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Author for correspondence:
Arghir Zarnescu
e-mail: azarnescu@bcamath.org

Mathematical problems of nematic liquid crystals: between dynamical and stationary problems

Arghir Zarnescu[1,2,3]

[1]IKERBASQUE, Basque Foundation for Science, Plaza Euskadi 5, 48009, Bilbao, Bizkaia, Spain
[2]BCAM, Basque Center for Applied Mathematics, Mazarredo, 14, E48009 Bilbao, Bizkaia, Spain
[3]'Simion Stoilow' Institute of the Romanian Academy, 21 Calea Griviței, 010702 Bucharest, Romania

AZ, 0000-0002-3620-6196

Mathematical studies of nematic liquid crystals address in general two rather different perspectives: that of fluid mechanics and that of calculus of variations. The former focuses on dynamical problems while the latter focuses on stationary ones. The two are usually studied with different mathematical tools and address different questions. The aim of this brief review is to give the practitioners in each area an introduction to some of the results and problems in the other area. Also, aiming to bridge the gap between the two communities, we will present a couple of research topics that generate natural connections between the two areas.

This article is part of the theme issue 'Topics in mathematical design of complex materials'.

1. Introduction

Liquid crystals are a state of matter which exhibits some properties specific to fluids (for instance they flow) and also some properties (such as optical ones) more common to solids. Since their discovery in 1888 [1] a large number of classes and types of liquid crystals have been discovered and synthesized [2]. The most popular from a technological point of view and the most studied mathematically are the *nematic liquid crystals (NLC)*. We will limit our discussion to these, specifically to the *thermotropic* NLC, that change phase subject to a change of temperature.

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The NLC materials have rod-like molecules. At a high enough temperature, the centres of mass of the molecules are isotropically distributed and there is no preferred orientational distribution; the material behaves essentially like an *isotropic fluid*. Upon lowering the temperature one would reach in an ordinary material the solid phase, with localized centres of mass and orientations of the molecules. The specific feature of the NLC is that between the temperatures characteristic to the isotropic and the solid phases there is a special range of temperatures. For these temperatures, the material exhibits *the nematic phase*, namely the centres of mass are isotropically distributed but there is a long-range orientational order, that is locally the molecules have a preferred direction.

There exist several competing models that aim to provide a continuum-level description of NLC [3,4]. These models describe the material as functions defined on Ω, an open set in $\mathbb{R}^d$, $d = 2, 3$ (modelling the space filled with NLC material) and taking values into *order parameter* spaces, namely sets that attempt to encode mathematically the local ordering of the molecules. Thus we have:

— Oseen–Frank (OF) theory, working with $n : \Omega \to \mathbb{S}^2$ where $\mathbb{S}^2 := \{y \in \mathbb{R}^3; |y| = 1\}$, see [4,5].
— Ericksen (E) theory, working with $(n, s) : \Omega \to \mathbb{S}^2 \times [-1/2, 1]$ see [4,6].
— Landau de Gennes (LDG) theory, using $Q : \Omega \to \mathcal{S}_0$ with $\mathcal{S}_0 := \{Q \in \mathbb{R}^{3\times 3}; Q = Q^t; \mathrm{tr}(Q) = 0\}$ the space of Q-tensors, see [3,7,8].

The OF model describes just the nematic phase, excluding certain physical features such as local isotropic melting, which is allowed in the E theory. The LDG theory allows for describing the phase transitions, the non-orientable configurations (discussed in §3), the local isotropic melting as well as the so-called biaxial phases [7,8].

The mathematics of liquid crystals has developed extraordinarily, particularly in recent years, with more than a thousand papers being listed on Mathscinet with reference to liquid crystals. Most of these study thermotropic NLC. In this brief review, limited by the space constraints, we will focus on the LDG model, as it is the most comprehensive, briefly mentioning other models and the specific differences between the models. Moreover, we will not aim to provide a comprehensive overview of the current literature, but merely to make some introductory points (biased by the author's preferences) particularly relevant to highlighting the interactions between the fluid mechanics and calculus of various perspectives.

2. Fluid mechanics perspectives

Nematic liquid crystals are most comprehensively described, from the point of view of rational mechanics, as complex non-Newtonian fluids. As such, their evolution is subject to certain conservation laws, that lead to equations for the nematic director $Q(t, x)$ coupled with the equations for the velocities $u(t, x)$ of the centres of mass, with t being the time variable and x the spatial one.

The director equations result out of the angular momentum conservation and in the Beris–Edwards (BE) model (see [9], here following the notations and formalism from [10]) take the form (assuming a non-dimensionalized setting, see [11]):

$$D_t Q - S(\nabla u, Q) = -\Gamma \frac{\partial \mathcal{F}_{\mathrm{LDG}}}{\partial Q} \tag{2.1}$$

with $\Gamma > 0$. Here $D_t Q = \partial_t Q + u \cdot \nabla Q$ is the material derivative of Q while

$$\mathcal{F}_{\mathrm{LDG}}(Q) = \int \frac{L}{2}|\nabla Q|^2 + f_B(Q)\,\mathrm{d}x \tag{2.2}$$

is the free energy of the liquid crystal molecules. Here, we denoted with $f_B \overset{\mathrm{def}}{=} -(a/2)\,\mathrm{tr}(Q^2) - (b/3)\mathrm{tr}(Q^3) + (c/4)(\mathrm{tr}(Q^2))^2$ the *bulk potential* and by $\partial \mathcal{F}_{\mathrm{LDG}}/\partial Q = -L\Delta Q - aQ - b[Q^2 - (\mathrm{tr}(Q^2)/3)Id] + cQ\mathrm{tr}(Q^2)$ the variational derivative within $\mathcal{S}_0$. The L, a, b, c constants are specific to the material with $L > 0$ and $a, b \in \mathbb{R},\ c > 0$.

If $u=0$ the Q-tensor equation would simply be a gradient flow of the free energy. For $u\neq 0$, the molecules are transported by the flow (as indicated by the convective derivative D_t) as well as being tumbled and aligned by the flow, a fact described by the term:

$$S(\nabla u, Q) \stackrel{\text{def}}{=} (\xi D + \Omega)\left(Q+\frac{1}{3}Id\right) + \left(Q+\frac{1}{3}Id\right)(\xi D - \Omega) - 2\xi\left(Q+\frac{1}{3}Id\right)\mathrm{tr}(Q\nabla u), \tag{2.3}$$

where $D \stackrel{\text{def}}{=} 1/2(\nabla u + (\nabla u)^T)$ and $\Omega \stackrel{\text{def}}{=} 1/2(\nabla u - (\nabla u)^T)$ are, respectively, the symmetric part and the antisymmetric part, of the velocity gradient matrix ∇u. The constant ξ is a material dependent constant, the case $\xi = 0$ being referred to as the *co-rotational case*.

The equations for the flow u resulting out of the linear momentum conservation satisfy the forced Navier–Stokes system:

$$\left.\begin{aligned} &\partial_t u + (u\cdot\nabla)u = \nu\Delta u + \nabla p + \lambda\nabla\cdot T\\ &\nabla\cdot u = 0, \end{aligned}\right\} \tag{2.4}$$

where ν, $\lambda > 0$ with λ measuring the ratio of the elastic effects (produced by the liquid crystal molecules) to that of the diffusive effects. The forcing is provided by the additional stress caused by the anisotropy of the liquid crystal molecules, more specifically we have:

$$\begin{aligned} T \stackrel{\text{def}}{=} {} & \xi\left(Q+\frac{1}{3}Id\right)\frac{\partial\mathcal{F}_{\mathrm{LDG}}}{\partial Q} + \xi\frac{\partial\mathcal{F}_{\mathrm{LDG}}}{\partial Q}\left(Q+\frac{1}{3}Id\right) - 2\xi\left(Q+\frac{1}{3}Id\right)Q\frac{\partial\mathcal{F}_{\mathrm{LDG}}}{\partial Q}\\ & - L\nabla Q\odot\nabla Q + \frac{\partial\mathcal{F}_{\mathrm{LDG}}}{\partial Q}Q - Q\frac{\partial\mathcal{F}_{\mathrm{LDG}}}{\partial Q}. \end{aligned} \tag{2.5}$$

The coupled systems exhibit a dissipation law, which for smooth enough solutions and under suitable boundary conditions ([12,13]) takes the form:

$$\frac{\mathrm{d}}{\mathrm{d}t}E[u,Q] + \nu\int\frac{1}{2}|\nabla u|^2 + \Gamma\int\mathrm{tr}\left(\frac{\partial\mathcal{F}_{\mathrm{LDG}}}{\partial Q}\right)^2 = 0 \tag{2.6}$$

where the energy $E[u,Q]$ is the sum of the kinetic and free energy $E[u,Q] = (1/2)\int|u|^2\,\mathrm{d}x + \mathcal{F}_{\mathrm{LDG}}(Q)$.

Various other models. *[Q-tensor models]* Other models with a similar structure are the MacMillan (MM) one [14,15] and the Qiang–Shen (QS) one [16]. A couple of models, including one with two different types of Q- tensors, and a thorough derivation of the models are available in [17].

[Ericksen-Leslie model] The most widely accepted model uses the OF formalism, thus replacing a matrix-valued field Q with a unit-length vector field $n\in\mathbb{S}^2$. It was proposed by Ericksen in [18] and then refined by Leslie in [19,20] thus being nowadays referred to as the Ericksen–Leslie (EL) model. Usually, the OF theory refers just to the statical aspects of this theory.

[Relaxed-unit-length Ericksen-Leslie models] The complexity of the EL model as well as the analytical and computational challenges generated by the unit-length constraint have led to the existence of relaxed models, in which the Lagrange multipliers corresponding to the unit-length constraint are replaced by a term of the form $(1/\varepsilon)\nabla F(n)$ with F a suitable function that attains a minimum for $|n|=1$, most commonly $F(n) = (1-|n|^2)^2$. Such a relaxation is sometimes referred to as being a Ginzburg–Landau relaxation, based on the similarities with superconductor models, mentioned in the next section. An alternative, that allows L^∞ bounds in the more complex models to be enforced, is provided by the so-called *singular potentials*, that is potentials that blow-up outside a bounded set, a physical range, see for instance for definition [21–23] and for uses [24,25].

A first such model was the Lin–Liu (LL) model [26] and afterwards, based on an energetic variational approach, the more complex Sun–Liu (SL) model [27]. The SL model shares many analytical similarities with the BE model mentioned before.

[Ericksen model] The E model addresses the challenges induced by the unit-length constraint by introducing an additional variable, a scalar order parameter $s\in[-(1/2),1]$ referred to as a *degree of orientation*. The theory is then built in a manner that works with both degrees of freedom, the

order parameter s and the unit-vector n. The set where s vanishes is interpreted physically as the place where one has no preferred direction, an isotropic melting set. The model was introduced in [6] with a more concise description available in [28]. Physically consistent relaxed-unit-length EL models are very close to the E model.

Analytical studies. The presence of the Navier–Stokes part brings in the analytical difficulties associated with the celebrated system. There is no known instance where the presence of the additional stress tensor would provide better regularity estimates for the velocity u in the coupled system than for the standard Navier–Stokes system. As such the best regularity estimates, existence and uniqueness results that one can hope for are those which use the same level of regularity for the velocity u as for the velocity in the standard Navier–Stokes system.

For the BE system existence and regularity in the whole space was initially proved in [12,13] with subsequent developments in [25,29–35]. In these studies, one often restricts to the co-rotational case $\xi = 0$ which, although not particularly relevant physically, does simplify the system significantly. The problem in bounded domains was studied in [36–39], with studies of numerical schemes available in [40–44]. Long-time behaviour was studied in [45–48]. For the QS model, some results are available in [49–52]. The E system is studied analytically in [28] and numerically in [53,54].

There is a large body of literature on the EL system usually focused on existence in various functional spaces under various assumptions on the coefficients. Fewer results are available in the constrained case (unit-length vector) [55,56] with a large body of the literature in the relaxed case, see [57,58] and the references therein. The most natural assumptions on the coefficients are those physically based, and the best up to date analysis of the necessary conditions, together with suitable analytical results, is contained in [55].

An active direction is studying the inertial effects, which amount to having a second material derivative in the Q-tensor equation (or the n equation in the director models) [49,50,59]. Several works consider extensions adding thermal effects, which amount to having an energy balance, instead of an energy dissipation at the expense of having weaker regularity of the solutions [24,55,60]. Compressible models, although not physically accepted in general, are proving to be popular in all types of models, particularly EL and BE; see [58,61,62] and the references therein.

From a broader scientific perspective, it should be noted that material scientists in general aim to obtain a qualitative understanding of the capacities of the models. Thus they usually use the simpler models that we will present next, in the calculus of variations part. However, there are some notable exceptions, one of them being the work on polymeric liquid crystal flows, relating the theoretical work of F.L. Leslie with that of S. Kwolek, the discoverer of the Kevlar fibre. Such early research, leading to the work of A. Beris, is presented in [63]. Another direction is that of liquid crystal based active matter (e.g. bacteria flow and actin filaments), see for instance [64,65].

3. Calculus of variations perspectives

The main focus, from a calculus of variations perspective, is on the stationary solutions of (2.1) with the flow velocity formally set to 0, namely:

$$L\Delta Q = -aQ - b\left[Q^2 - \tfrac{1}{3}|Q|^2 I_3\right] + cQ|Q|^2 \tag{3.1}$$

with $|Q| \overset{\text{def}}{=} \sqrt{\text{tr}(Q^2)}$ and the term $(1/3)|Q|^2 I_3$ being a Lagrange multiplier enforcing the trace-free constraint on Q.

These are critical points of the free energy functional (2.2) and their study heavily revolves around the patterns they are able to generate and their energetic stability.

From a physical point of view, the most striking and characteristic optical feature of nematic liquid crystals is provided by the *defect patterns*. These appear when one passes polarized light through a thin layer of liquid crystals, and manifest themselves as very localized changes in the intensity and colour of the light passing through the material. They are classified as point, line or wall defects, depending on their dimension. The precise details of defect cores are not

known as they occur on a scale that is too small to probe by the currently available experimental techniques. However, their understanding, study and prediction is of great interest for all the scientific communities involved in the study of liquid crystals.

From a mathematical point of view, it is of paramount importance to understand to what extent the mathematical models are capable of predicting and describing such defect patterns. However, different models have different interpretations of defects. In the OF theory, they are defined as discontinuities of the director. A major drawback of this theory is that it only allows for point defects (in three-dimensional domains) with finite energy, while line and wall defects have infinite energy [66]. The E theory interprets defects as regions of *isotropic melting* that is where the scalar order parameter s vanishes. It allows for both line and wall defects [4,67] but misses potential effects of biaxiality. The LDG theory that uses Q-tensors does not have a universally accepted definition of defects, yet in general regions of *high gradients* and/or regions where one has *eigenvalue crossings* or *eigenframe discontinuities* are regarded as good candidates for the definition of defects [68–70].

A prototypical example of $2D$ defect is obtained by considering solutions $Q : B_R(0) \to \mathcal{S}_0$ of (3.1) where $B_R(0) = \{x \in \mathbb{R}^2; |x| \leq R\}$. The boundary conditions are taken to be:

$$Q_b(x) := s_+ \left(n_b(x) \otimes n_b(x) - \tfrac{1}{3} I_3 \right) \quad \text{as } |x| = R \tag{3.2}$$

where the map $n_b : \partial B_R(0) \to \mathbb{S}^2$ is given in the polar coordinates by

$$n_b(R\cos\varphi, R\sin\varphi) = \left(\cos\left(\frac{k}{2}\varphi\right), \sin\left(\frac{k}{2}\varphi\right), 0 \right), \varphi \in [0, 2\pi), \tag{3.3}$$

with $k \in \mathbb{Z}$. Here, $s_+ = (b + \sqrt{b^2 + 24ac})/4c$ is such that Q_b is minimizing the bulk potential f_B.

It should be noted that Q_b remains invariant if we replace n_b by $-n_b$ at each point in its definition. Thus Q_b depends in fact on the pair $\{-n_b, n_b\}$ not on n_b alone. It can be observed that the set of matrices having the representation of Q_b (for some $n_b \in \mathbb{S}^2$) give a way of embedding the *space of lines*, namely the real projective plane $\mathbb{R}P^2$, into the space of Q-tensors $\mathcal{S}_0$. We can thus think of Q_b taking values into $\mathbb{R}P^2$ (in fact into $\mathbb{R}P^1$ given the specific form of n_b as $n_b \cdot e_3 = 0$).

Moreover, one notes that the number $k/2$ for k even represents the number of times n_b 'winds' around the circle ∂B_R, the topological degree of this map (see for instance [71]). Furthermore, one can observe that if k is odd then $n_b(R\cos\varphi, R\sin\varphi) = -\lim_{\varepsilon\to 0} n_b(R\cos((2\pi - \varepsilon) + \varphi), R(\sin(2\pi - \varepsilon) + \varphi))$ that is after a rotation of 2π around the circle $\partial B_R(0)$ there will be a discontinuity for n_b. However, $Q_b(R\cos\varphi, R\sin\varphi) = \lim_{\varepsilon\to 0} Q_b(R\cos((2\pi - \varepsilon) + \varphi), R(\sin(2\pi - \varepsilon) + \varphi))$ so a similar phenomenon will not happen for Q_b. Thus Q_b provides an example of *non-orientable* boundary condition, namely a *continuous* $\mathbb{R}P^1$-valued map which cannot be simplified into a *continuous* $\mathbb{S}^1$-valued map (see [72] for formal definitions). Nevertheless if we consider Q_b as an $\mathbb{R}P^1$-valued map on $\mathbb{R}^2\backslash\{0\}$, then it has degree $k/2$ about the origin. (For a definition of the degree for $\mathbb{R}P^1$-valued maps, see for instance [66], pp. 685–686). An introduction into these topological aspects is provided in [72,73].

This model can be seen as the $2D$ reduction of the physical situation of a $3D$ cylindrical boundary domain, where the configurations are invariant in the vertical direction (see for instance [74]). It can be checked [75–77] that subject to these boundary conditions we have solutions for (3.1) with the structure

$$Q(x) = u(|x|)\sqrt{2}\left(n(x) \otimes n(x) - \frac{1}{2} I_2 \right) + v(|x|)\sqrt{\frac{3}{2}}\left(e_3 \otimes e_3 - \frac{1}{3} I_3 \right), \tag{3.4}$$

where the vector field n is given by

$$n(r\cos\varphi, r\sin\varphi) = \left(\cos\left(\frac{k}{2}\varphi\right), \sin\left(\frac{k}{2}\varphi\right), 0 \right), \quad r > 0, \varphi \in [0, 2\pi), \tag{3.5}$$

I_3 is the 3×3 identity matrix, $I_2 = I_3 - e_3 \otimes e_3$, and the pair of scalars (u, v) satisfies on $(0, R)$ the following coupled system of ODEs:

$$\begin{cases} u'' + \dfrac{u'}{r} - \dfrac{k^2 u}{r^2} = u\Big[-a + \sqrt{\dfrac{2}{3}} bv + c\left(u^2 + v^2\right) \Big] \\ v'' + \dfrac{v'}{r} = v\Big[-a - \dfrac{1}{\sqrt{6}} bv + c\left(u^2 + v^2\right) \Big] + \dfrac{1}{\sqrt{6}} bu^2, \end{cases} \tag{3.6}$$

It can be checked that this prototypical example of defect exhibits an eigenvector discontinuity and eigenvalue crossing at the origin and also for the physically relevant regime $L \to 0$ (see next section) one has high gradients at zero (see for instance [78]).

The physically relevant question is the physical stability of such defects, because only those defects that are stable are experimentally observed (in the absence of other stabilizing effects such as fields). Mathematically this amounts to checking the positivity of the second variation, that is to check that $\mathcal{L}[Q](P) \geq 0$ for *any* variation $P \in C_c^\infty(B_R, \mathcal{S}_0)$ where

$$\begin{aligned} \mathcal{L}[Q](P) &= \frac{\mathrm{d}^2}{\mathrm{d}t^2}\Big|_{t=0} \int_{B_{R'}} \left\{ \frac{1}{2} |\nabla(Q + tP)|^2 + f_{\text{bulk}}(Q + tP) \right\} \mathrm{d}x \\ &= \int_{B_R} \left\{ |\nabla P|^2 - a|P|^2 - 2b\,\mathrm{tr}(P^2 Q) + c\left(|Q|^2 |P|^2 + 2|\mathrm{tr}(QP)|^2 \right) \right\} \mathrm{d}x. \end{aligned} \tag{3.7}$$

The stability analysis requires a fine understanding of both the scalar profiles u and v as well as of the geometry of the matrix space. Two techniques are particularly relevant: a suitable, space-dependent, basis decomposition of the solution (see [75,76]), and the so-called *Hardy trick* decomposition (see in particular the appendix of [79]) which is essentially a decomposition of an arbitrary perturbation P along a fixed sign profile u (or v) for the pair (u, v) of solutions of (3.6).

There is a large and growing literature on defects, studying various aspects, including: their stability [76,77,79–83], the OF limit [78,84–86], point defects (see [79] and references therein), line defects (see [87] and references therein), deep nematic regime ([88]), uniaxiality ([89]) and anisotropic energies [90–92].

The stationary models studied with calculus of variations models and the full dynamical models have in common an energetical perspective. As such, the stability results obtained in the stationary case should provide a good basis for addressing the effect of the flow on the stability of the prototypical defects. It is natural to consider studying:

> **Research topics 1:** Consider the coupled system (2.1) and (2.4) in a geometry specific to prototypical defects, as mentioned before. Determine the stability of such defects for the coupled system, i.e. if a solution starting near such a prototypical defect will stay in near the defect in the long-time limit.

A recent and strongly developing direction, stimulated by the interest from current intensive physics studies, concerns the study of colloids. This amounts to considering energy functionals of the type

$$\mathcal{F}_{LDGs}(Q) = \int_{\Omega \setminus \mathcal{C}} \frac{L}{2} |\nabla Q|^2 + f_B(Q)\,\mathrm{d}x + \int_{\partial \mathcal{C}} f_s(Q, \nu)\,\mathrm{d}s, \tag{3.8}$$

where $\mathcal{C} \subset \Omega$ are the colloidal particles included in the NLC environment and $f_s(Q, \nu)$ is a surface energy quantifying the interaction between the NLC and the colloids (here ν stands for the exterior derivative). The equations corresponding to critical points of $\mathcal{F}_{\text{LDGs}}$ are the same as (3.1) but on $\Omega \setminus \mathcal{C}$ with boundary conditions on $\partial \mathcal{C}$ of Robin type (coming out of the surface energy term, see for instance [93–95]). There exist a number of works in this direction studying either the case of a single coloidal particle and the qualitative structure of defects around it [93,94,96] or

many particles and the homogenization effects [95,97–99]. It is natural to understand what is the effect of the flow in such a context, but a first step is to obtain some solid well-posedness results, which motivates the next:

Research topics 2: Consider the coupled system (2.1) and (2.4) on a domain with $\Omega\backslash\mathcal{C}$ with $\mathcal{C}\subset\Omega$ being the colloid(s) (i.e. one or more connected sets). Assume no-slip boundary conditions on $\partial\mathcal{C}$ for the u part and Robin boundary conditions corresponding to surface energy on the Q-tensor part (see [93–95]). Study the well-posedness of the coupled system and the limit when the size of colloids tends to zero.

4. Relationships between models

A natural question is: what are the differences in the predictions of the models? From a physical point of view different models are justifiable for use at different scales and thus the OF model is seen as providing more macroscopic information than the LDG one which is more mesoscopic, providing a better description at small scales. To some extent this intuition can be justified mathematically. Indeed, suitable non-dimensionalizations of the models lead naturally to the existence of certain small parameters. For the LDG formalism in the stationary case such a non-dimensionalization is presented in [100], see also the appendix of [101]. For the BE equation, a non-dimensionalization is provided in [11]. The mathematical study of the vanishing limits of these small parameters leads sometimes to an understanding on how some models are related to each other.

A prototypical case is that of the LDG to OF limit in [102]. Dividing by L and subtracting a constant from the bulk term f_B (operations which will not change the critical points) one can rewrite the energy $\mathcal{F}_{\mathrm{LDG}}(Q)$ in (2.2) as:

$$\widetilde{\mathcal{F}}_{\mathrm{LDG}}(Q)=\int_\Omega \frac{1}{2}|\nabla Q|^2(x)+\frac{1}{L}\tilde{f}_B(Q(x))\,\mathrm{d}x, \tag{4.1}$$

where we define $\tilde{f}_B(Q)\overset{\mathrm{def}}{=}f_B(Q)-\min_{Q\in\mathcal{S}_0}f_B(Q)$.

We have $\tilde{f}_B(Q)\geq 0$ with the minimum, zero, attained on the set $\mathcal{S}_*=\{Q\in\mathcal{S}_0; Q=s_+(n\otimes n-(1/3)I_3),\ \text{for some } n\in\mathbb{S}^2\}$ (a set homeomorphic to $\mathbb{R}P^2$ as pointed before) with $s_+=(b+\sqrt{b^2+24ac})/4c$. Then, heuristically, in the limit $L\to 0$ (physically motivated in [100,101]), one would want to minimize the gradient part subject to keeping $Q\in\mathcal{S}_*$, i.e. to minimize the energy $\mathcal{F}_{OF*}(Q)=\int_\Omega(1/2)|\nabla Q|^2(x)\,dx$ in the set $W^{1,2}(\Omega;\mathcal{S}_*)=\{Q\in W^{1,2}(\Omega;\mathbb{R}^{3\times 3}); Q(x)\in\mathcal{S}_*\ \text{a. e. } x\in\Omega\}$. For simply connected domains Ω, it can be showed (see for instance [72,73]) that for any $Q\in W^{1,2}(\Omega;\mathcal{S}_*)$ one can choose $n_Q\in W^{1,2}(\Omega;\mathbb{S}^2)$ such that $Q=s_+(n_Q\otimes n_Q-(1/3)I_3)$ a.e. in Ω and a straightforward calculation shows $\mathcal{F}_{OF*}(Q)=s_+^2\int_\Omega|\nabla n_Q|^2\,dx$. Thus, with modulo topological considerations (developed in [72]) in the limit $L\to 0$ one recovers the OF energy out of the LDG one.

The sense in which the minimizers behave in the limit was first analysed in [102] and later on refined in various other papers, such as [78,84–86,101,103]. The limit has strong formal similarities with the celebrated Ginzburg–Landau (GL) problem in superconductors [104,105] where one studies minimizers of the energy $F_{GL}(u)=\int_\Omega(1/2)|\nabla u|^2+(1/4\varepsilon^2)(1-|u|^2)^2\,\mathrm{d}x$ for $u:\Omega\subset\mathbb{R}^2\to\mathbb{R}^2$ in the limit $\varepsilon\to 0$. Thus many techniques used in GL have relevance in studying the LDG problems. However, the finite energy of point defects and the higher dimensionality of the target space, in the LDG problems, generate significant levels of additional complexity, when compared to the GL problems.

The study of the similar limit in the dynamical problems has generated several notable results such as [52] (QS to EL), [106] (LDG to EL), [107] (LDG to harmonic maps), [103,108–111]

(molecular theories to OF). However, the presence of the flow adds formidable difficulties to the study of this limit for weak solution, see in particular in the relaxed EL problem context the Open Problem 2.4 in [58]. Thus in order to consider the specific features brought by the tensorial description of NLC, one can look into the following:

> **Research topics 3:** Consider the coupled system (2.1) and (2.4) with either periodic boundary conditions or in the whole space and assume a 'tame regime' for the Navier–Stokes part (i.e. either small and highly regular initial data or large ν). Consider the asymptotic setting in works such as [106,107], and determine the rate of convergence to the limit and the next order terms in the asymptotic expansion.

Basically, the above question aims to extend to a regime with flow the studies done in [101, 112] on the rate of convergence and the next order term in the asymptotic expansion. These are important for two reasons: to understand quantitatively the approximation of one model by the other and also the effects that the more complex model is able to capture, and are not present in the simpler, limit model. This requires a good understanding of the geometry of the Q-tensors, as done in [101,112], together with an understanding of the effects produced by the flow.

Another relevant direction, as provided by the study of asymptotic limits, is that of model reduction. Indeed, often the limit models are simpler in some sense (for instance, the OF model is more constrained, more geometrical than the LDG one) and thus these limits provide effective ways of obtaining a model reduction in a physically relevant manner. An interesting such limit, which has been only crudely explored so far, is that from [11]. There it was shown that in the limit of *large spatial scales* the physical regime which allows us to see the localized defect patters, one has a decoupling of the BE system, namely the limit consists of a Euler equation without any forcing term coupled with an equation for the Q-tensors that includes also some terms coming from the Euler flow part. The limit system allows an understanding of the dynamical emergence of defects, and a number of interesting questions are left there open for further study.

5. Flow effects

The time-independent models that ignore the effect of the fluid velocity can be formally obtained from the full models just by setting formally the flow velocity u to be identically zero and also ignoring the time dependence. This provides the equations for the director, but leaves however a gap in the self-consistency of the model, namely in the flow part. One can note in equation (2.4) that setting $u = 0$ leaves the equation

$$\nabla p = -\lambda \nabla \cdot T \tag{5.1}$$

with the additional stress tensor T from (2.5) provided in terms of Q. Thus in principle not all the solutions for the Q-tensor part would be valid, but only those that satisfy the additional constraint (5.1).

It can be checked that at least in the BE formalism stationary solutions of the Q-tensor equations, i.e. satisfying (3.1), automatically satisfy the constraint (5.1). This is no longer the case for time-dependent solutions. In fact, J.L. Ericksen, considering the case when the inertia is present (thus having also a second time-derivative in (2.1)) and working in the EL formalism, called these solutions 'twist-waves' [113]. These are solutions which exhibit dynamic behaviour of the directors, such that they do not create a velocity flow. They represent an interesting and important limit behaviour of the system, as such it is important to understand (in various theories (BE, EL, relaxed EL, . . .)): the following:

Research topics 4: Provide necessary and sufficient conditions for the existence solutions of (2.1) (considering also the case with an inertial term as in [113], i.e. a second-order time derivative) that also satisfy the additional constraint (5.1).

Another important direction of research concerns the effect that the flow has on the dynamics of the Q-tensor equations. The issue to understand is to what extent the presence of the flow modifies the dynamics, when compared with the case without flow. More specifically, it is important to understand what is the difference in the dynamics when one considers the same initial data Q_0 and (2.1) coupled with the equation (2.4) for the flow velocity u, compared with the case when one considers just (2.1) with $u \equiv 0$. In the physics literature this is referred to as the 'backflow effect', namely to understand what is the effect of the flow (produced under the influence of directors, through the additional stress tensor T) on the dynamics of the directors. Various studies show that the backflow has a genuine quantitative and qualitative effect, for instance, modifying the velocity of defects [114–116].

Another direction of study is to understand to what extent the very presence of the flow is responsible for the emergence of defects, that otherwise would not appear. A first direction towards understanding *the dynamic emergence of the defects* is provided in [11]. The framework presented there allows us to understand the emergence of defects for simple solutions of the Euler equations, particularly in dimension two.

More generally, the most natural starting point from a calculus of variations point of view would be to understand the effect of the simplest types of flows:

Research topics 5: Consider the coupled system (2.1) and (2.4). Assume that the flow takes a simple form (e.g. strain, shear, vortex,. . . see for instance Ch. 1 and 2 in [117]). For the Q-tensor equations (2.1) consider the prototypical defects geometry and boundary conditions presented in §3. Determine the stability of these prototypical defects, by extending the analysis done in the case without flow.

A research direction such as proposed above is natural from the point of view of rational mechanics and in rheological studies (because such simple flows can be regarded as building blocks of general, arbitrary flows). Such a direction was considered by E. MacMillan in his works [14,118] focusing mostly on symmetry considerations.

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