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Models for biaxial nematic liquid crystals

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Abstract. In the Landau-de Gennes theory, the order parameter describing a biaxial nematic liquid crystal is, at each point of the region occupied by the system, a symmetric, traceless 3 × 3 matrix with three distinct eigenvalues. In the constrained case of matrices with constant eigenvalues, the order parameter space identifies with an eightfold quotient of the 3-sphere, and a configuration of a biaxial nematic liquid crystal is described by a map into such a quotient. We express the (simplest form of the) Landau-de Gennes elastic free-energy density of biaxial nematics as a density on maps into the 3-sphere, whose functional dependence is restricted by the requirements that it is well-defined on the class of configuration maps (residual symmetry) and is independent of arbitrary superposed rigid rotations (frame indifference). This is a report on joint work with D. Mucci [18], to which we refer for more details and applications.

1. The Landau–de Gennes Q-tensor model for nematic liquid crystals
A liquid crystal is a state of matter, called mesomorphic, intermediate between the crystal state and the liquid state, in which the molecules retain preferential orientations relative to one another over large distances. There are many different types of liquid crystals, the main classes being nematics, cholesterics and smectics. Nematic liquid crystals consist of rod-like molecules which have a locally preferred direction of orientation.

In the Landau–de Gennes theory [7, 16], the state of alignment of a nematic liquid crystal occupying a region Ω is described, at each point of Ω, by an order parameter, Q, the so-called Q-tensor, which is a symmetric, traceless 3 × 3 matrix. By definition, Q vanishes in the isotropic phase and thus measures the extent to which the system is ordered in the region Ω. In a general nematic phase, Q has five degrees of freedom, two of them specify the degree of order, while the remaining three are the angles needed to specify the principal directions. A nematic phase is said biaxial when Q has three distinct eigenvalues, uniaxial when Q has two non-zero equal eigenvalues. While uniaxial nematics has been known to exist for more than a century, the experimental evidence of biaxial nematics is more recent [13].

A general Q-tensor can be written as

\[ Q = S_1 \left( n \otimes n - \frac{1}{3} I \right) + S_2 \left( m \otimes m - \frac{1}{3} I \right), \quad S_1, S_2 \in \mathbb{R}, \quad n, m \in S^2, \]

(1)

where n, m are orthonormal eigenvectors of Q and S_1, S_2 are scalar order parameters given by S_1 = λ_1 - λ_3 = 2λ_2 + λ_3, S_2 = λ_2 - λ_3 = λ_1 + 2λ_2 in terms of the eigenvalues λ_1, λ_2, λ_3 of Q. We may assume λ_1 ≤ λ_2 ≤ λ_3 and λ_1, λ_2, λ_3 ∈ (-\frac{1}{3}, \frac{2}{3}) (see [2]). In the uniaxial case, Q takes the form

\[ Q = s \left( r \otimes r - \frac{1}{3} I \right), \quad s \in \mathbb{R}, \quad r \in S^2, \]

(2)
where $s$ is the only scalar order parameter. The Landau–de Gennes free-energy functionals are nonlinear integral functionals of $\mathbf{Q}$ and its spatial derivatives. In general, it is required that any energy density $\Psi = \Psi(\mathbf{Q}, \nabla \mathbf{Q})$ satisfy the condition of frame indifference which amounts to

$$\Psi(\mathbf{Q}, \nabla \mathbf{Q}) = \Psi( M \mathbf{Q} M^T, \mathbf{D}^*) \quad \forall M = (M^i_j) \in SO(3),$$

(3)

where $\mathbf{D}^*$ denotes a third order tensor such that $\mathbf{D}^*_{ijk} = M^i_l M^j_m M^k_p \mathbf{Q}_{lmp}$, and $\mathbf{Q}_{ij,k} = \frac{\partial}{\partial x_k} \mathbf{Q}_{ij}$ denote the first order partial derivatives of $\mathbf{Q}$ (compare, for example, [1]).

A commonly used expression for the free energy of a nematic liquid crystal is [7, 6, 16, 20]

$$\mathcal{F}(\mathbf{Q}, \Omega) := \int_\Omega [\psi(\mathbf{Q}, \nabla \mathbf{Q}) + f_B(\mathbf{Q})] \, dx,$$

(4)

where $f_B(\mathbf{Q}) = f_B(\text{tr}(\mathbf{Q}^2), \text{tr}(\mathbf{Q}^3))$ is the bulk part (a function of the principal invariants of $\mathbf{Q}$) and

$$\psi(\mathbf{Q}, \nabla \mathbf{Q}) = L_1 I_1 + L_2 I_2 + L_3 I_3 + L_4 I_4$$

(5)

is the elastic free-energy density; the $I_i$ are material constants and the $I_i$ are elastic invariants,

$$I_1 = Q_{i,j,j} Q_{i,k,k}, \quad I_2 = Q_{i,k,j} Q_{i,j,k}, \quad I_3 = Q_{i,j,k} Q_{i,j,k}, \quad I_4 = Q_{i,k,l} Q_{i,j,l} Q_{i,j,k}$$

(6)

(summation over repeated indices is assumed). The bulk energy $f_B(\mathbf{Q})$ is invariant under the $SO(3)$-action by conjugation on the five-dimensional space of $\mathbf{Q}$-tensors, so that the critical points of the bulk energy form an orbit of solutions in the space of $\mathbf{Q}$-tensors. Clearly, a $\mathbf{Q}$-tensor taking values in a group orbit has constant scalar order parameters $S_1, S_2$. In many applications, it suffices to work in the constrained Landau–de Gennes theory, in which $\mathbf{Q}$ has constant $S_1, S_2$, independent of $x \in \Omega$, and hence constant eigenvalues [3, 14]. In the constrained theory, the bulk energy is constant and one only has to consider the elastic free energy.

2. The Oseen–Frank vector model for uniaxial nematics

In the Oseen–Frank theory [10, 19], a configuration of a liquid crystal is described by a unit vector field $\mathbf{r} : \Omega \to S^2$, which represents the direction of preferred molecular alignment. This theory has received much analytical and computational attention, but is not sufficiently general to represent biaxial states. In this model, the elastic energy density associated to $\mathbf{r}$ is given by

$$w(\mathbf{r}, \nabla \mathbf{r}) = K_1 (\text{div} \mathbf{r})^2 + K_2 (\mathbf{r} \cdot \text{curl} \mathbf{r})^2 + K_3 |\mathbf{r} \times \text{curl} \mathbf{r}|^2 + (K_2 + K_4)[\text{tr}[(\nabla \mathbf{r})^2] - (\text{div} \mathbf{r})^2],$$

where the $K_i$ are elastic constants. This energy density satisfies the invariance properties

$$w(\mathbf{r}, \nabla \mathbf{r}) = w(-\mathbf{r}, -\nabla \mathbf{r}); \quad w(\mathbf{r}, \nabla \mathbf{r}) = w(H \mathbf{r}, H \nabla \mathbf{r} H^T), \quad \forall H \in O(3),$$

(7)

so that the corresponding functional is well defined on vector fields in $\Omega$, regardless of the orientation. The first equation in (7) accounts for the lack of polarity of nematics, while the second expresses the frame indifference of the energy density and the material symmetry condition corresponding to the lack of chirality of nematics. Requiring that the second condition in (7) hold for $SO(3)$ only, is equivalent to the frame indifference condition (3) for constrained uniaxial $\mathbf{Q}$-tensors. The vector approach has been further developed in [8, 9, 12]. The Oseen–Frank model does not respect the “head-to-tail” symmetry, in which $\mathbf{r}$ and $-\mathbf{r}$ represent the same state; instead, $\mathbf{r}$ should take values in $S^2$ with antipodal points identified, i.e., in the projective plane $\mathbb{R}P^2$. The constrained uniaxial $\mathbf{Q}$-tensor representation (2) clearly respects this symmetry.

In the constrained uniaxial case, formally calculating the energy density (5) in terms of $\mathbf{r}$ and $\nabla \mathbf{r}$, it can be checked (see [3, 16, 18]) that the Landau-de Gennes elastic free-energy density
\(\psi(Q, \nabla Q)\) reduces to the Oseen-Frank energy density \(w(r, \nabla r)\), that is, it is possible to choose the \(L_i\) and the \(K_i, i = 1, 2, 3, 4\), so that

\[
\psi(Q, \nabla Q) = w(r, \nabla r).
\]

However, according to [3], although the elastic energies can be taken to be the same in the two theories, the result of the energy minimization might be different. For the related problems of line field orientability and map lifting in the Sobolev setting, we refer the reader to [3, 17].

3. Constrained theory of biaxial nematic liquid crystals

Let \(Q(\lambda_1, \lambda_2, \lambda_3)\) be the set of all constrained biaxial \(Q\)-tensors of the form (1) with distinct constant eigenvalues \(\lambda_1, \lambda_2, \lambda_3\). Any element \(Q \in Q(\lambda_1, \lambda_2, \lambda_3)\) can be written in the form \(Q = \mathbf{G} \mathbf{A} \mathbf{G}^T\), for some \(\mathbf{G} \in SO(3)\), where \(\mathbf{A} = \text{diag}(\lambda_1, \lambda_2, \lambda_3)\) is the diagonal matrix of the eigenvalues. Thus, \(Q(\lambda_1, \lambda_2, \lambda_3)\) coincides with the orbit of \(\mathbf{A}\) with respect to the \(SO(3)\)-action by conjugation on the space of \(Q\)-tensors, and can be identified with the homogeneous space \(SO(3)/D_2\), where \(D_2\) is the abelian four-element dihedral group ([15]). Using the identification of \(S^3\) with the Lie group of unit quaternions, \(Sp(1)\), and the 2:1 covering map \(\Phi: S^3 \to SO(3)\), the order parameter space of constrained biaxial nematics is then diffeomorphic to the homogeneous manifold \(S^3/\mathcal{H}\), where \(\mathcal{H} = \{\pm 1, \pm i, \pm j, \pm k\}\) is the non-abelian eight-element quaternion group. In this model, a configuration of a biaxial nematic liquid crystal is described by a map from \(\Omega\) to \(S^3/\mathcal{H}\), as opposed to the constrained uniaxial case where the order parameter space is \(\mathbb{R}P^2\).

4. A vector model for the elastic energy of constrained biaxial nematics

Motivated by (8) in the constrained uniaxial case, our purpose is to express, in the constrained biaxial case, the Landau-de Gennes elastic free-energy density \(I_3(Q, \nabla Q)\) as a density on maps \(q : \Omega \to S^3\). For, we need first to identify the conditions on a generic energy density \(f: S^3 \times M_{4 \times 3} \to [0, +\infty)\), depending on \(q: \Omega \to S^3\) and its first derivatives, in order that: (a) \(f\) is independent of arbitrary superposed rigid rotations (frame indifficulty condition); (b) \(f\) is well defined on the class of configuration maps \(\Omega \to S^3/\mathcal{H}\) (residual symmetry condition), that corresponds to the “head-to-tail” symmetry in the uniaxial case. As for condition (a), we say that \(f: S^3 \times M_{4 \times 3} \to [0, +\infty)\) satisfies the frame invariance condition if, for any \(q \in S^3 \cong Sp(1)\),

\[
f(w, H) = f(qw, L(q)H\Phi(q)^T) \quad \forall (w, H) \in S^3 \times M_{4 \times 3},
\]

where \(L(q)\) is the matrix of the \(\mathbb{R}\)-linear map \(w \mapsto qw\) on the algebra of quaternions \(\mathbb{H}\), relative to \(\{1, i, j, k\}\), and \(\Phi(q)\) is the rotation induced by \(q\) via the 2:1 covering map \(\Phi: S^3 \to SO(3)\). We prove that this invariance condition is indeed equivalent to the frame indifficulty condition in the sense of \(Q\)-tensors (see [18]). The proof uses the identification \(S^3 \cong Sp(1)\) and the relations between quaternions and rotations in \(\mathbb{R}^3\) and \(\mathbb{R}^4\). As for condition (b), we say that \(f: S^3 \times M_{4 \times 3} \to [0, +\infty)\) satisfies the residual symmetry property if, for any \(q \in \mathcal{H}\), one has

\[
f(w, H) = f(qw, L(q)H) \quad \forall (w, H) \in S^3 \times M_{4 \times 3}.
\]

Given that, we express the Landau-de Gennes energy density \(I_3\) in terms of maps \((u, v) : \Omega \to S^3\), namely, we explicitly compute \(f_3: S^3 \times M_{4 \times 3} \to [0, +\infty)\), so that

\[
I_3(Q, \nabla Q) = f_3((u, v), \nabla(u, v)),
\]

provided that \(Q\) corresponds to \((u, v)\), that is, \(Q = \mathbf{G} \mathbf{A} \mathbf{G}^T\) with \(\mathbf{G} = \Phi((u, v))\). For \((u, v) \in S^3\) and \(H \in M_{4 \times 3}\), the function \(f_3: S^3 \times M_{4 \times 3} \to [0, +\infty)\) is given by

\[
f_3((u, v), H) := (k_1 - k_2 + k_3)|H|^2 - k_1 A((u, v), H)^2 + k_2 B((u, v), H)^2 - k_3 C((u, v), H)^2,
\]
where $H = (H^j_i)$, $j = 0, 1, 2, 3; i = 1, 2, 3$, $|H|^2 := \sum_{i=1}^{3} \sum_{j=0}^{3} (H^j_i)^2$, $k_1 := 8S_1(S_1 - S_2)$, $k_2 := 8S_2(S_1 - S_2)$, $k_3 := 8S_1S_2 (k_1, k_2, k_3 > 0$ and $(k_1 - k_2 + k_3) = 8(S_1^2 + S_2^2 - S_1S_2) > 0)$, and

\[
\begin{align*}
A((u, v), H)^2 &:= \sum_{i=1}^{3} (-v_1 H^i_1 + u H^i_1 + v_3 H^i_2 - v_2 H^i_3)^2, \\
B((u, v), H)^2 &:= \sum_{i=1}^{3} (-v_2 H^i_1 - v_3 H^i_2 + u H^i_3 + v_1 H^i_1)^2, \\
C((u, v), H)^2 &:= \sum_{i=1}^{3} (-v_3 H^i_1 + v_2 H^i_1 - v_1 H^i_2 + u H^i_3)^2.
\end{align*}
\]

In particular, the energy density model $f_3((u, v), \nabla (u, v))$ is proved to satisfy the above mentioned frame indifference and residual symmetry conditions. Therefore, $f_3$ may be interpreted as the elastic energy density model for the configuration maps $(u, v): \Omega \to \mathbb{S}^3/\mathcal{H}$ of a constrained biaxial nematic liquid crystal. (In principle, similar calculations can be performed also for the elastic invariants $I_1$, $I_2$ and $I_3$, see [6, 18, 21].) The corresponding elastic energy functional

\[
\mathcal{F}_3((u, v), \Omega) := \int_{\Omega} f_3((u, v)(x), \nabla (u, v)(x)) \, dx
\]

is well defined, for instance, on Sobolev maps $(u, v): \Omega \to \mathbb{S}^3/\mathcal{H}$, where $\Omega$ is a bounded domain of $\mathbb{R}^3$. This representation is also used to prove the coercivity of the energy density. This yields, for instance, that the class of measurable and a.e. weakly differentiable functions from $\Omega$ to $\mathbb{S}^3/\mathcal{H}$ with finite $\mathcal{F}_3$-energy agrees with the Sobolev class $W^{1,2}(\Omega, \mathbb{S}^3/\mathcal{H})$. A general lifting technique described by Bethuel and Chiron in [5], combined with a strong density result of Bethuel [4], are then used to prove results on lower semicontinuity and strong density of smooth maps (see [18] for more details).

References

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