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Biaxial escape in nematics at low temperature

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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 $f_T(Q)$:

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