

A novel Landau-de Gennes model with quartic elastic terms†

DMITRY GOLOVATY¹, MICHAEL NOVACK² and PETER STERNBERG²

¹*Department of Mathematics, University of Akron, Akron, OH 44325, USA*
email: dmitry@uakron.edu

²*Department of Mathematics, Indiana University, Bloomington, IN 47405, USA*
emails: mrnovack@indiana.edu; sternber@indiana.edu

(Received 19 June 2019; revised 21 February 2020; accepted 27 February 2020; first published online 24 March 2020)

Within the framework of the generalised Landau-de Gennes theory, we identify a Q -tensor-based energy that reduces to the four-constant Oseen–Frank energy when it is considered over orientable uniaxial nematic states. Although the commonly considered version of the Landau-de Gennes theory has an elastic contribution that is at most cubic in components of the Q -tensor and their derivatives, the alternative offered here is quartic in these variables. One clear advantage of our approach over the cubic theory is that the associated minimisation problem is well-posed for a significantly wider choice of elastic constants. In particular, this quartic energy can be used to model nematic-to-isotropic phase transitions for highly disparate elastic constants. In addition to proving well-posedness of the proposed version of the Landau-de Gennes theory, we establish a rigorous connection between this theory and its Oseen–Frank counterpart via a Γ -convergence argument in the limit of vanishing nematic correlation length. We also prove strong convergence of the associated minimisers.

Key words: Nematic liquid crystal, Gamma-convergence, Landau-de Gennes theory, Q -tensor, disparate elastic constants, nematic-to-isotropic phase transition

2010 Mathematics Subject Classification: 35J50, 35B36, 49K20, 76A15

1 Introduction

Two well-regarded and heavily researched mathematical models for nematic liquid crystals are the director-based Oseen–Frank model [14, 31, 32, 34] and the Q -tensor-based Landau-de Gennes theory [9, 10, 29, 32]. In this article, we present a version of Landau-de Gennes which enables us to make a rigorous and relatively simple asymptotic connection between the two theories in the limit of Landau-de Gennes with vanishing non-dimensional nematic correlation length. In [28], the authors carry out such a program in the so-called ‘equal-constants’ setting where the elastic energy of both models is given by the Dirichlet integral. Here, we identify an elastic energy density involving certain terms that are quartic in the Q -tensor and its derivatives such that the corresponding Landau-de Gennes energy approaches, in the sense of Γ -convergence, the full Oseen–Frank energy.

† D. G. acknowledges the support from NSF DMS-1729538. M. N. and P. S. acknowledge the support from a Simons Collaboration grant 585520.

We recall now the form of the Oseen–Frank energy,

$$F_{OF}(n) := \int_{\Omega} \left(\frac{K_1}{2} (\operatorname{div} n)^2 + \frac{K_2}{2} ((\operatorname{curl} n) \cdot n)^2 + \frac{K_3}{2} |(\operatorname{curl} n) \times n|^2 + \frac{K_2 + K_4}{2} (\operatorname{tr} (\nabla n)^2 - (\operatorname{div} n)^2) \right) dx, \tag{1.1}$$

where K_1, K_2, K_3 and K_4 are material constants, $\Omega \subset \mathbb{R}^3$ represents the sample domain and the director n maps Ω to \mathbb{S}^2 .

We also recall the standard Landau-de Gennes model defined for $Q : \Omega \rightarrow \mathcal{S}$, where

$$\mathcal{S} := \{Q \in M^{3 \times 3} : Q^T = Q, \operatorname{tr} Q = 0\}.$$

It is given by

$$F_{LdG}(Q) := \int_{\Omega} \left(\frac{L_1}{2} |\nabla Q|^2 + \frac{L_2}{2} Q_{ij,j} Q_{ik,k} + \frac{L_3}{2} Q_{ik,j} Q_{ij,k} + W(Q) \right) dx, \tag{1.2}$$

where $Q_{ij,k} = \partial Q_{ij} / \partial x_k$ and repeated indices are summed from one to three. Here, the bulk Landau-de Gennes energy density is

$$W(Q) := a \operatorname{tr} (Q^2) - \frac{2b}{3} \operatorname{tr} (Q^3) + \frac{c}{2} (\operatorname{tr} (Q^2))^2, \tag{1.3}$$

cf. [16]. The coefficient a is temperature-dependent and, in particular, is negative for sufficiently low temperatures. Throughout this article, we will assume that we are in a temperature regime where $a < \frac{b^2}{27c}$, an inequality implying that Q -tensors in the minimal set \mathcal{N} of W are in a uniaxial nematic state describable in terms of a director as follows:

$$\mathcal{N} := \left\{ s_0 \left(n \otimes n - \frac{1}{3} \mathbf{I} \right) : n \in \mathbb{S}^2 \right\}. \tag{1.4}$$

Here, s_0 is given explicitly in terms of the coefficients a, b and c , and by subtracting an appropriate constant from W , one can take W to vanish along this minimal set. We will ignore this constant and simply assume without loss of generality that W vanishes along this minimal set of states.

The effort to find a connection between F_{OF} and a corresponding Q -tensor-based elastic energy has a long history, going back at least to [7] and includes the contributions of [11, 25, 30]. However, these studies are premised on the observation that one can obtain F_{OF} from a Q -tensor model for certain values of the elastic constants by adding to the standard Landau-de Gennes energy (1.2) an additional elastic term that is cubic in Q and its derivatives, namely,

$$\int_{\Omega} Q_{lk} \partial_k Q_{ij} \partial_l Q_{ij} dx.$$

As pointed out, for instance, in [2, p. 21], this choice represents one of the six possible linearly independent cubic terms that are quadratic in ∇Q and respect the necessary symmetries. From the standpoint of energy minimisation, unfortunately, such a version of Landau-de Gennes becomes problematic, since the inclusion of the cubic term leads to an energy which is unbounded from below [4]. Indeed, quoting [25], ‘In the presence of biaxial fluctuations the general third-order theory in $Q_{\alpha\beta}$ becomes unstable and thus is thermodynamically incorrect. One has to include higher-order terms (or neglect third-order ones) to preserve stability of the free energy’.

Alternatively, one can impose a constraint through a choice of bulk potential that penalises large Q and prevents the cubic elastic term(s) from overtaking the quadratic ones [4, 6, 13, 22].

Not surprisingly, this deficiency then also leads to instabilities in attempts to capture dynamics through the corresponding gradient flow. Along these lines, we mention the work of [21] where the authors overcome this impediment to obtain a dynamical well-posedness result under an assumption of sufficiently small initial data, while also showing blow-up for large initial data.

In contrast to these sizable troubles to be overcome when taking a cubic elastic energy density for Landau-de Gennes, we propose a version of Landau-de Gennes, in the spirit of the quotation from [25] above, involving a quartic elastic energy density that presents none of these technical difficulties. As usual, it is defined over the class \mathcal{S} . In a prototypical form, the energy is given by

$$\begin{aligned} \mathcal{F}_{LdG}(Q) := & \int_{\Omega} \left(\frac{L_1}{2} \left| \left(\frac{s_0}{3} \mathbf{I} + Q \right) \operatorname{div} Q \right|^2 + \frac{L_2}{2} \left| \left(\frac{s_0}{3} \mathbf{I} + Q \right) \operatorname{curl} Q \right|^2 \right. \\ & + \frac{L_3}{2} \left| \left(\frac{2s_0}{3} \mathbf{I} - Q \right) \operatorname{div} Q \right|^2 + \frac{L_4}{2} \left| \left(\frac{2s_0}{3} \mathbf{I} - Q \right) \operatorname{curl} Q \right|^2 \\ & \left. + W(Q) \right) dx. \end{aligned} \tag{1.5}$$

Here, the elastic constants $\{L_i\}$ are taken to be positive, and we assume W is still given by (1.3). We point out that our model is still *quadratic* in its dependence on the gradient of Q .

Before explaining how we arrive at \mathcal{F}_{LdG} , we want to be clear on our motivation for seeking such a version of Landau-de Gennes energy. Our criteria were

- For a reasonable range of elastic constants, one should be able to recover the four-term Oseen–Frank energy among uniaxial Q -tensors as in (1.4). This range should, in particular, allow for the regime of extreme disparity between the K_i s, since we wish to use the model to explore various types of liquid crystals for which some subset of the three deformations splay, twist and bend is far more favourable energetically than others. For example, we seek a model capable of capturing the formation of tactoids in nematic/isotropic phase transitions. (See e.g. [17, 18, 19].)
- Minimisation of \mathcal{F}_{LdG} via the direct method should be achievable, and in particular, the energy should be bounded from below and coercive.
- Any elastic terms should respect the necessary symmetries and so be selected from the list to be found, for example, in [24]. Among the quartic choices – that is, quadratic in both Q and ∇Q – there are 13 to work with.
- One should strive for as simple a choice as possible that meets the previous three criteria.

To arrive at \mathcal{F}_{LdG} , we begin by considering $Q \in \mathcal{N}$ where the corresponding director field n is sufficiently smooth. We show that each elastic term in the Oseen–Frank energy can be realised through projections of $\operatorname{div} Q$ and $\operatorname{curl} Q$ on n and on the plane perpendicular to n . This allows us to rewrite F_{OF} in terms of the divergence and curl of $Q \in \mathcal{N}$. We subsequently relax the constraint $Q(x) \in \mathcal{N}$ to allow biaxial states as well by assuming simply that Q takes values in \mathcal{S} and add $W(Q)$ to the elastic energy density to force energy minimising configurations to have values close to \mathcal{N} . While we certainly do not claim that our choice is unique, this version of Landau-de Gennes model leads to a variational problem that is well-posed under minimisation and rigorously reduces to F_{OF} in the limit of vanishing non-dimensional nematic correlation

length. Indeed, we feel that the resulting energy \mathcal{F}_{LdG} given in (1.5) meets all the criteria listed above.

Though in this article we do not address dynamics, in [17], we carry out computations in the context of an associated gradient flow in a thin film limit. The computations are performed for a director that lies in the plane of the film and in the regime where splay is heavily penalised, that is, where L_1 in \mathcal{F}_{LdG} is much larger than the other elastic coefficients. In doing so, we also pursue a temperature regime for the Landau-de Gennes potential W where both the nematic and isotropic states are preferable. We find nice agreement with certain experimentally observed morphologies associated with tactoid evolution and defect splitting. Indeed, this highlights another favourable feature of the energy \mathcal{F}_{LdG} , namely, that it allows one to model nematic/isotropic phase transitions in such a way that in the uniaxial nematic region, the energy agrees with Oseen–Frank.

We emphasise again that the model we propose here is not the only possible higher-order extension of the Landau-de Gennes elastic energy. Indeed, although we choose to retain up to quartic terms in Q , we neither explored all possible combinations of cubic and quartic elastic terms nor considered terms of even higher order. We conjecture nevertheless that, if one chooses to cut-off the expansion of the elastic energy at terms of an odd power in Q , the energy would not be bounded from below. Further, because we retain the standard version of the Landau-de Gennes potential, our expression for the Landau-de Gennes energy would still suffer from the usual deficiencies of the Landau-de Gennes approach at low temperatures [26, 27].

The plan of the paper is as follows. In Proposition 2.6, we show that for Q in the uniaxial minimising set given by (1.4), $\mathcal{F}_{LdG}(Q)$ reduces to precisely $F_{OF}(n)$ for a particular set of constants $\{L_i\}$ given in terms of $\{K_i\}$. More precisely, we can assert this equivalence when Q is orientable, in the sense that $Q \in H^1(\Omega, \mathcal{N})$ is representable as $Q = s_0(n \otimes n - I/3)$ for some ‘lifting’ $n \in H^1(\Omega; \mathbb{S}^2)$, a property that, in particular, always holds when Ω is taken to be simply connected, cf. [5]. After a non-dimensionalisation, leading to a dimensionless version of \mathcal{F}_{LdG} , namely \mathcal{F}_ε given in (3.4) below, we argue that this form of Landau-de Gennes is coercive over $H^1(\Omega; S)$, and weakly lower semicontinuous, making it well suited for minimisation via the direct method in the calculus of variations when a Dirichlet (strong anchoring) condition is imposed on $\partial\Omega$, cf. Theorem 3.3. As described at the outset of Section 3, the parameter ε appearing in the non-dimensionalisation represents a ratio of the nematic correlation length to a characteristic length scale of the domain.

To make rigorous the asymptotic connection between \mathcal{F}_ε and F_{OF} in the limit of small nematic correlation length, we then establish Γ -convergence and compactness with respect to weak H^1 -convergence, cf. Theorem 3.4 and Proposition 3.5. From standard Γ -convergence theory, this implies the weak H^1 -convergence of minimisers of Landau-de Gennes to a minimiser of Oseen–Frank. In our last result, Theorem 3.6, we upgrade this convergence to strong H^1 -convergence.

2 Tensor formulation of the Oseen–Frank energy

In this section, we present several calculations which establish equalities between the terms in the Oseen–Frank energy of an \mathbb{S}^2 -valued vector field n and quartic terms in $n \otimes n$ and $\nabla(n \otimes n)$. These calculations form the basis for our choice of elastic terms for a Landau-de Gennes energy. Let us first establish the notation used throughout this section and the rest of the manuscript.

Definition 2.1 For a function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$, we define ∇f to be matrix of partial derivatives $\nabla f = (\partial f_i / \partial x_j) \in \mathbb{R}^{m \times n}$.

When f is scalar-valued, we will for convenience sometimes treat ∇f as a column vector as opposed to a row vector, to aid in calculations.

We will often use the notation A_j for the j th row of a matrix A .

Definition 2.2 For a smooth, matrix-valued map $A : \mathbb{R}^n \rightarrow \mathbb{R}^{n \times n}$, the vector field $\operatorname{div} A : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is given by

$$\operatorname{div} A = \sum_{j=1}^n (\operatorname{div} A_j) e_j,$$

so that the j th entry of $\operatorname{div} A$ is the divergence of the j th row of A .

Definition 2.3 We define the curl of a tensor field A by

$$(\operatorname{curl} A)v := \operatorname{curl}(A^T v) \quad \text{for all } v \in \mathbb{R}^3, \tag{2.1}$$

which is equivalent to defining $\operatorname{curl} A$ via

$$\operatorname{curl} A = \varepsilon_{ijk} A_{mj,i} e_k \otimes e_m.$$

Hence, the j th column of $\operatorname{curl} A$ is the curl A_j .

In order to calculate terms involving the curl of a symmetric tensor, we need the following lemma, the proof of which is immediate from the previous definition.

Lemma 2.1 1. For any smooth vector field m , we have

$$\operatorname{curl}(m \otimes m) = ((\operatorname{curl} m_j m)_i) \in \mathbb{R}^{3 \times 3}.$$

That is, the j th column of $\operatorname{curl}(m \otimes m)$ is $\operatorname{curl}(m_j m)$.

2. For any tensor field Q taking values in the space of symmetric matrices, if we refer to the j th row of Q as Q_j , we have

$$\operatorname{curl} Q = ((\operatorname{curl} Q_j)_i) \in \mathbb{R}^{3 \times 3}. \tag{2.2}$$

We begin our analysis with expressions for the K_1 , K_2 and K_3 elastic terms from Oseen–Frank in terms of derivatives of $n \otimes n$.

Proposition 2.2 Let n be a smooth vector field defined on an open subset of \mathbb{R}^3 and taking values in \mathbb{S}^2 . Then

$$(\operatorname{div} n)^2 = |(n \otimes n) \operatorname{div}(n \otimes n)|^2. \tag{2.3}$$

Proof Let us first note that

$$0 = \frac{1}{2} \nabla(|n|^2) = \nabla n^T n, \tag{2.4}$$

which follows from the fact that $|n| = 1$ everywhere. We now use (2.4) to write

$$\begin{aligned}
 (\operatorname{div} n)n &= (\operatorname{div} n)n + \nabla n^T n \\
 &= (\operatorname{div} n)n + (n \cdot \nabla n^T n)n \\
 &= (\operatorname{div} n)n + (\nabla n n \cdot n)n \\
 &= (n \otimes n)(\operatorname{div} n)n + (n \otimes n)(\nabla n n) \\
 &= (n \otimes n) \operatorname{div} (n \otimes n).
 \end{aligned}
 \tag{2.5}$$

Taking $|\cdot|^2$ on both sides yields (2.3). □

Proposition 2.3 *Let n be a smooth vector field defined on an open subset of \mathbb{R}^3 and taking values in \mathbb{S}^2 . Then*

$$((\operatorname{curl} n) \cdot n)^2 = |(n \otimes n) \operatorname{curl} (n \otimes n)|^2,
 \tag{2.6}$$

where for any matrix M , $|M|^2$ denotes the sum of the squares of the entries.

Proof Let us first record

$$(n \otimes n)(\nabla n_j \times n) = (n \cdot (\nabla n_j \times n))n = (\nabla n_j \cdot (n \times n))n = 0.
 \tag{2.7}$$

In the following calculation, we will use the fact that $|n|^2 = 1$ in the first and third lines and use (2.7) once to add 0 in the fourth line. We write

$$\begin{aligned}
 ((\operatorname{curl} n) \cdot n)^2 &= |((\operatorname{curl} n) \cdot n)n|^2 \\
 &= |(n \otimes n)(\operatorname{curl} n)|^2 \\
 &= \sum_j |n_j(n \otimes n)(\operatorname{curl} n)|^2 \\
 &= \sum_j |n_j(n \otimes n)(\operatorname{curl} n) + (n \otimes n)(\nabla n_j \times n)|^2 \\
 &= \sum_j |(n \otimes n)(n_j \operatorname{curl} n + \nabla n_j \times n)|^2 \\
 &= \sum_j |(n \otimes n) \operatorname{curl} (n_j n)|^2.
 \end{aligned}
 \tag{2.8}$$

But $\operatorname{curl} (n_j n)$ is precisely the j th column of $\operatorname{curl} (n \otimes n)$, so that

$$\sum_j |(n \otimes n) \operatorname{curl} (n_j n)|^2 = |(n \otimes n) \operatorname{curl} (n \otimes n)|^2.$$

Combining this with (2.8) finishes the proof of (2.6). □

Proposition 2.4 *Let n be a smooth vector field defined on an open subset of \mathbb{R}^3 and taking values in \mathbb{S}^2 . Then,*

$$|(\operatorname{curl} n) \times n|^2 = |(I - n \otimes n) \operatorname{div} (n \otimes n)|^2.
 \tag{2.9}$$

Proof Using the calculation from (2.5) of $(n \otimes n) \operatorname{div} (n \otimes n)$, let us first write

$$\begin{aligned} (I - n \otimes n) \operatorname{div} (n \otimes n) &= \operatorname{div} (n \otimes n) - (\operatorname{div} n)n \\ &= \nabla n n + (\operatorname{div} n)n - (\operatorname{div} n)n \\ &= \nabla n n. \end{aligned}$$

Now recalling (2.4), we may subtract $\nabla n^T n = 0$ from the right-hand side of previous equation to obtain

$$\begin{aligned} (I - n \otimes n) \operatorname{div} (n \otimes n) &= \nabla n n - \nabla n^T n \\ &= \begin{pmatrix} 0 & n_{1,y} - n_{2,x} & n_{1,z} - n_{3,x} \\ n_{2,x} - n_{1,y} & 0 & n_{2,z} - n_{3,y} \\ n_{3,x} - n_{1,z} & n_{3,y} - n_{2,z} & 0 \end{pmatrix} n \\ &= \begin{pmatrix} 0 & -(\operatorname{curl} n)_3 & (\operatorname{curl} n)_2 \\ (\operatorname{curl} n)_3 & 0 & -(\operatorname{curl} n)_1 \\ -(\operatorname{curl} n)_2 & (\operatorname{curl} n)_1 & 0 \end{pmatrix} n \\ &= \begin{pmatrix} (\operatorname{curl} n)_2 n_3 - (\operatorname{curl} n)_3 n_2 \\ (\operatorname{curl} n)_3 n_1 - (\operatorname{curl} n)_1 n_3 \\ (\operatorname{curl} n)_1 n_2 - (\operatorname{curl} n)_2 n_1 \end{pmatrix} \\ &= (\operatorname{curl} n) \times n. \end{aligned}$$

Taking $|\cdot|^2$ on both sides completes the proof. □

Proposition 2.5 *Let n be a smooth vector field defined on an open subset of \mathbb{R}^3 and taking values in \mathbb{S}^2 . Then*

$$|\nabla n|^2 = |(I - n \otimes n) \operatorname{curl} (n \otimes n)|^2. \tag{2.10}$$

Proof Let us first calculate $|\operatorname{curl} (n \otimes n)|^2$, after which we can use Proposition 2.3 to find $|(I - n \otimes n) \operatorname{curl} (n \otimes n)|^2$. Invoking Lemma 2.1 and then expanding, we write

$$\begin{aligned} |\operatorname{curl} (n \otimes n)|^2 &= \sum_j |\operatorname{curl} (n_j n)|^2 \\ &= \sum_j |\nabla n_j \times n + n_j (\operatorname{curl} n)|^2 \\ &= \sum_j |\nabla n_j \times n|^2 + \sum_j n_j^2 |\operatorname{curl} n|^2 + \sum_j 2(\nabla n_j \times n) \cdot (n_j \operatorname{curl} n) \\ &=: I + II + III. \end{aligned} \tag{2.11}$$

For I , we use Lagrange’s identity and the identity $(\operatorname{curl} n) \times n = \nabla n n$ from the previous lemma to write

$$\begin{aligned} I &= \sum_j (|\nabla n_j|^2 |n|^2 - (\nabla n_j \cdot n)^2) \\ &= \left(\sum_j |\nabla n_j|^2 \right) |n|^2 - |\nabla n n|^2 \\ &= |\nabla n|^2 |n|^2 - |(\operatorname{curl} n) \times n|^2. \end{aligned} \tag{2.12}$$

Moving on to *II*, we immediately see that

$$II = |\operatorname{curl} n|^2. \tag{2.13}$$

Finally, *III* vanishes since

$$III = \sum_j (\nabla(|n_j|^2) \times n) \cdot (\operatorname{curl} n) = (\nabla(|n|^2) \times n) \cdot (\operatorname{curl} n) = 0. \tag{2.14}$$

Substituting (2.12)–(2.14) into (2.11) yields

$$|\operatorname{curl}(n \otimes n)|^2 = |\nabla n|^2 - |(\operatorname{curl} n) \times n|^2 + |\operatorname{curl} n|^2 = |\nabla n|^2 + ((\operatorname{curl} n) \cdot n)^2. \tag{2.15}$$

But with the aid of Lemma 2.3, we can also calculate $|\operatorname{curl}(n \otimes n)|^2$ as

$$\begin{aligned} & |(\mathbf{I} - n \otimes n) \operatorname{curl}(n \otimes n)|^2 + |(n \otimes n) \operatorname{curl}(n \otimes n)|^2 \\ &= |(\mathbf{I} - n \otimes n) \operatorname{curl}(n \otimes n)|^2 + ((\operatorname{curl} n) \cdot n)^2. \end{aligned} \tag{2.16}$$

Equating (2.15) and (2.16) equal and subtracting $((\operatorname{curl} n) \cdot n)^2$, we arrive at (2.10). □

For uniaxial Q such that $W(Q) = 0$, we can use the preceding propositions to establish an equality between \mathcal{F}_{LdG} and the Oseen–Frank energy F_{OF} .

Proposition 2.6 *Let Ω be an open set in \mathbb{R}^n and suppose $W(Q) = 0$ and $Q \in H^1(\Omega; \mathcal{N})$ is orientable, so that $Q = s_0(n \otimes n - \mathbf{I}/3)$ for $n \in H^1(\Omega; \mathbb{S}^2)$. Then, we have the equivalence*

$$\begin{aligned} \mathcal{F}_{LdG}(Q) &= \int_{\Omega} \left(\frac{L_1}{2} \left| \left(\frac{s_0}{3} \mathbf{I} + Q \right) \operatorname{div} Q \right|^2 + \frac{L_2}{2} \left| \left(\frac{s_0}{3} \mathbf{I} + Q \right) \operatorname{curl} Q \right|^2 \right. \\ &\quad \left. + \frac{L_3}{2} \left| \left(\frac{2s_0}{3} \mathbf{I} - Q \right) \operatorname{div} Q \right|^2 + \frac{L_4}{2} \left| \left(\frac{2s_0}{3} \mathbf{I} - Q \right) \operatorname{curl} Q \right|^2 \right) dx \\ &= \int_{\Omega} \left(\frac{K_1}{2} (\operatorname{div} n)^2 + \frac{K_2}{2} ((\operatorname{curl} n) \cdot n)^2 + \frac{K_3}{2} |(\operatorname{curl} n) \times n|^2 \right. \\ &\quad \left. + \frac{K_2 + K_4}{2} (\operatorname{tr}(\nabla n)^2 - (\operatorname{div} n)^2) \right) dx = F_{OF}(n), \end{aligned} \tag{2.17}$$

where $s_0^4 L_4 = K_2 + K_4$ and $s_0^4(L_i + L_4) = K_i$ for $1 \leq i \leq 3$.

Proof Rearranging $Q = s_0(n \otimes n - \mathbf{I}/3)$, we arrive at

$$s_0 n \otimes n = \frac{s_0}{3} \mathbf{I} + Q \text{ and } s_0(\mathbf{I} - n \otimes n) = \frac{2s_0}{3} \mathbf{I} - Q. \tag{2.18}$$

Substituting the equations in (2.18) into the left-hand side of (2.17) and using the equalities (2.3), (2.6) and (2.9)–(2.10) yields

$$\begin{aligned} & \int_{\Omega} \left(\frac{L_1}{2} \left| \left(\frac{s_0}{3} \mathbf{I} + Q \right) \operatorname{div} Q \right|^2 + \frac{L_2}{2} \left| \left(\frac{s_0}{3} \mathbf{I} + Q \right) \operatorname{curl} Q \right|^2 \right. \\ & \quad \left. + \frac{L_3}{2} \left| \left(\frac{2s_0}{3} \mathbf{I} - Q \right) \operatorname{div} Q \right|^2 + \frac{L_4}{2} \left| \left(\frac{2s_0}{3} \mathbf{I} - Q \right) \operatorname{curl} Q \right|^2 \right) dx \end{aligned}$$

$$\begin{aligned}
 &= \int_{\Omega} \left(\frac{s_0^4 L_1}{2} |(n \otimes n) \operatorname{div} (n \otimes n)|^2 + \frac{s_0^4 L_2}{2} |(n \otimes n) \operatorname{curl} (n \otimes n)|^2 \right. \\
 &\quad \left. + \frac{s_0^4 L_3}{2} |(I - n \otimes n) \operatorname{div} (n \otimes n)|^2 + \frac{s_0^4 L_4}{2} |(I - n \otimes n) \operatorname{curl} (n \otimes n)|^2 \right) dx \\
 &= \int_{\Omega} \left(\frac{s_0^4 L_1}{2} (\operatorname{div} n)^2 + \frac{s_0^4 L_2}{2} ((\operatorname{curl} n) \cdot n)^2 + \frac{s_0^4 L_3}{2} |(\operatorname{curl} n) \times n|^2 \right. \\
 &\quad \left. + \frac{s_0^4 L_4}{2} |\nabla n|^2 \right) dx.
 \end{aligned}$$

Recalling the identity

$$|\nabla n|^2 = (\operatorname{div} n)^2 + ((\operatorname{curl} n) \cdot n)^2 + |(\operatorname{curl} n) \times n|^2 + \operatorname{tr} (\nabla n)^2 - (\operatorname{div} n)^2$$

for smooth $n : \Omega \rightarrow \mathbb{S}^2$, we can rewrite the last integral as

$$\begin{aligned}
 &\int_{\Omega} \left(\frac{s_0^4(L_1 + L_4)}{2} (\operatorname{div} n)^2 + \frac{s_0^4(L_2 + L_4)}{2} ((\operatorname{curl} n) \cdot n)^2 \right. \\
 &\quad \left. + \frac{s_0^4(L_3 + L_4)}{2} |(\operatorname{curl} n) \times n|^2 + \frac{s_0^4 L_4}{2} (\operatorname{tr} (\nabla n)^2 - (\operatorname{div} n)^2) \right) dx. \quad \square
 \end{aligned}$$

We will refer to the elastic energy density terms in \mathcal{F}_{LDG} as

$$\begin{aligned}
 \sigma(Q) := &\frac{L_1}{2} \left| \left(\frac{s_0}{3} I + Q \right) \operatorname{div} Q \right|^2 + \frac{L_2}{2} \left| \left(\frac{s_0}{3} I + Q \right) \operatorname{curl} Q \right|^2 \\
 &+ \frac{L_3}{2} \left| \left(\frac{2s_0}{3} I - Q \right) \operatorname{div} Q \right|^2 + \frac{L_4}{2} \left| \left(\frac{2s_0}{3} I - Q \right) \operatorname{curl} Q \right|^2. \quad (2.19)
 \end{aligned}$$

Remark 1 It is straightforward that σ satisfies the requisite frame indifference and material symmetry conditions; cf. Lemma 4.1. Moreover, in the Appendix, we identify each term in σ as an appropriately weighted sum of terms from the generalised Landau-de Gennes theory [24]. For example, the term $\left| \left(\frac{s_0}{3} I + Q \right) \operatorname{div} Q \right|^2$ corresponds to the $L_2^{(2)}$ -, $L_3^{(3)}$ - and $L_6^{(4)}$ -invariants.

Remark 2 To ensure that σ is non-negative, it is natural to require that each L_i is non-negative. In fact, as we will see in the upcoming Proposition 3.1, when each L_i is positive, \mathcal{F}_{LDG} is coercive over H^1 . Conversely, if one of the L_i s is negative, then one can construct a map Q such that $\sigma(Q) < 0$. For example, if $L_1 < 0$, a curl-free map Q can be constructed which satisfies

$$\frac{|L_1|}{2} \left| \left(\frac{s_0}{3} I + Q \right) \operatorname{div} Q \right|^2 > \frac{L_3}{2} \left| \left(\frac{2s_0}{3} I - Q \right) \operatorname{div} Q \right|^2$$

pointwise and ensures that $\sigma(Q) < 0$.

Remark 3 The Oseen–Frank elastic constants K_i and our constants L_i are related to each other as follows:

$$L_4 = \frac{K_2 + K_4}{s_0^4}, \text{ and } L_i = \frac{K_i - K_2 - K_4}{s_0^4} \text{ for } 1 \leq i \leq 3,$$

or

$$K_i = s_0^4(L_i + L_4) \text{ for } 1 \leq i \leq 3, \text{ and } K_4 = -s_0^4 L_2.$$

In the equal elastic constant case, $K_1 = K_2 = K_3 = K$, $K_4 = 0$, so that

$$F_{OF}(n) = \frac{K}{2} \int |\nabla n|^2 / 2,$$

each L_i vanishes except for L_4 . If we include the additional term $\int_{\Omega} L_5 |\nabla Q|^2 / 2$, then the equal elastic constant case yields a Q -tensor model in which only L_4 - and L_5 -terms survive, satisfying $L_4 + 2L_5/s_0^2 = K$. As a special case, one may choose $L_4 = 0$, so that the elastic energy is just the Dirichlet energy for the Q -tensor.

Remark 4 One might inquire as to the relationship between the inequalities $L_i \geq 0$ and Ericksen’s inequalities

$$2K_1 \geq K_2 + K_4, K_2 \geq |K_4|, K_3 \geq 0 \tag{2.20}$$

for F_{OF} , which guarantee that the energy density in F_{OF} is non-negative [12]. It is quickly checked that if each L_i is non-negative, then (2.20) is satisfied. Conversely, if $\{K_i\}$ satisfies (2.20), it can be checked that the additional assumptions

$$K_1 \geq K_2 + K_4, K_3 \geq K_2 + K_4, K_4 \leq 0$$

are needed so that each L_i is non-negative. It is possible that these additional assumptions can be relaxed through the inclusion of more quartic terms identified by [24], but we do not pursue this issue further.

3 Analysis and Γ -convergence of \mathcal{F}_{LdG}

Motivated by Proposition 2.6, we combine the quartic Q -tensor elastic terms with the bulk potential W given by (1.3) to obtain the following generalised Landau-de Gennes energy with quartic elastic energy density, defined over $Q \in H^1(\Omega; \mathcal{S})$:

$$\begin{aligned} \mathcal{F}_{LdG}(Q) := & \int_{\Omega} \left(\frac{L_1}{2} \left| \left(\frac{s_0}{3} \mathbf{I} + Q \right) \operatorname{div} Q \right|^2 + \frac{L_2}{2} \left| \left(\frac{s_0}{3} \mathbf{I} + Q \right) \operatorname{curl} Q \right|^2 \right. \\ & + \frac{L_3}{2} \left| \left(\frac{2s_0}{3} \mathbf{I} - Q \right) \operatorname{div} Q \right|^2 + \frac{L_4}{2} \left| \left(\frac{2s_0}{3} \mathbf{I} - Q \right) \operatorname{curl} Q \right|^2 \\ & \left. + W(Q) \right) dx. \end{aligned}$$

We assume that $L_i > 0$ for each i . This will ensure that our energy is coercive over $H^1(\Omega; \mathcal{S})$; cf. Proposition 3.1. Let us point out that Q merely belonging to $H^1(\Omega; \mathcal{S})$ is not enough to conclude that $\mathcal{F}_{LdG}(Q) < \infty$. If, for example, $Q \in (L^\infty \cap H^1)(\Omega; \mathcal{S})$ or $W^{1,4}(\Omega; \mathcal{S})$; however, then \mathcal{F}_{LdG} is necessarily finite.

In order to establish a meaningful asymptotic connection between this generalised Landau-de Gennes model and Oseen–Frank, we next non-dimensionalise the energy \mathcal{F}_{LdG} by scaling the spatial coordinates

$$\bar{x} = x/D,$$

where $D := \text{diam}(\Omega)$. We also rescale Q by letting

$$\bar{Q}(\bar{x}) := Q(x)/s_0.$$

Although the order parameter Q is already dimensionless, dividing by the dimensionless parameter s_0 enables us to eliminate it from the elastic energy density. Let $\zeta := L_1 s_0^4 / D^2$ and define a dimensionless elastic energy density via

$$\bar{\sigma}(\bar{Q}) := \frac{1}{\zeta} \sigma(Q).$$

Then, in the \bar{x} -coordinates,

$$\begin{aligned} \bar{\sigma}(\bar{Q}) = & \frac{\bar{L}_1}{2} |(1/3 + \bar{Q}) \text{div } \bar{Q}|^2 + \frac{\bar{L}_2}{2} |(1/3 + \bar{Q}) \text{curl } \bar{Q}|^2 \\ & + \frac{\bar{L}_3}{2} |(2I/3 - \bar{Q}) \text{div } \bar{Q}|^2 + \frac{\bar{L}_4}{2} |(2I/3 - \bar{Q}) \text{curl } \bar{Q}|^2, \end{aligned} \tag{3.1}$$

where $\bar{L}_i := L_i / L_1$ for $1 \leq i \leq 4$. Next, we rescale the Landau-de Gennes potential W by introducing

$$\bar{W}(\bar{Q}) := \bar{a} \text{tr}(\bar{Q}^2) - \frac{2\bar{b}}{3} \text{tr}(\bar{Q}^3) + \bar{c} (\text{tr}(\bar{Q}^2))^2, \tag{3.2}$$

where $\bar{a} = a s_0^2 / c$, $\bar{b} = b s_0^3 / c$ and $\bar{c} = s_0^4 / 2$. Then, setting $\varepsilon := \sqrt{\frac{\zeta}{c}}$, we have

$$\bar{W}(\bar{Q}) = \frac{\varepsilon^2}{\zeta} W(Q).$$

Recall that we are assuming the global minimum of \bar{W} is 0, and it is now achieved along the set

$$\left\{ n \otimes n - \frac{1}{3} I : n \in \mathbb{S}^2 \right\}, \tag{3.3}$$

which we will still refer to as \mathcal{N} . If we write $\bar{\Omega} := \Omega / D$, then the total energy is given by

$$\int_{\Omega} (\sigma(Q) + W(Q)) \, dx = \zeta D^3 \int_{\bar{\Omega}} \left(\bar{\sigma}(\bar{Q}) + \frac{1}{\varepsilon^2} \bar{W}(\bar{Q}) \right) \, d\bar{x}.$$

Finally, noting that ζD^3 has the dimensions of energy, we define the non-dimensionalised energy via

$$\mathcal{F}_{\varepsilon}(\bar{Q}) := \int_{\bar{\Omega}} \left(\bar{\sigma}(\bar{Q}) + \frac{1}{\varepsilon^2} \bar{W}(\bar{Q}) \right) \, d\bar{x}.$$

The parameter ε can be interpreted as ξ_{NI} / D , where ξ_{NI} is the nematic correlation length that determines isotropic core size [16]. With a slight abuse of notation, we will dispose of the bars for the rest of the paper, so that the non-dimensionalised energy is written as

$$\mathcal{F}_{\varepsilon}(Q) = \int_{\Omega} \left(\sigma(Q) + \frac{1}{\varepsilon^2} W(Q) \right) \, dx, \tag{3.4}$$

with $\sigma(Q)$ henceforth given by (3.1) and $W(Q)$ given by (3.2). We will consider the $\varepsilon \rightarrow 0$ limit for \mathcal{F}_ε , which should be understood as the limit in which the nematic correlation length is vanishingly small compared to the size of the domain.

Finally, we will require throughout the rest of the article that admissible competitors for \mathcal{F}_ε are subject to a Dirichlet boundary condition

$$g \in \text{Lip}(\partial\Omega; \mathcal{S}).$$

For such g , the set $H_g^1(\Omega; \mathcal{S})$ contains competitors which are also Lipschitz, so that the infimum of \mathcal{F}_ε among $H_g^1(\Omega; \mathcal{S})$ is not infinity. Later on, when we are considering the asymptotic behaviour of \mathcal{F}_ε as $\varepsilon \rightarrow 0$, we will further require that g takes values in \mathcal{N} .

Proposition 3.1 (Coercivity of \mathcal{F}_ε) *There exist constants $C_1 = C_1(\{L_i\}) > 0$ and $C_2 = C_2(g)$ such that for any $Q \in H_g^1(\Omega; \mathcal{S})$,*

$$\|Q\|_{H^1}^2 \leq C_1 \mathcal{F}_\varepsilon(Q) + C_2. \tag{3.5}$$

Proof It is standard to bound $\|Q\|_{L^2}^2$ from above by the potential term in the energy \mathcal{F}_ε , so we focus on σ . First, recall that for any symmetric matrix M and vectors v_1, v_2 ,

$$\langle Mv_1, v_2 \rangle = \langle v_1, Mv_2 \rangle.$$

Using this fact, we calculate

$$\begin{aligned} & |(I/3 + Q) \operatorname{div} Q|^2 + |(2I/3 - Q) \operatorname{div} Q|^2 \\ &= \langle \operatorname{div} Q, (I/3 + Q)^2 \operatorname{div} Q \rangle + \langle \operatorname{div} Q, (2I/3 - Q)^2 \operatorname{div} Q \rangle \\ &= \langle \operatorname{div} Q, (2Q^2 - 2Q/3 + 5I/9) \operatorname{div} Q \rangle \\ &= \langle \operatorname{div} Q, (I/2 + 2(Q - I/6)^2) \operatorname{div} Q \rangle \\ &= |\operatorname{div} Q|^2/2 + 2|(Q - I/6) \operatorname{div} Q|^2. \end{aligned} \tag{3.6}$$

Similarly, we have

$$\begin{aligned} & |(I/3 + Q) \operatorname{curl} Q|^2 + |(2I/3 - Q) \operatorname{curl} Q|^2 \\ &= |\operatorname{curl} Q|^2/2 + 2|(Q - I/6) \operatorname{curl} Q|^2. \end{aligned} \tag{3.7}$$

The equalities (3.6)–(3.7) imply that

$$\frac{1}{2} \min_i \frac{L_i}{2} (|\operatorname{div} Q|^2 + |\operatorname{curl} Q|^2) \leq \sigma(Q). \tag{3.8}$$

To bound this from below using $|\nabla Q|^2$, we need the identity

$$|\nabla Q|^2 = \sum_j ((\operatorname{div} Q_j)^2 + |\operatorname{curl} Q_j|^2 + \operatorname{tr}(\nabla Q_j)^2 - (\operatorname{div} Q_j)^2) \tag{3.9}$$

cf. [20, Lemma 1.4], where Q_j is the j th row of Q . Therefore, with $C_1 = 4/(\min_{1 \leq i \leq 4} L_i)$, we can combine (3.8) and (3.9) to arrive at

$$\int_\Omega |\nabla Q|^2 dx \leq C_1 \int_\Omega \sigma(Q) dx + \int_\Omega \sum_j (\operatorname{tr}(\nabla Q_j)^2 - (\operatorname{div} Q_j)^2) dx.$$

The remainder on the right-hand side is a null Lagrangian, and since the boundary data g is Lipschitz, it can be written as

$$\int_{\partial\Omega} \left(\sum_j (\nabla_{\tan} g_j) g_j - (\text{tr } \nabla_{\tan} g_j) g_j \right) \cdot \nu \, d\mathcal{H}^2, \tag{3.10}$$

which is a constant C_2 independent of $Q \in H_g^1(\Omega; S)$. We refer the reader to [20, Lemma 1.2] for the derivation of this formula. \square

To prove the existence of minimisers of \mathcal{F}_ε among $H_g^1(\Omega; S)$ and to prove a Γ -convergence result, we will need the following proposition.

Proposition 3.2 (Lower semicontinuity of σ) *For any sequence Q_n which converges weakly in $H^1(\Omega; S)$ to $Q \in H^1(\Omega; S)$, we have*

$$\int_{\Omega} \sigma(Q) \, dx \leq \liminf_{n \rightarrow \infty} \int_{\Omega} \sigma(Q_n) \, dx. \tag{3.11}$$

Proof We focus on the term $|(I/3 + Q_n) \text{div } Q_n|^2$; the argument for the other terms is the same. Let us assume that the right-hand side of (3.11) is finite; if it is not, the proof is trivial. The essence of the subsequent proof is the real analysis fact

$$\begin{aligned} f_n \rightarrow f \text{ strongly in } L^2, \quad g_n \rightarrow g \text{ weakly in } L^2, \quad \|f_n g_n\|_{L^2} \leq C < \infty \\ \implies f_n g_n \rightarrow fg \text{ weakly in } L^2. \end{aligned}$$

Without loss of generality, we can assume (by restricting to a subsequence) that $\liminf \int_{\Omega} |(I/3 + Q_n) \text{div } Q_n|^2 \, dx$ is finite, and the sequence of integrals converges to its limit inferior. Let us first recall that weak convergence in $H^1(\Omega; S)$ entails strong convergence in $L^2(\Omega; S)$, so that

$$I/3 + Q_n \rightarrow I/3 + Q \text{ in } L^2(\Omega; S). \tag{3.12}$$

Next, since $\text{div } Q_n$ converges weakly in $L^2(\Omega; \mathbb{R}^3)$ to $\text{div } Q$ and $I/3 + Q_n$ converges strongly in $L^2(\Omega; S)$ to $I/3 + Q$, we have for any $\phi \in L^\infty(\Omega; \mathbb{R}^3)$:

$$\begin{aligned} \int_{\Omega} (I/3 + Q_n) \text{div } Q_n \cdot \phi &= \int_{\Omega} [(I/3 + Q_n) - (I/3 + Q)] \text{div } Q_n \cdot \phi \\ &\quad + \int_{\Omega} (I/3 + Q) \text{div } Q_n \cdot \phi \rightarrow \int_{\Omega} (I/3 + Q) \text{div } Q \cdot \phi. \end{aligned}$$

Thus,

$$(I/3 + Q_n) \text{div } Q_n \rightarrow (I/3 + Q) \text{div } Q \text{ weakly in } L^1(\Omega; \mathbb{R}^3).$$

Now from the uniform L^2 bound on $(I/3 + Q_n) \text{div } Q_n$, we have that (up to a subsequence)

$$(I/3 + Q_n) \text{div } Q_n \rightarrow h \text{ weakly in } L^2(\Omega; \mathbb{R}^3)$$

for some $h \in L^2(\Omega; \mathbb{R}^3)$. But from the previous observation and the uniqueness of weak limits, we deduce that the weak L^2 -limit h must coincide with $(I/3 + Q) \text{div } Q$, the weak L^1 -limit. The

inequality

$$\int_{\Omega} |(I/3 + Q) \operatorname{div} Q|^2 dx \leq \liminf_{n \rightarrow \infty} \int_{\Omega} |(I/3 + Q_n) \operatorname{div} Q_n|^2 dx$$

now follows from the lower semicontinuity of the L^2 -norm under weak convergence. Repeating the same argument for the other terms in σ concludes the proof. \square

Remark 5 *The proposition 3.2 should hold for other quartic elastic energies, provided the energy is strongly lower semicontinuous and convex [8]. This would also allow for generalisation of the Γ -convergence result (Theorem 3.4) to other models with quartic elastic energies.*

Next, we turn our attention to the existence of minimisers of \mathcal{F}_ε .

Theorem 3.3 (Existence of a minimiser) *For any $\varepsilon > 0$ and Lipschitz $g : \partial\Omega \rightarrow \mathcal{S}$, there exists Q_0 which minimises \mathcal{F}_ε within $H_g^1(\Omega; \mathcal{S})$.*

Proof Fix $\varepsilon > 0$ and g as stated in the theorem. By virtue of the previous two propositions, the existence of a minimiser will follow without difficulty from the direct method in the calculus of variations.

Let $\{Q_n\}$ be a sequence such that

$$\lim_{n \rightarrow \infty} \mathcal{F}_\varepsilon(Q_n) = \inf\{\mathcal{F}_\varepsilon(Q) : Q \in H_g^1(\Omega; \mathcal{S})\}.$$

As noted earlier, since g is Lipschitz, the infimum is not ∞ . Then by Proposition 3.1, we have a uniform H^1 bound on $\{Q_n\}$ and a subsequence, which we still refer to as $\{Q_n\}$, converging weakly in H^1 to some $Q_0 \in H_g^1(\Omega; \mathcal{S})$. Proposition 3.2 then yields

$$\int_{\Omega} \sigma(Q_0) dx \leq \liminf_{n \rightarrow \infty} \int_{\Omega} \sigma(Q_n) dx. \tag{3.13}$$

By Rellich’s theorem, we may assume as well that Q_n converge in L^4 to Q_0 , from which we deduce

$$\int_{\Omega} W(Q_0) dx = \lim_{n \rightarrow \infty} \int_{\Omega} W(Q_n) dx. \tag{3.14}$$

The minimality of Q_0 is now a consequence of (3.13) and (3.14). \square

We are now interested in the asymptotic behaviour of minimisers of \mathcal{F}_ε as $\varepsilon \rightarrow 0$. Let us begin by identifying a limiting functional. In the limit $\varepsilon \rightarrow 0$, it is clear that competitors with finite energy will have to take values in \mathcal{N} , the well of W , cf. (3.3). Assume that in addition to being Lipschitz, the boundary data g take values in \mathcal{N} , so that $W(g) = 0$. The set of satisfactory boundary data includes, for example, g which are formed using a Lipschitz vector field $n : \partial\Omega \rightarrow \mathbb{S}^2$ and considering the tensor field

$$n \otimes n - \frac{1}{3}I : \partial\Omega \rightarrow \mathcal{N}, \tag{3.15}$$

cf. [20, Lemma 1.1]. The limiting functional \mathcal{F}_0 is then defined by

$$\mathcal{F}_0(Q) = \begin{cases} \int_{\Omega} \sigma(Q) \, dx & \text{if } Q \in H_g^1(\Omega; \mathcal{N}), \\ \infty & \text{otherwise,} \end{cases}$$

with σ given by (3.1).

Let us point out a key feature of the limiting model: \mathcal{F}_0 coincides with the Oseen–Frank model, in the sense of Proposition 2.6. The question of when minimising \mathcal{F}_0 among Q -tensor fields coincides with minimising the version of the Oseen–Frank energy above is more delicate. There may well be strictly more competitors in the space of Q -tensors than in the space of \mathbb{S}^2 -valued fields n due to the possible ‘non-orientability’ of a Q -tensor field. It has been shown in [5] that when $\Omega \subset \mathbb{R}^k$ is simply connected and $k = 2, 3$, every $Q \in H^1(\Omega; \mathcal{N})$ has a lifting $n^Q \in H^1(\Omega; \mathbb{S}^2)$ such that

$$Q = n^Q \otimes n^Q - I/3.$$

If Ω is not simply connected or if $p < 2$, then there might exist tensor fields which cannot be ‘oriented’ to produce a globally defined corresponding director. We refer the reader to [5] for a more detailed treatment.

We state the first of two theorems regarding the asymptotic behaviour of \mathcal{F}_ε and its minimisers.

Theorem 3.4 (Γ -convergence) *For any choice of boundary data g as above, the sequence $\{\mathcal{F}_\varepsilon\}$ Γ -converges in the weak topology of $H_g^1(\Omega; S)$ to \mathcal{F}_0 . That is,*

1. For any $Q \in H_g^1(\Omega; S)$ and for any sequence $\{Q_\varepsilon\}$ in $H_g^1(\Omega; S)$,

$$Q_\varepsilon \rightharpoonup Q \text{ in } H_g^1(\Omega; S) \text{ implies } \liminf_{\varepsilon \rightarrow 0} \mathcal{F}_\varepsilon(Q_\varepsilon) \geq \mathcal{F}_0(Q), \tag{3.16}$$

and

2. For each $Q \in H_g^1(\Omega; S)$, there exists a recovery sequence $\{Q_\varepsilon\}$ in $H_g^1(\Omega; S)$ satisfying

$$Q_\varepsilon \rightharpoonup Q \text{ in } H_g^1(\Omega; S), \tag{3.17}$$

$$\lim_{\varepsilon \rightarrow 0} \mathcal{F}_\varepsilon(Q_\varepsilon) = \mathcal{F}_0(Q). \tag{3.18}$$

Before we present the proof, we state a compactness proposition, which follows immediately from Proposition 3.1.

Proposition 3.5 (Compactness) *Let $\{Q_\varepsilon\}$ be a sequence of maps from Ω to S , and assume that the sequence of energies $\mathcal{F}_\varepsilon(Q_\varepsilon)$ is uniformly bounded. Then, there exists a subsequence $\{Q_{\varepsilon_j}\}$ and $Q \in H_g^1(\Omega; \mathcal{N})$ such that $Q_{\varepsilon_j} \rightharpoonup Q$ in $H^1(\Omega; S)$.*

Proof of Theorem 3.4 The lower semicontinuity condition (3.16) has been proved in Proposition 3.2. For the construction of a recovery sequence given some Q_0 , we can simply take $Q_\varepsilon = Q_0$ for all ε . □

Finally, we prove that

Theorem 3.6 (*H¹-convergence of a subsequence of minimisers*) *For any sequence of minimisers {Q_ε} of F_ε, there exists Q₀ ∈ H_g¹(Ω; N) which minimises F₀ and a subsequence {Q_{ε_j} converging to Q₀ strongly in H_g¹(Ω; S).}*

Proof We will prove the theorem under the assumption that

$$\min_{1 \leq i \leq 4} L_i = L_1 = 1 > 0; \tag{3.19}$$

the proof when one of the other *L_i*s is the smallest is similar. Appealing to Proposition 3.5 yields a subsequence {Q_{ε_j}}, which we will call {Q_{*j*}} for convenience, such that Q_{*j*} converges weakly in H¹(Ω; S) to some Q₀ ∈ H_g¹(Ω; N) of F₀. It is a classical fact from the theory of Γ-convergence that Q₀ minimises F₀. To show the strong convergence of Q_{*j*}, we will use the fact that weak convergence together with convergence of norms implies strong convergence.

It will be necessary to first extend our maps to compactly supported Sobolev maps on a larger domain. Let Ω' ⊂ ℝ³ be a smooth domain such that Ω is compactly contained in Ω', and let P : Ω' \ Ω → S be an H¹ function such that its trace on ∂Ω is *g* and its trace on ∂Ω' is 0. We extend each Q_{*j*} to a map Q̃_{*j*} ∈ H₀¹(Ω'; S) via

$$\tilde{Q}_j(x) = \begin{cases} Q_j(x) & x \in \Omega, \\ P(x) & x \in \Omega' \setminus \Omega, \end{cases}$$

and similarly for Q₀. We will now use the calculations (3.6)–(3.7) from Proposition 3.1 to extract a |∇Q|² term from σ. First, from (3.6)–(3.7), we have

$$\begin{aligned} & \int_{\Omega'} \left(\frac{1}{2} |(I/3 + \tilde{Q}_j) \operatorname{div} \tilde{Q}_j|^2 + \frac{L_2}{2} |(I/3 + \tilde{Q}_j) \operatorname{curl} \tilde{Q}_j|^2 \right. \\ & \quad \left. + \frac{L_3}{2} |(2I/3 - \tilde{Q}_j) \operatorname{div} \tilde{Q}_j|^2 + \frac{L_4}{2} |(2I/3 - \tilde{Q}_j) \operatorname{curl} \tilde{Q}_j|^2 \right) dx \\ &= \frac{1}{2} \int_{\Omega'} \left(|(I/3 + \tilde{Q}_j) \operatorname{div} \tilde{Q}_j|^2 + |(I/3 + \tilde{Q}_j) \operatorname{curl} \tilde{Q}_j|^2 \right. \\ & \quad \left. + |(2I/3 - \tilde{Q}_j) \operatorname{div} \tilde{Q}_j|^2 + |(2I/3 - \tilde{Q}_j) \operatorname{curl} \tilde{Q}_j|^2 \right. \\ & \quad \left. + \frac{L_2 - 1}{2} |(I/3 + \tilde{Q}_j) \operatorname{curl} \tilde{Q}_j|^2 + \frac{L_3 - 1}{2} |(2I/3 - \tilde{Q}_j) \operatorname{div} \tilde{Q}_j|^2 \right. \\ & \quad \left. + \frac{L_4 - 1}{2} |(2I/3 - \tilde{Q}_j) \operatorname{curl} \tilde{Q}_j|^2 \right) dx \\ &= \frac{1}{2} \int_{\Omega'} \left((|\operatorname{div} \tilde{Q}_j|^2 + |\operatorname{curl} \tilde{Q}_j|^2) / 2 + 2|(\tilde{Q}_j - I/6) \operatorname{div} \tilde{Q}_j|^2 \right. \\ & \quad \left. + 2|(\tilde{Q}_j - I/6) \operatorname{curl} \tilde{Q}_j|^2 + \frac{L_2 - 1}{2} |(I/3 + \tilde{Q}_j) \operatorname{curl} \tilde{Q}_j|^2 \right. \\ & \quad \left. + \frac{L_3 - 1}{2} |(2I/3 - \tilde{Q}_j) \operatorname{div} \tilde{Q}_j|^2 + \frac{L_4 - 1}{2} |(2I/3 - \tilde{Q}_j) \operatorname{curl} \tilde{Q}_j|^2 \right) dx. \end{aligned}$$

But for any smooth Q ∈ H₀¹(Ω'; S), we have by (3.9) and (3.10)

$$\begin{aligned} \int_{\Omega'} (|\operatorname{div} Q|^2 + |\operatorname{curl} Q|^2) dx &= \int_{\Omega'} (|\nabla Q|^2 + \text{null Lagrangian}) dx \\ &= \int_{\Omega'} |\nabla Q|^2 dx. \end{aligned} \tag{3.20}$$

Hence (3.20) holds for all $Q \in H_0^1(\Omega'; \mathcal{S})$ by density. Plugging this equality into our expression for $\int_{\Omega'} \sigma(\tilde{Q}_j) dx$ gives

$$\begin{aligned} & \int_{\Omega'} \sigma(\tilde{Q}_j) dx \tag{3.21} \\ &= \frac{1}{2} \int_{\Omega'} \left(|\nabla \tilde{Q}_j|^2 / 2 + 2|(\tilde{Q}_j - I/6) \operatorname{div} \tilde{Q}_j|^2 \right. \\ &\quad + 2|(\tilde{Q}_j - I/6) \operatorname{curl} \tilde{Q}_j|^2 + \frac{L_2 - 1}{2} \left| (I/3 + \tilde{Q}_j) \operatorname{curl} \tilde{Q}_j \right|^2 \\ &\quad \left. + \frac{L_3 - 1}{2} \left| (2I/3 - \tilde{Q}_j) \operatorname{div} \tilde{Q}_j \right|^2 + \frac{L_4 - 1}{2} \left| (2I/3 - \tilde{Q}_j) \operatorname{curl} \tilde{Q}_j \right|^2 \right) dx. \end{aligned}$$

Define $\tilde{\sigma}(\tilde{Q}_j)$ to be the sum of the integrands of the right-hand side of (3.21), so that

$$\int_{\Omega'} \sigma(\tilde{Q}_j) dx = \int_{\Omega'} \tilde{\sigma}(\tilde{Q}_j) dx.$$

By the exact same argument as in Proposition 3.2, each of the individual terms in $\int_{\Omega'} \tilde{\sigma}(\tilde{Q}_j) dx$ is lower semicontinuous with respect to weak H^1 -convergence. Therefore,

$$\int_{\Omega'} \tilde{\sigma}(\tilde{Q}_0) dx \leq \liminf_{j \rightarrow \infty} \int_{\Omega'} \tilde{\sigma}(\tilde{Q}_j) dx. \tag{3.22}$$

But since Q_j minimises $\mathcal{F}_{\varepsilon_j}$, we also have

$$\begin{aligned} \limsup_{j \rightarrow \infty} \int_{\Omega'} \tilde{\sigma}(\tilde{Q}_j) dx &= \limsup_{j \rightarrow \infty} \int_{\Omega'} \sigma(\tilde{Q}_j) dx \\ &\leq \limsup_{j \rightarrow \infty} \int_{\Omega'} \left(\sigma(\tilde{Q}_j) + \frac{1}{\varepsilon_j} W(\tilde{Q}_j) \right) dx \\ &\leq \int_{\Omega'} \sigma(\tilde{Q}_0) dx \\ &= \int_{\Omega'} \tilde{\sigma}(\tilde{Q}_0) dx. \end{aligned} \tag{3.23}$$

Together, (3.22) and (3.23) give

$$\int_{\Omega'} \tilde{\sigma}(\tilde{Q}_0) dx = \lim_{j \rightarrow \infty} \int_{\Omega'} \tilde{\sigma}(\tilde{Q}_j) dx.$$

Since each separate term in $\tilde{\sigma}$ is lower semicontinuous, it must be the case that

$$\int_{\Omega'} |\nabla \tilde{Q}|^2 = \lim_{j \rightarrow \infty} \int_{\Omega'} |\nabla \tilde{Q}_j|^2 dx. \tag{3.24}$$

From the weak H^1 -convergence, we know that $\nabla \tilde{Q}_j \rightarrow \nabla \tilde{Q}_0$ weakly in L^2 , which in conjunction with (3.24) implies that

$$\nabla \tilde{Q}_j \rightarrow \nabla \tilde{Q}_0 \text{ in } L^2(\Omega'; \mathcal{S}).$$

Since $\tilde{Q}_j = P = Q_0$ on $\Omega' \setminus \Omega$, we have shown that in fact

$$\nabla Q_j \rightarrow \nabla Q_0 \text{ in } L^2(\Omega; \mathcal{S}),$$

and the proof is complete under the assumption that $1 = L_1 \leq L_i$ for $2 \leq i \leq 4$. If $\min_i L_i$ is achieved by some L_i where $i \neq 1$, the proof follows almost exactly as above, with the second integral in (3.21) replaced by a similar expression involving the three largest L_i s and their corresponding elastic terms. \square

4 Discussion

We have introduced a version of Landau-de Gennes model involving a quartic elastic energy that reduces to the four-constant Oseen–Frank energy for uniaxial Q -tensors. This version has several advantages, as laid out in the introduction, in addition to being capable of recovering the full Oseen–Frank energy.

From the mathematical standpoint, it is far more stable than the frequently used cubic model since the energy is bounded from below and coercive. From the physical viewpoint, we have found this form of Landau-de Gennes is particularly useful in modelling liquid crystalline states with coexisting isotropic and nematic phases, specifically in the context of lyotropic chromonic liquid crystals (LCLCs) [23, 33]. To this end, in order to capture nematic-to-isotropic phase transitions, a Q -tensor has to vanish in a part of the physical domain while being in a uniaxial, $\mathbb{R}P^2$ -valued nematic state elsewhere. Clearly, this setup falls outside of the scope of an S^2 -valued director theory such as that of Oseen and Frank. What is more, because in the Oseen–Frank limit, the standard quadratic Landau-de Gennes model (1.2) reduces to a director model with two equal elastic constants, the quadratic Landau-de Gennes framework is not adequate when the contributions from splay, twist and bend all incur different costs. In fact, it is well known experimentally that for certain liquid crystals, including LCLCs, the elastic constants for splay, bend and twist can vary dramatically. It is thus a keen interest of ours to explore the effects of strong elastic disparity on evolution of interfaces and nematic singularities in isotropic-to-nematic transitions. We are encouraged by the results of gradient flow simulations using our model which exhibit good qualitative agreement with experiments, including the capture of such features as phase boundary singularities – the so-called ‘boojums’ – and vortex splitting, cf. [17].

Example 4.1 (LCLCs) Let us compare the standard quadratic Landau-de Gennes energy (1.2), a cubic Landau-de Gennes energy [4] and the quartic energy proposed here in terms of modelling the LCLCs with highly disparate elastic constants considered in [33]. The authors in [33] measured the values of the Oseen–Frank elastic constants for disodium cromoglycate and found that the coefficients K_1 and K_3 for splay and bend are of the order 10 pN, while the twist coefficient is about 10 times smaller. However, the values of K_1 and K_3 are not equal. In Fig. 4 of [33], the ratio K_1/K_3 varies between approximately 0.4 and 1.2, depending on temperature and concentration. Therefore, modelling this liquid crystal using the standard quadratic model (1.2) is not feasible, since the values of K_1 and K_3 in terms of L_i for this model are equal, cf. [3, equation (4.17)]. If one were to attempt to use the cubic model with modified potential from [4], a necessary condition for minimisation is that one of the coefficients, L'_1 , is positive, cf. [3, equation (5.16)]. In terms of the Oseen–Frank constants K_i [3, equation 4.18], this condition is equivalent to

$$(1 - s_0)(K_1 - K_3) + 3s_0 K_2 > 0, \quad (4.1)$$

when $K_3 > K_1$. If, for instance, one has $10K_2 \approx K_1 \approx K_3/2$ from the experiment and s_0 is in the typically observed interval (0.6, 0.7) [2], this inequality does not hold. Thus, the standard Landau-de Gennes model and its variants are ill-suited to modelling in this scenario, since

they are not well-posed. In contrast, for the quartic model proposed here, the restrictions $K_1 > K_2 + K_4$, $K_3 > K_2 + K_4$ needed in order to guarantee coercivity do not present any obstacles. Furthermore, these inequalities are consistent with commonly observed values of K_i [15].

Finally, we wish to emphasise that there are surely many, many other choices of elastic energy densities beside those we take in (1.5) capable of recovering the four-constant Oseen–Frank energy for uniaxial Q . This should not cause concern since what is physically measurable are the Frank constants K_1 , K_2 , K_3 and K_4 . Given that there are 6 different allowable cubic terms, 13 quartic terms, and even more terms if one ventures into higher order, it is clear that there are myriad combinations of terms in a Q -tensor-based elastic energy density that can reduce to the four-constant Oseen–Frank energy when Q is uniaxial. Of course, what may differ from one choice to another are the constraints on the coefficients under which the particular version is well-posed. On this point, it should be noted that one should expect *any* such choice of elastic energy density to impose restrictions more stringent than those dictated by the Ericksen inequalities on the K_i s, cf. (2.20), since one is seeking well-posedness over a much broader class of competitors than just uniaxials.

References

- [1] BALL, J. M. (2010) The Q-tensor theory of liquid crystals. <https://people.maths.ox.ac.uk/ball/teaching/benjamin%20summer%20school-%202010.pdf>.
- [2] BALL, J. M. (2017) Liquid crystals and their defects. *Mathematical Thermodynamics of Complex Fluids*, Lecture Notes in Math., 2200, Fond. CIME/CIME Found. Subser., Springer, Cham, pp. 1–46.
- [3] BALL, J. M. (2017) Mathematics and liquid crystals. *Mol. Cryst. Liq. Cryst.* **647**(1), 1–27.
- [4] BALL, J. M. & MAJUMDAR, A. (2010) Nematic liquid crystals: from Maier-Saupe to a continuum theory. *Mol. Cryst. Liq. Cryst.* **525**(1), 1–11.
- [5] BALL, J. M. & ZARNESCU, A. (2011) Orientability and energy minimization in liquid crystal models. *Arch. Ration. Mech. Anal.* **202**(2), 493–535.
- [6] BAUMAN, P. & PHILLIPS, D. (2016) Regularity and the behavior of eigenvalues for minimizers of a constrained Q -tensor energy for liquid crystals. *Calc. Var. Partial Differ. Equ.* **55**(4), Article No. 81, 22.
- [7] BERREMAN, D. W. & MEIBOOM, S. (1984) Tensor representation of Oseen–Frank strain energy in uniaxial cholesterics. *Phys. Rev. A* **30**, 1955–1959.
- [8] DAVIS, T. A. & GARTLAND, JR., E. C. (1998) Finite element analysis of the Landau-de Gennes minimization problem for liquid crystals. *SIAM J. Numer. Anal.* **35**(1), 336–362.
- [9] DE GENNES, P. G. (1971) Short range order effects in the isotropic phase of nematics and cholesterics. *Mol. Cryst. Liq. Cryst.* **12**(3), 193–214.
- [10] DE GENNES, P. G. & PROST, J. (1995) *The Physics of Liquid Crystals*. International Series of Monogr. Clarendon Press, Oxford.
- [11] DICKMANN, S. (1995) *Numerische Berechnung von Feld und Molekülausrichtung in Flüssigkristallanzeigen*. PhD thesis, University of Karlsruhe.
- [12] ERICKSEN, J. L. (1966) Inequalities in liquid crystal theory. *Phys. Fluids* **9**(6), 1205–1207.
- [13] FATKULLIN, I. & SLASTIKOV, V. (2008) On spatial variations of nematic ordering. *Physica D* **237**(20), 2577–2586.
- [14] FRANK, F. C. (1958) I. Liquid crystals. On the theory of liquid crystals. *Discuss. Faraday Soc.* **25**, 19–28.
- [15] GARTLAND, JR., E. C. (2013) An overview of the Oseen–Frank elastic model. <https://www.newton.ac.uk/files/seminar/20130108090009401-153462.pdf>.
- [16] GARTLAND, JR., E. C. (2018) Scalings and limits of Landau–de Gennes models for liquid crystals: a comment on some recent analytical papers. *Math. Model. Anal.* **23**(3), 414–432.

- [17] GOLOVATY, D., KIM, Y.-K., LAVRETOVICH, O. D., NOVACK, M. & STERNBERG, P. (2019) Phase transitions in nematics: textures with tactoids and disclinations. *arXiv e-prints* [arXiv:1902.06342](https://arxiv.org/abs/1902.06342).
- [18] GOLOVATY, D., NOVACK, M., STERNBERG, P. & VENKATRAMAN, R. (2018) A model problem for nematic-isotropic transitions with highly disparate elastic constants. *arXiv e-prints* [arXiv:1811.12586](https://arxiv.org/abs/1811.12586).
- [19] GOLOVATY, D., STERNBERG, P. & VENKATRAMAN, R. (2019) A Ginzburg-Landau type problem for highly anisotropic nematic liquid crystals. *SIAM J. Math. Anal.* **51**(1), 276–320.
- [20] HARDT, R., KINDERLEHRER, D. & LIN, F.-H. (1986) Existence and partial regularity of static liquid crystal configurations. *Comm. Math. Phys.* **105**(4), 547–570.
- [21] IYER, G., XU, X. & ZARNESCU, A. D. (2015) Dynamic cubic instability in a 2D Q -tensor model for liquid crystals. *Math. Models Methods Appl. Sci.* **25**(8), 1477–1517.
- [22] KATRIEL, J., KVENTSEL, G. F., LUCKHURST, G. R. & SLUCKIN, T. J. (1986) Free energies in the Landau and molecular field approaches. *Liq. Cryst.* **1**(4), 337–355.
- [23] KIM, Y.-K., SHIYANOVSKII, S. V. & LAVRETOVICH, O. D. (2013) Morphogenesis of defects and tactoids during isotropic–nematic phase transition in self-assembled lyotropic chromonic liquid crystals. *J. Phys.: Condens. Matter* **25**(40), 404202.
- [24] LONGA, L., MONSELESAN, D. & TREBIN, H.-R. (1987) An extension of the Landau-Ginzburg-de Gennes theory for liquid crystals. *Liq. Cryst.* **2**(6), 769–796.
- [25] LONGA, L. & TREBIN, H. (1989) Structure of the elastic free energy for chiral nematic liquid crystals. *Phys. Rev. A* **39**(4), 2160–2168.
- [26] LUCKHURST, G. R., NAEMURA, S., SLUCKIN, T. J., THOMAS, K. S. & TURZI, S. S. Molecular-field-theory approach to the Landau theory of liquid crystals: uniaxial and biaxial nematics. *Phys. Rev. E* **85**, 031705.
- [27] MAJUMDAR, A. (2010) Equilibrium order parameters of nematic liquid crystals in the Landau-de Gennes theory. *Eur. J. Appl. Math.* **21**(2), 181–203.
- [28] MAJUMDAR, A. & ZARNESCU, A. (2010) Landau-De Gennes theory of nematic liquid crystals: the Oseen-Frank limit and beyond. *Arch. Ration. Mech. Anal.* **196**(1), 227–280.
- [29] MOTTRAM, N. J. & NEWTON, C. J. P. (2014) Introduction to Q -tensor theory. *ArXiv e-prints*.
- [30] NAKAGAWA, M. (1997) On the relation between tensor and vector approaches of nematodynamics. *Liq. Cryst.* **23**(4), 561–567.
- [31] OSEEN, C. W. (1933) The theory of liquid crystals. *Trans. Faraday Soc.* **29**, 883–899.
- [32] VIRGA, E. G. (1994) *Variational Theories for Liquid Crystals*, Applied Mathematics and Mathematical Computation, Vol. 8. Chapman & Hall, London.
- [33] ZHOU, S., NEUPANE, K., NASTISHIN, Y. A., BALDWIN, A. R., SHIYANOVSKII, S. V., LAVRETOVICH, O. D. & SPRUNT, S. (2014) Elasticity, viscosity, and orientational fluctuations of a lyotropic chromonic nematic liquid crystal disodium cromoglycate. *Soft Matter* **10**, 6571–6581.
- [34] ZOCHER, H. (1933) The effect of a magnetic field on the nematic state. *Trans. Faraday Soc.* **29**, 945–957.

Appendix. Relationship with generalized Landau-de Gennes elastic free energy

Here, we elucidate the relationship between the energy (2.19) and the independent elastic invariants in [24]. First, we observe that

$$\left| \left(\frac{s_0}{3} \mathbf{I} \pm \mathcal{Q} \right) \operatorname{div} \mathcal{Q} \right|^2 = \frac{s_0^2}{9} |\operatorname{div} \mathcal{Q}|^2 \pm \frac{2s_0}{3} \operatorname{div} \mathcal{Q} \cdot \mathcal{Q} \operatorname{div} \mathcal{Q} + |\mathcal{Q} \operatorname{div} \mathcal{Q}|^2 \quad (\text{A.1})$$

and, utilising the anticommutator $\{A, B\} := AB + BA$,

$$\begin{aligned} \left| \left(\frac{s_0}{3} \mathbf{I} \pm \mathcal{Q} \right) \operatorname{curl} \mathcal{Q} \right|^2 &= \frac{1}{2} \sum_{j=1}^3 \left| \left\{ \frac{s_0}{6} \mathbf{I} \mp \mathcal{Q}, \nabla \mathcal{Q}_j - \nabla \mathcal{Q}_j^T \right\} \right|^2 \\ &= \frac{s_0^2}{9} \sum_{j=1}^3 \left(|\nabla \mathcal{Q}_j|^2 - \nabla \mathcal{Q}_j \cdot \nabla \mathcal{Q}_j^T \right) \end{aligned}$$

$$\mp \frac{S_0}{3} \sum_{j=1}^3 \left(\nabla Q_j - \nabla Q_j^T \right) \cdot \left(Q \left(\nabla Q_j - \nabla Q_j^T \right) + \left(\nabla Q_j - \nabla Q_j^T \right) Q \right) + \left| \left(Q \left(\nabla Q_j - \nabla Q_j^T \right) + \left(\nabla Q_j - \nabla Q_j^T \right) Q \right) \right|^2. \tag{A.2}$$

The terms in (A.1) can be written as

$$\begin{aligned} |\operatorname{div} Q|^2 &= Q_{ij,j} Q_{ik,k}, \\ \operatorname{div} Q \cdot Q \operatorname{div} Q &= Q_{im} Q_{ij,j} Q_{ml,l}, \\ |Q \operatorname{div} Q|^2 &= Q_{ik} Q_{ii} Q_{kj,j} Q_{lm,m}. \end{aligned}$$

These correspond to the invariants $[L_2^{(2)}]$, $[L_3^{(3)}]$ and $[L_6^{(4)}]$ in [24], respectively. Expanding the terms quadratic in Q in (A.2) results in expressions

$$\begin{aligned} |\nabla Q_j|^2 &= Q_{ij,k} Q_{ij,k}, \\ \nabla Q_j \cdot \nabla Q_j^T &= Q_{ij,k} Q_{kj,i}, \end{aligned}$$

corresponding to $[L_1^{(2)}]$ and $[L_3^{(2)}]$ in [24]. The cubic terms in (A.2) are

$$\begin{aligned} \nabla Q_j \cdot Q \nabla Q_j &= Q_{il} Q_{ij,m} Q_{lj,m}, \\ \nabla Q_j \cdot Q \nabla Q_j^T &= Q_{il} Q_{ij,m} Q_{mj,l}, \\ \nabla Q_j \cdot \nabla Q_j Q &= Q_{il} Q_{mj,i} Q_{mj,l}, \end{aligned}$$

and these are, respectively, the invariants $[L_4^{(3)}]$, $[L_6^{(3)}]$ and $[L_7^{(3)}]$ in [24]. Note that $[L_7^{(3)}]$ is not an independent invariant (cf. [24]) because it can be written as

$$[L_7^{(3)}] = 2[L_6^{(3)}] + [L_5^{(3)}] - 2[L_4^{(3)}] + [L_3^{(3)}] + 2[L_2^{(3)}] - 2[L_1^{(3)}].$$

Finally, the fourth-order terms in (A.2) are as follows:

$$\begin{aligned} Q \nabla Q_j \cdot Q \nabla Q_j &= Q_{il} Q_{im} Q_{lj,p} Q_{mj,p}, \\ Q \nabla Q_j \cdot Q \nabla Q_j^T &= Q_{il} Q_{lm} Q_{ik,p} Q_{pk,m}, \\ Q \nabla Q_j^T \cdot Q \nabla Q_j^T &= Q_{il} Q_{lm} Q_{kj,i} Q_{kj,m}, \\ Q \nabla Q_j \cdot \nabla Q_j Q &= Q_{ik} Q_{lm} Q_{lj,i} Q_{mj,k}, \\ Q \nabla Q_j \cdot \nabla Q_j^T Q &= Q_{ik} Q_{ml} Q_{lj,i} Q_{kj,m}. \end{aligned}$$

The first term in this list is the invariant $[L_9^{(4)}]$, the second term is $[L_9^{(4)}]$ and the fourth term is $[L_{11}^{(4)}]$. The third and fifth terms do not belong to the list of independent invariants in [24], and thus must be linear combinations of the invariants $[L_1^{(4)}]$ through $[L_{13}^{(4)}]$ in [24], cf. the following lemma. We will not pursue the issue of finding the coefficients of these combinations further.

Lemma 4.1 *The terms*

$$Q \nabla Q_j^T \cdot Q \nabla Q_j^T = Q_{il} Q_{lm} Q_{kj,i} Q_{kj,m} \tag{A.3}$$

and

$$Q \nabla Q_j \cdot \nabla Q_j^T Q = Q_{ik} Q_{ml} Q_{lj,i} Q_{kj,m} \tag{A.4}$$

are frame indifferent and materially symmetric, and so can each be written as a linear combination of the 13 quartic $[L_j^{(4)}]$ invariants in [24].

Proof We begin with the first term (A.3) and follow the discussion in [1]. Both conditions involve invariance of (A.3) under different coordinate changes $x \rightarrow z$, with corresponding measurements of the tensor Q, Q^* in the $x = (x_1, x_2, x_3)$ (standard Cartesian) and $z = (z_1, z_2, z_3)$ (Cartesian after a change of variables) coordinates, respectively. More precisely, the frame indifference condition entails that for $\bar{x} \in \Omega, \tilde{R} \in SO(3)$ and $z = \bar{x} + \tilde{R}(x - \bar{x})$,

$$Q \nabla_x^T Q \cdot Q \nabla_x^T Q = Q^* \nabla_z^T Q^* \cdot Q^* \nabla_z^T Q^*. \tag{A.5}$$

Material symmetry is similar, except that $z = \bar{x} + \hat{R}(x - \bar{x})$, where \hat{R} is the reflection $\hat{R} = -I + 2e \otimes e, |e| = 1$. Since any $R \in O(3)$ can be expressed as $\hat{R}\tilde{R}$ for a reflection \hat{R} and $\tilde{R} \in SO(3)$, verifying these two conditions can be combined and simplified into a single calculation, cf. [1]. Therefore, we must check that (A.5) holds for $R \in O(3)$. We will start on the right-hand side of (A.5) and simplify, using the relation $R_{\gamma\alpha}R_{\gamma\beta} = \delta_{\alpha\beta}$ and the identities

$$\begin{aligned} Q_{ab}^* &= R_{af}Q_{fg}R_{bg}, & Q_{de,a}^* &= R_{do}R_{ep}R_{aq}Q_{op,q}, \\ Q_{bc}^* &= R_{bh}Q_{hn}R_{cn}, & Q_{de,c}^* &= R_{dr}R_{es}R_{ct}Q_{rs,t}, \end{aligned}$$

which can be derived as in [1]. Here, $\delta_{\alpha\beta}$ is the usual Kronecker delta, and the first relation is a restatement of the identity $R^T R = I$ for an orthogonal matrix. We write

$$\begin{aligned} &Q^* \nabla_z^T Q^* \cdot Q^* \nabla_z^T Q^* \\ &= Q_{ab}^* Q_{bc}^* Q_{de,a}^* Q_{de,c}^* \\ &= R_{af}Q_{fg}R_{bg}R_{do}R_{ep}R_{aq}Q_{op,q}R_{bh}Q_{hn}R_{cn}R_{dr}R_{es}R_{ct}Q_{rs,t} \\ &= R_{af}R_{aq}R_{bg}R_{bh}R_{do}R_{dr}R_{ep}R_{es}R_{ct}R_{cn}Q_{fg}Q_{hn}Q_{op,q}Q_{rs,t} \\ &= \delta_{fq}\delta_{gh}\delta_{or}\delta_{ps}\delta_{tn}Q_{fg}Q_{hn}Q_{op,q}Q_{rs,t} \\ &= Q_{fg}Q_{gt}Q_{op,f}Q_{op,t}. \end{aligned}$$

Of course, the indices f, g, t, o, p can be replaced by i, j, k, l, m , and we have shown that $Q^* \nabla_z^T Q^* \cdot Q^* \nabla_z^T Q^* = Q \nabla_x^T Q \cdot Q \nabla_x^T Q$.

Moving on to the second term, we first record the identities

$$\begin{aligned} Q_{ab}^* &= R_{af}Q_{fg}R_{bg}, & Q_{de,a}^* &= R_{do}R_{ep}R_{aq}Q_{op,q}, \\ Q_{cd}^* &= R_{ch}Q_{hn}R_{dn}, & Q_{be,c}^* &= R_{br}R_{es}R_{ct}Q_{rs,t}. \end{aligned}$$

We may now calculate

$$\begin{aligned} &Q^* \nabla_z Q_j^* \cdot \nabla_z^T Q_j^* Q^* \\ &= Q_{ab}^* Q_{cd}^* Q_{de,a}^* Q_{be,c}^* \\ &= R_{af}Q_{fg}R_{bg}R_{ch}Q_{hn}R_{dn}R_{do}R_{ep}R_{aq}Q_{op,q}R_{br}R_{es}R_{ct}Q_{rs,t} \\ &= R_{af}R_{aq}R_{bg}R_{br}R_{ch}R_{ct}R_{dn}R_{do}R_{ep}R_{es}Q_{fg}Q_{hn}Q_{op,q}Q_{rs,t} \\ &= \delta_{fq}\delta_{gr}\delta_{ht}\delta_{no}\delta_{ps}Q_{fg}Q_{hn}Q_{op,q}Q_{rs,t} \\ &= Q_{fg}Q_{hn}Q_{np,f}Q_{gp,h} \\ &= Q \nabla Q_j \cdot \nabla Q_j^T Q. \end{aligned} \quad \square$$