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Remarks on uniaxial solutions in the Landau–de Gennes theory

Apala Majumdar [a,*], Yiwei Wang [b]

[a] *Department of Mathematical Sciences, University of Bath, Bath BA2 7AY, UK*
[b] *School of Mathematical Sciences, Peking University, Beijing 100871, China*

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ABSTRACT

We study uniaxial solutions of the Euler–Lagrange equations for a Landau–de Gennes free energy for nematic liquid crystals, with a fourth order bulk potential, with and without elastic anisotropy. These uniaxial solutions are characterised by a director and a scalar order parameter. In the elastic isotropic case, we show that (i) all uniaxial solutions, with a director field of a certain specified symmetry, necessarily have the radial-hedgehog structure modulo an orthogonal transformation, (ii) the "escape into third dimension" director cannot correspond to a purely uniaxial solution of the Landau–de Gennes Euler–Lagrange equations and we do not use artificial assumptions on the scalar order parameter and (iii) we use the structure of the Euler–Lagrange equations to exclude non-trivial uniaxial solutions with $\mathbf{e}_z$ as a fixed eigenvector i.e. such uniaxial solutions necessarily have a constant eigenframe. In the elastic anisotropic case, we prove that all uniaxial solutions of the corresponding "anisotropic" Euler–Lagrange equations, with a certain specified symmetry, are strictly of the radial-hedgehog type, i.e. the elastic anisotropic case enforces the radial-hedgehog structure (or the degree +1-vortex structure) more strongly than the elastic isotropic case and the associated partial differential equations are technically far more difficult than in the elastic isotropic case.

1. Introduction

Nematic liquid crystals are classical examples of mesophases intermediate in physical character between conventional solids and liquids [6,20]. Nematics are often viewed as complex liquids with long-range orientational order or distinguished directions of preferred molecular alignment, referred to as directors in the literature. The orientational anisotropy of nematics makes them the working material of choice for a range of optical devices, notably they form the backbone of the multi-billion dollar liquid crystal display industry.

Continuum theories for nematics are well-established in the literature and we work within the powerful Landau–de Gennes (LdG) theory for nematic liquid crystals. The LdG theory describes the nematic phase

* Corresponding author.
E-mail addresses: A.Majumdar@bath.ac.uk (A. Majumdar), yiweiwang@pku.edu.cn (Y. Wang).

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by a macroscopic order parameter, the **Q**-tensor order parameter that describes the orientational anisotropy in terms of the preferred directions of alignment and "scalar order parameters" that measure the degree of order about these directions. Mathematically, the **Q**-tensor is a symmetric, traceless 3×3 matrix, with five degrees of freedom [6,20], i.e.

$$\mathbf{Q} \in \mathcal{S} = \left\{ \mathbf{Q} \in M^{3\times3}(\mathbb{R}) \mid \mathbf{Q} = \mathbf{Q}^{\mathrm{T}}, \operatorname{tr}(\mathbf{Q}) = 0 \right\}. \tag{1.1}$$

A nematic phase is said to be (i) *isotropic* if $\mathbf{Q} = 0$, (ii) *uniaxial* if **Q** has two degenerate non-zero eigenvalues with a single distinguished eigenvector and (iii) *biaxial* if **Q** has three distinct eigenvalues. In particular, if **Q** is uniaxial or isotropic, then

$$\mathbf{Q} \in \mathcal{U} = \left\{ s\left(\mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{I}}{3}\right) \;\middle|\; s \in \mathbb{R}, \quad \mathbf{n} \in \mathbb{S}^2 \right\}, \tag{1.2}$$

where **n** is the distinguished eigenvector with the non-degenerate eigenvalue, labelled as the "uniaxial" director, s is a scalar order parameter that measures the degree of order about **n**, and **I** is the 3×3 identity matrix [17]. The eigenvalues of the uniaxial **Q** are $\frac{2s}{3}, -\frac{s}{3}, -\frac{s}{3}$ respectively and $s = 0$ describes a locally isotropic point. The uniaxial **Q**-tensor only has three degrees of freedom and the mathematical analysis of uniaxial **Q**-tensors has strong analogies with Ginzburg–Landau theory, since we can treat uniaxial **Q**-tensors as $\mathbb{R}^3 \to \mathbb{R}^3$ maps [17].

As with most variational theories in materials science, the experimentally observed equilibria are modelled by either global or local minimizers of a LdG energy functional [6,19,20]. The LdG energy typically comprises an elastic energy and a bulk potential; the elastic energy penalizes spatial inhomogeneities and the bulk potential dictates the isotropic-nematic phase transition as a function of the temperature [19,20]. There are several forms of the elastic energy; the Dirichlet energy is referred to as the "isotropic" or "one-constant" elastic energy and elastic energies with multiple elastic constants are labelled as "anisotropic" in the sense that they have different energetic penalties for different characteristic deformations [5]. These equilibria are classical solutions of the associated Euler–Lagrange equations, which are a system of five elliptic, non-linear partial differential equations for reasonable choices of the elastic constants [5]. We study and classify uniaxial solutions with either specified symmetries or certain properties in this paper i.e. can we give a complete characterization of uniaxial solutions of the LdG Euler–Lagrange equations for certain model problems, under certain restrictions on either the director field or the eigenframe of the uniaxial solution? We treat the isotropic and anisotropic cases separately. The classification of all uniaxial solutions of the LdG Euler–Lagrange equations is a highly non-trivial analytic question; uniaxial **Q**-tensors only have three degrees of freedom and to date, there are few explicit examples of uniaxial solutions for this highly coupled system. Our results are forward steps in this challenging study.

Our computations build on the results in [17] and [15], although both papers focus on the elastic isotropic case. In the paper [17], the author derives the governing partial differential equations for the order parameter s and three-dimensional director field, **n** in (1.2) in the one-constant LdG case and studies uniaxial minimizers (if they exist) of the corresponding energy functional in a certain asymptotic limit. In [15], the author addresses some general questions about the existence of uniaxial solutions for the one-constant LdG Euler–Lagrange equations. The author derives an "extra equation" that needs to be satisfied by the director in "non-isotropic" regions; this equation heavily constrains uniaxial equilibria. The author further shows that if the uniaxial solution is invariant in a given direction, then the uniaxial director is necessarily constant in every connected component of the domain; we refer to such uniaxial solutions as "trivial" uniaxial solutions. In [15], the author proves that for the model problem of a spherical droplet with radial boundary conditions, the "radial-hedgehog" solution is the unique uniaxial equilibrium for all temperatures, for a one-constant elastic energy density. The radial-hedgehog solution is analogous to the degree +1 vortex in the Ginzburg–Landau theory for superconductivity [2]; the director field **n** is simply the radial unit-vector