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Biaxial escape in nematics at low temperature

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ABSTRACT

In the present work, we study minimizers of the Landau–de Gennes free energy in a bounded domain $\Omega \subset \mathbb{R}^3$. We prove that at low temperature minimizers do not vanish, even for topologically non-trivial boundary conditions. This is in contrast with a simplified Ginzburg–Landau model for superconductivity studied by Bethuel, Brezis and Hélein. Merging this with an observation of Canevari we obtain, as a corollary, the occurrence of *biaxial escape*: the tensorial order parameter must become strongly biaxial at some point in Ω. In particular, while it is known that minimizers cannot be purely uniaxial, we prove the much stronger and physically relevant fact that they lie in a different homotopy class.

1. Introduction

Nematic liquid crystals are composed of rigid rod-like molecules which tend to align in a preferred direction. As a result of this orientational order, nematics present electromagnetic properties similar to those of crystals. A striking feature of nematics is the appearance of particular optical textures called *defects*. From the mathematical point

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of view, the study of these defects is carried out using a tensorial order parameter Q (introduced by P.G. de Gennes [4]). The Q-tensor takes values in the five-dimensional space

$$\mathcal{S} = \left\{Q \in \mathbb{R}^{3\times 3} \colon Q_{ij} = Q_{ji},\ \operatorname{tr} Q = 0\right\}, \tag{1}$$

of symmetric traceless 3×3 matrices. Endowing $\mathcal{S}$ with the usual euclidean norm

$$|Q|^2 = \operatorname{tr}(Q^2)$$

will allow us to identify $\mathcal{S}$ isometrically with $\mathbb{R}^5$. As a symmetric matrix, a Q-tensor has an orthonormal frame of eigenvectors: the eigendirections are the locally preferred mean directions of alignment of the molecules, and the eigenvalues measure the degrees of alignment along those directions. In this context, *uniaxial* states are described by Q-tensors with two equal eigenvalues, and *biaxial* states correspond to Q-tensors with three distinct eigenvalues.

The configuration of a nematic material contained in a domain $\Omega \subset \mathbb{R}^3$ is given by a map $Q \colon \Omega \to \mathcal{S}$. At equilibrium, Q should minimize the Landau–de Gennes free energy given by

$$F_T(Q) = \int_\Omega \left(\frac{L}{2}|\nabla Q|^2 + f_T(Q)\right) dx. \tag{2}$$

Here L is an elastic constant and $f_T(Q)$ is the bulk free energy density, usually considered to be of the form

$$f_T(Q) = \frac{\alpha(T - T_*)}{2}|Q|^2 - \frac{b}{3}\operatorname{tr}(Q^3) + \frac{c}{4}|Q|^4. \tag{3}$$

Above α, b and c are material-dependent positive constants, T is the absolute temperature and T_* a critical temperature. For $T < T_*$, the bulk free energy density $f_T(Q)$ attains its minimum exactly on the vacuum manifold $\mathcal{N}_T \subset \mathcal{S}$ composed of uniaxial Q-tensors with a certain fixed norm:

$$\begin{aligned} \mathcal{N}_T &= \left\{Q \in \mathcal{S} \colon Q = s_*\left(n \otimes n - \frac{1}{3}I\right),\ n \in \mathbb{S}^2\right\}, \\ s_* &= s_*(T) = \frac{b + \sqrt{b^2 - 24\alpha(T - T_*)c}}{4c}. \end{aligned} \tag{4}$$

Above, the notation $n \otimes n$ denotes the matrix $(n_i n_j)$. Note that $\mathcal{N}_T$ is diffeomorphic to the projective plane $\mathbb{RP}^2$. In this work we consider minimizers of $F_T(Q)$ subject to Dirichlet boundary conditions $Q_{b,T} \colon \partial\Omega \to \mathcal{N}_T$ minimizing the potential $f_T(Q)$:

$$Q_{b,T}(x) = s_*\left(n_b(x) \otimes n_b(x) - \frac{1}{3}I\right), \quad n_b \colon \partial\Omega \to \mathbb{S}^2. \tag{5}$$

In the London limit $L \to 0$, a minimizing Q-tensor must be close to an $\mathcal{N}_T$-valued harmonic map Q_*, that is a minimizer of the Dirichlet energy among maps with values in the manifold $\mathcal{N}_T$. This is analogous to the case of the simplified Ginzburg–Landau energy with prescribed topologically nontrivial boundary conditions studied in [2]; in this setting it is proved that minimizers of the corresponding energy converge to harmonic maps with values in $\mathbb{S}^1$, which are then forced to have singularities, known in that context as vortices.

The singularities of the director field n_* associated to the limit of minimizers of $F_T(Q)$ correspond to the optical defects observed in experiments. In the core of a defect, two possible behaviours are considered in the physics literature. The notion of *isotropic melting* refers to a Q-tensor vanishing in the core of the defect. This is comparable to the behaviour observed in the core of Ginzburg–Landau vortices, and can be achieved by remaining in a uniaxial state. Alternatively, Q-tensors may take advantage of the additional degrees of freedom offered by biaxiality: instead of vanishing in the core of the defect, the Q-tensor order parameter may become strongly biaxial. This last behaviour is referred to as *biaxial escape* [22].

Biaxial escape has been first proposed as a way to avoid singularities of the director field by Lyuksyutov [12]. The corresponding mechanism has been investigated in greater detail by Penzenstadler and Trebin [17], followed by a number of further studies (see e.g. [22,18,16,8]). These works indicate that biaxial escape should be energetically favourable when the bulk free energy (3) degenerates to a Ginzburg–Landau-like potential, which occurs for instance at low temperature.

Our main result states that, at low temperatures, isotropic melting is indeed avoided: the minimizing configurations do not vanish.

Theorem 1.1. *Let $\Omega \subset \mathbb{R}^3$ be a smooth bounded simply connected domain. Let $n_b\colon \partial\Omega \to \mathbb{S}^2$ be a smooth director field and $Q_{b,T}\colon \partial\Omega \to \mathcal{N}_T$ the associated boundary datum (5). Let Q_T be a solution of the variational problem*

$$\min\left\{F_T(Q)\colon Q \in H^1(\Omega;\mathcal{S}),\ Q = Q_{b,T} \text{ on } \partial\Omega\right\},$$

where F_T is the Landau–de Gennes free energy (2). Then, there exists $T_0 \in \mathbb{R}$ (depending on Ω, L, α, b, c), such that if $T < T_0$,

$$\inf_{\Omega} |Q_T| > 0,$$

i.e. Q_T does not vanish in Ω.

To prove Theorem 1.1, we use the fact that any zero x_T of Q_T must converge, as $T \to -\infty$, to a point $x_0 \in \Omega$; this follows from the analysis in [14]. After this, we take advantage of the degeneracy of the bulk potential to a Ginzburg–Landau potential in the low temperature limit. The Ginzburg–Landau potential $f_{GL}(Q) = (1 - |Q|^2)^2$ being minimized by $\mathbb{S}^4$-valued maps, we are able to relate Q_T to an $\mathbb{S}^4$-valued harmonic map. This is done through a blow-up analysis of Q_T at x_T which in turn leads to a local minimization problem in $\mathbb{R}^3$ for a limiting map Q_∞. Next, thanks to the study in [15] based on the work of Lin and Wang [10], a blow-down analysis of the limiting map using the minimality of Q_∞ yields strong convergence to a harmonic map with values in $\mathbb{S}^4$. The conclusion follows with the help of a regularity result for minimizing harmonic maps by Schoen and Uhlenbeck [21].

Next we explain how Theorem 1.1 is related to the phenomenon of biaxial escape. Of course, Theorem 1.1 is more interesting when the boundary condition n_b is topologically non-trivial. In that case, a recent remark of Canevari [3, Lemma 3.10] shows that the only way for Q_T to avoid vanishing is to be *strongly* biaxial. To give a precise meaning to this statement, we recall the definition of the biaxiality parameter for a Q-tensor,

$$\beta(Q) = 1 - 6\frac{(\mathrm{tr}(Q^3))^2}{|Q|^6}, \tag{6}$$

introduced in [7]. It holds that $0 \leq \beta(Q) \leq 1$, and Q is uniaxial for $\beta = 0$, biaxial for $\beta > 0$ and is said to be *maximally biaxial* for $\beta = 1$. Canevari's lemma implies the following corollary to our main result:

Corollary 1.2. *If the boundary datum $n_b\colon \partial\Omega \to \mathbb{S}^2$ is topologically non-trivial, then for low enough temperatures $T < T_0$, any minimizing configuration Q_T must be strongly biaxial:*

$$\beta(Q_T(x_0)) = 1$$

for some $x_0 \in \Omega$.

In fact, in [3] Canevari uses the aforementioned lemma to prove a theorem similar to Corollary 1.2, in the case of a two-dimensional domain. Our result is a three-dimensional analog of [3, Theorem 1.1], and could probably be adapted to provide a simpler proof of [3, Theorem 1.1].

Corollary 1.2 generalizes a recent result by Henao, Majumdar and Pisante [13]. In [13], the authors show that for low enough temperature, minimizers can not be purely uniaxial (that is, can not satisfy $\beta = 0$ everywhere). Note that this result does not exclude the existence of approximately uniaxial minimizers, which would satisfy $\beta \sim 0$ throughout Ω. On the other hand, Canevari's lemma shows that these configurations are not homotopically equivalent to those that satisfy the conclusion of Corollary 1.2 (see § 5 for more details). Thus, our main result settles the question of the essentially non-uniaxial nature of minimizers in the $T \to 0$ limit.

To further clarify the biaxial vs uniaxial discussion we remark that results of the second author in [9] indicate that the uniaxiality constraint is very rigid: non-existence of purely uniaxial solutions may not be specific to low temperature or energy minimization. In contrast, Corollary 1.2 is really specific to the low temperature limit.

The article is organized as follows. In Section 2 we reformulate the problem and recall some basic convergence properties of minimizers of F_T. In Section 3 we study the blown-up problem, obtain a limiting map and derive its minimal character. In Section 4 we conclude the proof of Theorem 1.1 with the aid of a blow-down analysis. Finally, in Section 5 we prove Corollary 1.2 and make some final remarks.

2. Properties of minimizing Q-tensors

2.1. Rescaling

Introducing the reduced temperature t and rescaled maps $\widetilde{Q}$:

$$t := \frac{-\alpha(T - T_*)c}{b^2}, \quad \widetilde{Q} := \frac{1}{s_*}\sqrt{\frac{3}{2}}Q,$$

we see that, for some constant $K = K(\alpha, b, c, T)$ which plays no role in the sequel,

$$F_T(Q) = \frac{s_*^2 b^2}{3c} \int\limits_\Omega \left(\frac{\widetilde{L}}{2}|\nabla\widetilde{Q}|^2 + \frac{t}{2}(|\widetilde{Q}|^2 - 1)^2 + \lambda(t)\, h(\widetilde{Q}) \right) dx \ + K,$$

where $\widetilde{L} = 3cL/b^2$,

$$\lambda(t) = \frac{\sqrt{24t+1}+1}{12} \underset{t\to+\infty}{\sim} \sqrt{\frac{t}{6}}, \tag{7}$$

and

$$h(\widetilde{Q}) = \frac{1}{6} - \frac{2\sqrt{2}}{\sqrt{3}}\mathrm{tr}(\widetilde{Q}^3) + \frac{1}{2}|\widetilde{Q}|^4. \tag{8}$$

It holds that $h(Q) \geq 0$ for every $Q \in \mathcal{S}$, and the potential h vanishes exactly at

$$\widetilde{\mathcal{N}} = \left\{ \sqrt{\frac{3}{2}}\left(n\otimes n - \frac{1}{3}I \right) : n \in \mathbb{S}^2 \right\}. \tag{9}$$

The limit $T \to -\infty$ corresponds to $t \to +\infty$. Therefore we may reformulate the problem: show that minimizers Q_t of the energy functional

$$\widetilde{F}_t(Q) = \int\limits_\Omega \left(\frac{\widetilde{L}}{2}|\nabla Q|^2 + \frac{t}{2}(|Q|^2 - 1)^2 + \lambda(t)\, h(Q) \right) dx \tag{10}$$

subject to the boundary condition

$$Q_t = \widetilde{Q}_b = \sqrt{\frac{3}{2}}\left(n_b \otimes n_b - \frac{1}{3}I\right) \quad \text{on } \partial\Omega, \tag{11}$$

do not vanish for large enough t.

We prove Theorem 1.1 by contradiction: we assume the existence of sequences $t_j \to +\infty$ and $(x_j) \subset \Omega$ such that Q_{t_j} minimizes (10)–(11) and $Q_{t_j}(x_j) = 0$. Note that any minimizer of $\widetilde{F}_t$ is smooth thanks to standard elliptic estimates (see e.g. [14, Proposition 13]), so that evaluation at x_j makes sense. Up to extracting a subsequence, we may assume in addition that $x_j \to x_* \in \overline{\Omega}$.

In the sequel we study the behaviour of the sequence (Q_{t_j}) and obtain a contradiction. To simplify the notations, we drop the subscript j: we write (Q_t) and (x_t) and it is always implied that a subsequence is considered.

2.2. Convergence

Since the set $H^1_{n_b}(\Omega;\mathbb{S}^2) = \{n \in H^1(\Omega;\mathbb{S}^2)\colon n_{|\partial\Omega} = n_b\}$ is not empty (see e.g. [5, Lemma 1.1]), we may use an $\widetilde{\mathcal{N}}$-valued comparison map and obtain the bound

$$\widetilde{F}_t(Q_t) = \int_\Omega \left(\frac{\widetilde{L}}{2}|\nabla Q_t|^2 + \frac{t}{2}(|Q_t|^2 - 1)^2 + \lambda(t)\, h(Q_t)\right) dx \le C. \tag{12}$$

In particular, we see that the sequence (Q_t) is bounded in $H^1(\Omega;\mathcal{S})$. Up to extracting a subsequence, we may therefore assume that Q_t converges weakly to a limiting map $Q_* \in H^1(\Omega;\mathcal{S})$ with $Q_* = Q_b$ on $\partial\Omega$. Moreover, since the bound (12) implies

$$\int_\Omega h(Q_t) \le C\lambda(t)^{-1} \sim C\sqrt{\frac{6}{t}},$$

we deduce that $h(Q_*) = 0$ a.e., so that Q_* is $\widetilde{\mathcal{N}}$-valued. From this point on, we can proceed as in [14, Lemma 3]. We conclude that Q_t converges to Q_* strongly in H^1 and Q_* is an $\widetilde{\mathcal{N}}$-valued harmonic map.[1] In particular, Q_* is smooth in $\Omega \setminus \Sigma$, where $\Sigma \subseteq \Omega$ is a finite set of interior point singularities [19,20].

As in the Ginzburg–Landau case [1], the convergence of Q_t towards Q_* can be improved away from the singularities Σ. The arguments in [1] have been adapted to the liquid crystal case in [14]. The asymptotic regime $L \to 0$ in [14] corresponds to the limit $t \to +\infty$ in the present work. The arguments in [14, Proposition 4] and [14, Proposition 6] are straightforward to adapt, and we obtain the convergence

$$\frac{1}{2}(|Q_t|^2 - 1)^2 + \frac{\lambda(t)}{t}\, h(Q_t) \longrightarrow 0, \quad \text{locally uniformly in } \overline{\Omega} \setminus \Sigma.$$

[1] In fact, $Q_* = \sqrt{\frac{3}{2}}\left(n_* \otimes n_* - \frac{1}{3}I\right)$ where $n_* \in H^1(\Omega;\mathbb{S}^2)$ is a minimizing harmonic map.

Since we have in addition, thanks to the maximum principle, $|Q_t| \leq 1$ (cf. e.g. [14, Proposition 3]), we deduce – using also (7) – that

$$|Q_t| \longrightarrow 1 \quad \text{locally uniformly in } \overline{\Omega} \setminus \Sigma. \tag{13}$$

Recall that by assumption, $Q_t(x_t) = 0$ for a sequence $x_t \to x_* \in \overline{\Omega}$. The uniform convergence (13) away from Σ implies that $x_* \in \Sigma$. In particular x_* lies well inside Ω. Our next step will consist in "blowing up" around x_t.

3. Blowing up

We fix $\delta > 0$ such that $B(x_t, \delta) \subset \Omega$ for all j. We consider the blown-up maps

$$\overline{Q}_t(x) = Q_t\left(x_t + \frac{x}{\sqrt{t}}\right), \quad x \in B_{\delta\sqrt{t}}.$$

The map $\overline{Q}_t$ minimizes the energy functional

$$E_t(Q; B_{\delta\sqrt{t}}) = \int_{B_{\delta\sqrt{t}}} \left(\frac{\widetilde{L}}{2}|\nabla Q|^2 + \frac{1}{2}(|Q|^2 - 1)^2\right) dx + \frac{\lambda(t)}{t} \int_{B_{\delta\sqrt{t}}} h(Q)\, dx, \tag{14}$$

with respect to its own boundary conditions. Fix any $R > 0$. For large enough t, $\overline{Q}_t$ is defined in B_R and solves the Euler–Lagrange equation

$$\widetilde{L}\Delta\overline{Q}_t = 2(|\overline{Q}_t|^2 - 1)\overline{Q}_t + \frac{\lambda(t)}{t}\nabla h(\overline{Q}_t).$$

The uniform bound $|\overline{Q}_t| \leq 1$ and standard elliptic estimates thus imply

$$|\nabla\overline{Q}_t| \leq C_R \quad \text{in } B_R,$$

where C_R is a constant that may depend on R but not on t. Therefore, up to extracting a subsequence, we may assume that $\overline{Q}_t$ converges locally uniformly, and weakly in H^1_{loc}, to a map $Q_\infty \in H^1_{\mathrm{loc}}(\mathbb{R}^3; \mathcal{S})$. Moreover, since the convergence is locally uniform, Q_∞ is continuous and satisfies

$$Q_\infty(0) = 0. \tag{15}$$

We claim that Q_∞ locally minimizes a Ginzburg–Landau energy:

Lemma 3.1. *For all $R > 0$, the limiting profile Q_∞ minimizes the energy functional*

$$E(Q; B_R) = \int_{B_R} \left(\frac{\widetilde{L}}{2}|\nabla Q|^2 + \frac{1}{2}(|Q|^2 - 1)^2\right) dx, \tag{16}$$

with respect to its own boundary condition.

Proof. Let $P \in H_0^1(B_R; \mathcal{S})$. Since $\overline{Q}_t$ is minimizing, it holds

$$0 \leq E_t(\overline{Q}_t + P; B_R) - E_t(\overline{Q}_t; B_R)$$

By elliptic regularity, $\overline{Q}_t$ converges to Q_∞ in C^1_{loc}, which then implies that

$$0 \leq E(Q_\infty + P; B_R) - E(Q_\infty; B_R),$$

as well by taking the limit $t \to +\infty$. Therefore Q_∞ minimizes (16), as claimed. □

Moreover, proceeding exactly as in the proof of [13, Theorem 1.(v)], we obtain the energy bound:

Lemma 3.2. *([13]) There exists $C > 0$ such that*

$$E(Q_\infty; B_R) \leq CR, \tag{17}$$

for all $R > 0$.

The bound (17) follows from two main ingredients: an energy monotonicity inequality for minimizers of (14) [14, Lemma 2], and an energy bound for $\mathbb{S}^2$-valued minimizing harmonic maps near their singularities (following from the energy monotonicity for minimizing harmonic maps, see e.g. [11, Lemma 2.2.5]).

4. Blowing down, proof of Theorem 1.1 completed

Our last step consists in "blowing down" Q_∞ around the origin, and eventually reaching a contradiction with (15). Let B_1 be the unit ball in $\mathbb{R}^3$. We consider the blown-down maps

$$\underline{Q}_R(x) = Q_\infty(Rx), \quad x \in B_1.$$

Note that (15) implies that

$$\underline{Q}_R(0) = 0, \quad \forall R > 0. \tag{18}$$

By definition, $\underline{Q}_R \in H^1(B_1)$ for all $R > 0$. We have:

Lemma 4.1. *Up to a subsequence,*

$$\underline{Q}_R \longrightarrow \underline{Q} \quad \text{in } H^1(B_1; \mathcal{S}),$$

for some $\mathbb{S}^4$-valued harmonic map $\underline{Q}$. Moreover, $|\underline{Q}_R| \longrightarrow 1$ uniformly in B_1.

Proof. Since Q_∞ minimizes (16), the map $\underline{Q}_R$ minimizes the energy functional

$$G_R(Q) = \int_{B_1} \left(\frac{\widetilde{L}}{2} |\nabla Q|^2 + \frac{R^2}{2} (|Q|^2 - 1)^2 \right) dx. \tag{19}$$

Moreover, the energy bound (17) implies the bound

$$G_R(\underline{Q}_R) \leq C, \tag{20}$$

so that we may extract a subsequence $R \to +\infty$ (indices are implicit), such that

$$\underline{Q}_R \longrightarrow \underline{Q} \quad \text{weakly in } H^1(B_1; \mathcal{S}). \tag{21}$$

The energy bound (20) also implies that $\underline{Q}$ is $\mathbb{S}^4$-valued. Now, thanks to Lemma 3.1, we can appeal to Proposition 4.2 in [15] to conclude that the convergence of $\underline{Q}_R$ to $\underline{Q}$ can be improved to strong convergence in H^1. In [15], the proof relies on [10, Theorem C] in the case of $\mathbb{R}^3$-valued maps converging to $\mathbb{S}^2$-valued maps. However, [10, Theorem C] is valid in greater generality and applies to our case. Moreover, the analysis in [15] does not make use of the dimension of the target space other than to provide an explicit constant in their computations.

Next, the minimizing character of $\underline{Q}$ follows from Step 1 in [15, Corollary 4.1], which also applies to our case without modifications. From this we conclude that $\underline{Q}$ is an $\mathbb{S}^4$-valued minimizing harmonic map. As a consequence, Schoen and Uhlenbeck's regularity result [21, Theorem 2.7] ensures that $\underline{Q}$ is smooth in B_1.

Since the proof of [15, Proposition 4.2] also shows that the convergence of $\underline{Q}_R$ towards $\underline{Q}$ is actually uniform away from the singularities of $\underline{Q}$, we obtain in particular that

$$|\underline{Q}_R| \longrightarrow 1 \quad \text{uniformly in } B_1, \tag{22}$$

which is the desired conclusion. □

We note that (22) contradicts (18) and thus the proof of Theorem 1.1 is complete. □

5. Proof of Corollary 1.2

In [3], Canevari makes the crucial observation that if Q is almost uniaxial, i.e.

$$\max_{\overline{\Omega}} \beta(Q) < 1, \tag{23}$$

then the Q-tensor must vanish. More precisely, in our case the following result holds.

Lemma 5.1. *([3, Lemma 3.11]) Let $Q \in C^1(\overline{\Omega}; \mathcal{S})$ with uniaxial boundary condition of the form (5). If $n_b \colon \partial\Omega \to \mathbb{S}^2$ is topologically non-trivial and (23) holds, then*

$$\min_{\overline{\Omega}} |Q| = 0.$$

In [3] the proof is carried out in the two-dimensional case but a careful reading shows that the argument still holds in the three-dimensional setting, since the result relies only on topological considerations in the target space $\mathcal{S}$. Indeed, the crucial observation leading to [3, Lemma 3.11] is the fact that, for any large C and small $\delta > 0$, the set

$$\{Q \in \mathcal{S} \colon \delta \le |Q| \le C, \ \beta(Q) \le 1 - \delta\} \subset \mathcal{S}$$

has two connected components, both topologically equivalent to $\mathcal{N}_T$, and exactly one component intersects $\mathcal{N}_T$.

As a consequence of Theorem 1.1 we see that, in light of Lemma 5.1, Q_T must be maximally biaxial at some point for sufficiently low temperature. The proof of Corollary 1.2 is complete. □

We finish with a few remarks. Theorem 1.1 implies the existence of a point where maximal biaxiality is achieved, however it does not provide a characterization of the location of this (or these) point(s) in terms of the domain or the boundary datum. Also the number of these points of biaxial escape cannot be deduced from the topological conclusion in [3, Lemma 3.11]. To finish, a more detailed description of the defect core is also an interesting matter worthy of pursuit. In this last direction, we mention the stability study of the radial hedgehog defect performed in [6].

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