathbb{C}P^3 = \mathbb{C}^4/\mathbb{C}^* = \mathbb{S}^7/\mathbb{S}^1$ , so the projection  $\tau : \mathbb{C}P^3 \to \mathbb{S}^4$  is nothing but the restriction to circles of the Hopf fibration  $\mathbb{S}^7 \to \mathbb{S}^4$ . If we write  $[z_0, z_1, z_2, z_3] \in \mathbb{C}P^3$ , with  $(z_0, z_1, z_2, z_3) \in \mathbb{C}^4 \setminus \{0\}$  the homogeneous coordinates in  $\mathbb{C}P^3$ , and we consider  $\mathbb{S}^4$  as the unit sphere of  $\mathbb{R} \oplus \mathbb{C} \oplus \mathbb{C}$ , then the twistor fibration  $\tau : \mathbb{C}P^3 \to \mathbb{S}^4$  turns out to be the map given by

$$\tau([z_0, z_1, z_2, z_3]) = \frac{(|z_0|^2 - |z_1|^2 - |z_2|^2 + |z_3|^2, 2(\overline{z_0}z_1 + \overline{z_2}z_3), 2(\overline{z_0}z_2 - \overline{z_1}z_3))}{|z_0|^2 + |z_1|^2 + |z_2|^2 + |z_3|^2}.$$
 (6.3)

Considering the  $\mathbb{S}^1$ -action on  $\mathbb{C}P^3$  defined by

 $R \cdot [z_0, z_1, z_2, z_3] := [z_0, e^{i\alpha} z_1, e^{2i\alpha} z_2, e^{3i\alpha} z_3] \qquad \forall R = e^{i\alpha} \in \mathbb{S}^1, \quad (6.4)$ 

and the (induced)  $\mathbb{S}^1$ -action on  $\mathbb{S}^4 \subseteq \mathbb{R} \oplus \mathbb{C} \oplus \mathbb{C}$  given by (6.1), the twistor map  $\boldsymbol{\tau}$  turns out to be equivariant.

This way, up to a possible application of the antipodal map as above and up to postcomposing with the twistor fibration  $\tau : \mathbb{C}P^3 \to \mathbb{S}^4$ , one has a one-to-one correspondence between harmonic spheres  $\omega : \mathbb{S}^2 \to \mathbb{S}^4$  and *horizontal*<sup>(2)</sup> algebraic curves  $\tilde{\omega} : \mathbb{C}P^1 \to \mathbb{C}P^3$  given by their twistor lift, and the commutative diagram

 $\mathbb{C}P^{3}$   $\downarrow^{\tau}$   $\mathbb{S}^{2} = \mathbb{C}P^{1} \xrightarrow{\omega} \mathbb{S}^{4}$ (6.5)

reflects the fact that  $\omega = \tau \circ \tilde{\omega}$ . In addition, the harmonic sphere  $\omega$  is equivariant if and only if its twistor lift is equivariant. As a consequence, specializing to the equivariant setting allows to classify the canonical lifts that in homogeneous coordinates  $[\lambda_0, \lambda_1] \in \mathbb{C}P^1$  can be written as

$$\widetilde{\omega}([\lambda_0,\lambda_1]) = \left[\lambda_0^3, \mu_1 \lambda_0^2 \lambda_1, \mu_2 \lambda_0 \lambda_1^2, -\frac{\mu_1 \mu_2}{3} \lambda_1^3\right] \in \mathbb{C}P^3, (\mu_1, \mu_2) \in \mathbb{C}^* \times \mathbb{C}^*.$$
(6.6)

Notice that according to [6], the energy of any harmonic sphere  $\omega$  is always quantized, namely  $\mathcal{E}_0(\omega) = 4\pi k$ , for some  $k \in \mathbb{N}$ . In view of equivariance we have  $k \in \{0, 1, 2, 3\}$ , where k = 0 corresponds to  $\omega \equiv \pm E_0$ , (6.2) describe the cases k = 1 or k = 2, and the case k = 3 is described in terms of (6.5) and (6.6).

<sup>&</sup>lt;sup>(2)</sup> Horizontality here means that at each point  $\widetilde{\omega}([\lambda_0, \lambda_1]) \in \mathbb{C}P^3$  the image of the differential  $d\widetilde{\omega}_{[\lambda_0, \lambda_1]}$  is orthogonal to the tangent space to the fiber  $\tau^{-1}(\omega([\lambda_0, \lambda_1]))$  with respect to the Fubini–Study metric.

As in Section 3 above, analyzing the second variation  $\mathcal{E}_0''(\cdot, Q)$  for the corresponding maps  $Q(x) = \omega(\frac{x}{|x|})$  in the class of  $\mathbb{S}^1$ -equivariant deformations a tricky but elementary argument gives the following result from [10].

THEOREM 6.1. — Let  $Q(x) = \omega(\frac{x}{|x|})$  be a nonconstant degree-zero homogeneous  $\mathbb{S}^1$ -equivariant harmonic maps into  $\mathbb{S}^4$  and  $\omega \in C^{\infty}(\mathbb{S}^2; \mathbb{S}^4)$  the corresponding harmonic sphere. Then the following holds.

- (1) For any  $s \in \mathbb{R}$ , if  $\mu_1 = e^{is}$  and  $\omega = \omega^{(1)}$  is the corresponding map in (6.2), then  $Q \in W^{1,2}_{loc}(\mathbb{R}^3; \mathbb{S}^4)$  is a minimizer of the Dirichlet integral  $\mathcal{E}_0$  with respect to compactly supported axially symmetric perturbations. In particular the map Q is stable.
- (2) All the other nonconstant degree-zero homogeneous S<sup>1</sup>-equivariant harmonic maps into S<sup>4</sup> are unstable.

In view of Theorems 5.1 and 6.1 above, the only possible profiles for axially symmetric minimizers of  $\mathcal{E}_{\lambda}$  at isolated singularities are of the form

$$Q^{(s)}(x) = \pm \frac{1}{|x|} (x_3, e^{is} x', 0), \qquad x = (x', x_3) \in \mathbb{R}^3 \setminus \{0\}, \quad s \in \mathbb{R}, \quad (6.7)$$

or in matrix form

$$Q^{(s)}(x) = \pm e^{is} \cdot \frac{1}{\sqrt{6}} \frac{1}{|x|} \begin{pmatrix} -x_3 & 0 & \sqrt{3}x_1 \\ 0 & -x_3 & \sqrt{3}x_2 \\ \sqrt{3}x_1 & \sqrt{3}x_2 & 2x_3 \end{pmatrix}, \quad x = (x_1, x_2, x_3) \in \mathbb{R}^3 \setminus \{0\}.$$

On the other hand, instability occurs as soon as for the harmonic map Q(x) the last component  $\mathbf{w}_2 \neq 0$ , therefore both  $Q(x) = \omega^{(2)}(\frac{x}{|x|})$  and all the tangent maps coming from linearly full harmonic spheres  $\omega = \tau \circ \widetilde{\omega}$  corresponding to (6.6) are unstable. In particular the homogeneous radial hedgehog

$$\overline{H}(x) = \sqrt{\frac{3}{2}} \left( \frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}I \right), \qquad x \in \mathbb{R}^3 \setminus \{0\}$$
(6.8)

is unstable.

## 7. Torus solutions vs split solutions

In this section we mention briefly a result from [11] about the presence or even the coexistence of smooth and singular minimizers of the energy functional  $\mathcal{E}_{\lambda}$  in the symmetric class  $\mathcal{A}_{Q_b}^{\text{sym}}$  defined in (5.4). More precisely, for  $\delta \in [-1, 1]$  we consider a continuous family  $\{\Omega_{\delta}\}_{\delta \in [-1, 1]}$  of S<sup>1</sup>-invariant smooth cylinder-type domains in  $\mathbb{R}^3$  together with the corresponding family of boundary data corresponding to radial anchoring,

$$\mathbf{Q}_{\mathrm{b}}^{(\delta)}(x) = \sqrt{\frac{3}{2}} \left( \vec{n}_{\delta}(x) \otimes \vec{n}_{\delta}(x) - \frac{1}{3}I \right) \,. \tag{7.1}$$

We assume each element  $\Omega_{\delta}$  of the family of cylidrical domains above is determined by two sidelenghts  $\ell_1 = \ell_1(\delta)$  and  $\ell_2 = \ell_2(\delta)$ , so that for each  $\delta \in [-1, 1]$ 

$$\Omega_{\delta} \approx \{ |x'| < \ell_1, \ |x_3| < \ell_2 \}, \qquad x = (x', x_3) \in \mathbb{R}^3,$$

and we analyze what happens to the minimizers  $Q_{\lambda}$  of  $\mathcal{E}_{\lambda}$  as the mutual ratio  $\ell_2/\ell_1$  varies continuously from  $\ell_2/\ell_1 \ll 1$  on the domain  $\Omega_{-1}$  to  $\ell_2/\ell_1 \gg 1$  on the domain  $\Omega_1$ . Here the intermediate domain  $\Omega_0$  corresponds by construction to the case  $\ell_1 \sim \ell_2$ , so that it should be euristically comparable to a nematic droplet. For simplicity we consider  $\ell_1$  constant for  $\delta \in [-1, 0]$  and  $\ell_2$  constant for  $\delta \in [0, 1]$ .

Notice that as  $\delta$  varies in [-1, 1] the domains vary smoothly together with the boundary conditions, hence the set of minimizers is compact in  $W^{1,2}$ topology (although some care is needed because the domain  $\Omega_{\delta}$  is varying) and, up to subsequences, minimizers converge to minimizers. As a consequence of the regularity theory and the analysis of the asymptotic profiles at singular point in Sections 5 and 6 it is not difficult to prove the following stability (closure) properties for the set of minimizers under deformation of the domain:

- the strong  $W^{1,2}$ -limit of smooth minimizers is a smooth minimizers;
- the strong  $W^{1,2}$ -limit of singular minimizers is a singular minimizers.

Notice that a simple consequence of these facts about energy minimizing configurations is that singularities cannot appear through a bifurcation mechanism from a smooth minimizer (no creation/annihilation mechanism for pairs of singularities is possible for minimizers).

The following is one of the main results in [11].

THEOREM 7.1. — Let  $\{\Omega_{\delta}\}_{\delta \in [-1,1]} \subseteq \mathbb{R}^3$  and  $\{Q_b^{(\delta)}\}_{\delta \in [-1,1]}$  as above and let  $Q_{\lambda}$  any minimizers of  $\mathcal{E}_{\lambda}$  in  $\mathcal{A}_{Q_b^{(\delta)}}^{\text{sym}}$  for some  $\delta \in [-1,1]$ . If  $\lambda$  is sufficiently small (depending only on  $a^2, b^2, c^2$  and L) then the following hold:

- (1) in the domain  $\Omega_{-1}$  if  $\ell_1 \sim 1$  and  $\ell_2 \gg 1$  is large enough (depending only on  $a^2, b^2, c^2$  and L) then any minimizers  $Q_{\lambda}$  is a split solution;
- (2) in the domain  $\Omega_1$  if  $\ell_2 \sim 1$  and  $\ell_1 \gg 1$  is large enough (depending only on  $a^2, b^2, c^2$  and L) then any minimizers  $Q_{\lambda}$  is a torus solution;

(3) there exists  $\delta^* \in (-1,1)$  such that in the domain  $\Omega_{\delta^*}$  the energy functional  $\mathcal{E}_{\lambda}$  has both a split solution and a torus solution as minimizing configurations with the same energy.

Some comments about the previous statement are in order. The first claim shows that in the energy minimization the presence of singularities may be energetically favourable and this fact is clearly reminiscent of the similar energy gap phenomenon discovered in [19] for maps into  $\mathbb{S}^2$ . Indeed, one can construct a singular competitor  $\widetilde{Q}$  with the same trace and energy strictly smaller than the one of any smooth map; for such a map on a long subinterval of the symmetry axis one has  $\widetilde{Q}(0,0,x_3) \equiv -E_0$  as opposed to the boundary value  $\widetilde{Q}(0,0,x_3) = E_0$  for  $x = (0,0,x_3) \in \partial \Omega_{-1}$  and even in a neighborhood of the boundary. The second claim reflects the fact that in the limit  $\ell_1 \to \infty$  one gets a minimizer in an infinite slab with constant boundary value, which is therefore constant; since regularity/singularities persist under strong convergence this clearly yields only torus solutions on the domain  $\Omega_1$  for  $\ell_1$  large enough. Finally, the same persistence properties recalled above through a continuity+compactness method allow to obtain an intermediate value  $\delta^* \in (-1, 1)$  such that both singular (split) and smooth (torus) solutions appear as minimizers on the same domain  $\Omega_{\delta^*}$  and with the same energy. It is not known whether this is the case for  $\delta = 0$ , i.e., whether or not on a domain similar or even equal to a nematic droplet minimizers among all axially symmetric maps are smooth or singular.

As a concluding remark, we observe that Theorem 7.1 together with Theorem 3.1 yield another very interesting consequence. Indeed, claim (1) in the theorem above implies that energy minimizers for  $\mathcal{E}_{\lambda}$  in the class  $\mathcal{A}_{Q_{b}^{(-1)}}$ being smooth, they cannot be axially symmetric even if the boundary condition  $Q_{b}$  satisfies this property. As a consequence, axial symmetry breaking and nonuniqueness phenomena must occur in the minimization of the energy functional  $\mathcal{E}_{\lambda}$ . Such phenomena are in agreement with the numerical simulations in [9] and are the natural counterpart for the Landau–De Gennes model of those known from [1] for minimizers of the Frank–Oseen energy.

# Bibliography

- JR. ALMGREN, FREDERICK J. & E. H. LIEB, "Singularities of energy minimizing maps from the ball to the sphere: examples, counterexamples, and bounds", Ann. Math. 128 (1988), no. 3, p. 483-530.
- [2] P. BAIRD & J. C. WOOD, Harmonic morphisms between Riemannian Manifolds, London Mathematical Society Monographs, vol. 29, London Mathematical Society, 2003.

- [3] J. M. BALL, "Liquid crystals and their defects", in *Mathematical thermodynamcis of complex fluids (Cetraro, Italy, June 2015)*, Lecture Notes in Mathematics, vol. 2200, Springer, 2017, p. 1-46.
- [4] J. M. BALL & A. ZARNESCU, "Orientability and energy minimization in liquid crystal models", Arch. Ration. Mech. Anal. 202 (2011), no. 2, p. 493-535.
- [5] H. BRÉZIS, J.-M. CORON & E. H. LIEB, "Harmonic maps with defects", Commun. Math. Phys. 107 (1986), p. 649-705.
- [6] E. CALABI, "Minimal immersions of surfaces in Euclidean spheres", J. Differ. Geom. 1 (1967), p. 111-125.
- [7] S.-Y. A. CHANG, L. WANG & P. C. YANG, "Regularity of harmonic maps", Commun. Pure Appl. Math. 52 (1999), no. 9, p. 1099-1111.
- [8] A. CONTRERAS & X. LAMY, "Biaxial escape in nematics at low temperature", J. Funct. Anal. 272 (2017), no. 10, p. 3987-3997.
- [9] G. DE LUCA & A. D. REY, "Point and ring defects in nematics under capillary confinement", J. Chem. Phys. 127 (2007), article no. 104902.
- [10] F. DIPASQUALE, V. MILLOT & A. PISANTE, "Torus-like solutions for the Landau-De Gennes model. Part II: topology of S<sup>1</sup>-equivariant minimizers", https://arxiv.org/ abs/2008.13676.
- [11] \_\_\_\_\_, "Torus-like solutions for the Landau–De Gennes model. Part III: torus solutions vs split solutions", in preparation.
- [12] —, "Torus like solutions for the Landau–De Gennes model. Part I: The Lyuksyutov regime", Arch. Ration. Mech. Anal. 239 (2021), p. 599-678.
- [13] L. C. EVANS, "Partial regularity for stationary harmonic maps into spheres", Arch. Ration. Mech. Anal. 116 (1991), no. 2, p. 101-113.
- [14] JR. GARTLAND, EUGENE C., "Scaling and limits of Landau-de Gennes models for liquid crystals: a comment on some recent analytical papers", *Math. Model. Anal.* 23 (2018), p. 414-432.
- [15] JR. GARTLAND, EUGENE C. & S. MKADDEM, "Instability of radial hedgehog configurations in nematic liquid crystals under Landau-de Gennes free-energy models", *Phys. Rev. E* 59 (1999), p. 563-567.
- [16] JR. GARTLAND, EUGENE C. & S. MKADDEM, "Fine structure of defects in radial nematic droplets", Phys. Rev. E 62 (2000), p. 6694-6705.
- [17] P.-G. DE GENNES & J. PROST, The Physics of Liquid Crystals, International Series of Monographs on Physics, vol. 83, Clarendon Press, 1993.
- [18] R. HARDT, D. KINDERLEHRER & F.-H. LIN, "Existence and partial regularity of static liquid crystal configurations", Commun. Math. Phys. 105 (1986), p. 547-570.
- [19] R. HARDT & F.-H. LIN, "A remark on H<sup>1</sup> mappings", Manuscr. Math. 56 (1986), p. 1-10.
- [20] D. HENAO, A. MAJUMDAR & A. PISANTE, "Uniaxial versus biaxial character of nematic equilibria in three dimensions", *Calc. Var. Partial Differ. Equ.* 56 (2017), no. 2, article no. 55 (22 pages).
- [21] 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), no. 5, p. 3390-3425.
- [22] ——, "Stability of the melting hedgehog in the Landau-de Gennes theory of nematic liquid crystals", Arch. Ration. Mech. Anal. 215 (2015), no. 2, p. 633-673.
- [23] M. KLÉMAN, "Defects in liquid crystals", Rep. Prog. Phys. 52 (1989), p. 267-311.
- [24] S. KRALJ & E. G. VIRGA, "Universal fine structure of nematic hedgehogs", J. Phys. A, Math. Gen. 34 (2001), no. 4, p. 829-838.
- [25] S. KRALJ, E. G. VIRGA & S. ŽUMER, "Biaxial torus around nematic point defects", *Phys. Rev. E* 60 (1999), p. 1858-1866.

- [26] X. LAMY, "Uniaxial symmetry in nematic liquid crystals", Ann. Inst. Henri Poincaré, Anal. Non Linéaire 32 (2015), no. 5, p. 1125-1144.
- [27] O. D. LAVRENTOVICH, P. PASINI, C. ZANNONI & S. ŽUMER (eds.), Defects in Liquid Crystals: Computer Simulations, Theory and Experiments, NATO Science Series II: Mathematics, Physics and Chemistry, vol. 43, Springer, 2012.
- [28] JR. LAWSON, H. BLAINE, "Surfaces minimales et la construction de Calabi-Penrose", in Séminaire Bourbaki 1983/84, Astérisque, vol. 121-122, Société Mathématique de France, 1985, p. 197-211.
- [29] L. LEMAIRE, "Applications harmoniques de surfaces Riemanniennes", J. Differ. Geom. 13 (1978), p. 51-78.
- [30] F.-H. LIN, "On nematic liquid crystals with variable degree of orientation", Commun. Pure Appl. Math. 44 (1991), no. 4, p. 453-468.
- [31] F.-H. LIN & C. WANG, The analysis of harmonic maps and their heat flows, World Scientific, 2008.
- [32] S. ŁOJASIEWICZ, "Une propriété topologique des sous-ensembles analytiques réels", in Les Équations aux Dérivées Partielles (Paris, 1962), Colloques internat., vol. 117, Éditions du Centre National de la Recherche Scientifique, 1962, p. 87-89.
- [33] S. LUCKHAUS, "Partial Hölder Continuity for Minima of Certain Energies among Maps into a Riemannian Manifold", Indiana Univ. Math. J. 37 (1988), no. 2, p. 349-367.
- [34] I. F. LYUKSYUTOV, "Topological instability of singularities at small distances in nematics", *Zh. Eksp. Teor. Fiz* **75** (1978), p. 358-360.
- [35] A. MAJUMDAR, "The radial-hedgehog solution in Landau-de Gennes theory for nematic liquid crystals", Eur. J. Appl. Math. 23 (2012), no. 1, p. 61-97.
- [36] A. MAJUMDAR & A. ZARNESCU, "Landau-De Gennes Theory of Nematic Liquid Crystals: the Oseen-Frank Limit and Beyond", Arch. Ration. Mech. Anal. 196 (2010), no. 1, p. 227-280.
- [37] C. B. J. MORREY, Multiple integrals in the calculus of variations, Grundlehren der Mathematischen Wissenschaften, vol. 130, Springer, 1966.
- [38] N. J. MOTTRAM & C. J. P. NEWTON, "Introduction to Q-tensor theory", https: //arxiv.org/abs/1409.3542, 2014.
- [39] E. PENZENSTADLER & H.-R. TREBIN, "Fine structure of point defects and soliton decay in nematic liquid crystals", J. Phys. France 50 (1989), p. 1027-1040.
- [40] C. SCHEVEN, "Variationally harmonic maps with general boundary conditions: boundary regularity", Calc. Var. Partial Differ. Equ. 25 (2006), no. 4, p. 409-429.
- [41] R. M. SCHOEN, "Analytic aspects of the harmonic map problem", in Seminar on nonlinear partial differential equations (Berkeley, Calif., 1983), Mathematical Sciences Research Institute Publications, vol. 2, Springer, 1983, p. 321-358.
- [42] R. M. SCHOEN & K. UHLENBECK, "A regularity theory for harmonic maps", J. Differ. Geom. 17 (1982), p. 307-335.
- [43] , "Boundary regularity and the Dirichlet problem for harmonic maps", J. Differ. Geom. 18 (1983), p. 253-268.
- [44] , "Regularity of minimizing harmonic maps into the sphere", *Invent. Math.* **78** (1984), p. 89-100.
- [45] L. SIMON, Theorems on Regularity and Singularity of Energy Minimizing Maps, Lectures in Mathematics, Birkhäuser, 2012.
- [46] E. G. VIRGA, Variational theories for liquid crystals, Applied Mathematics and Mathematical Computation, vol. 8, CRC Press, 1995.