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On the energy instability of liquid crystals

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The direct Lyapunov method is used to investigate the stability of general equilibria of a nematic liquid crystal. First, we prove the converse Lagrange theorem stating that an equilibrium is unstable to small perturbations if the distortion energy has no minimum at this equilibrium (i.e. if the second variation of the distortion energy evaluated at the equilibrium is not positive definite). The proof is constructive rather than abstract: we explicitly construct a functional that grows exponentially with time by virtue of linearized equations of motion provided the condition of the theorem is satisfied. We obtain an explicit formula that gives the dependence of the perturbation growth rate upon the equilibrium considered and the initial data for the perturbation. Secondly, we obtain the upper and lower bounds for growing solutions of the linearized problem, and we identify the initial data corresponding to the most unstable mode (i.e. to the perturbation with maximal growth rate). All results are obtained in quite a general formulation: a nematic is inside a three-dimensional domain of an arbitrary shape and strong anchoring on the boundary is supposed; the standard equations of nematodynamics are employed as the governing equations.

1 Introduction

Studies of the stability properties of various equilibrium configurations of liquid crystals have a long history [1] that may be traced back to the experiments by Freedericks & Zolina [2]. During the last two decades, the interest in instabilities of liquid crystal equilibria (especially in instabilities driven by external electro-magnetic fields) increased due to their applications to electro-optic display devices. The common recipe (which has been exploited in numerous publications [1, 3, 4]) for making a conclusion about stability or instability of a given equilibrium configuration is based on energy arguments: if the free energy of the distortion (plus magnetic energy if an external magnetic field is present) has a local minimum at the equilibrium considered then this equilibrium configuration is stable to small perturbations, otherwise it is unstable. The first (direct) part of this statement is an analogue of the Lagrange theorem in finite-dimensional mechanics and is certainly true. The exact meaning of 'stability' in this case will be addressed in §3 of the present paper. The second (converse) part concerning instability (called the converse Lagrange theorem) is less obvious and requires more careful treatment. Even though conclusions about instability in the case of no free energy minimum seem physically reasonable and are confirmed experimentally for many particular situations [5, 6], we cannot assert *a priori* that this is true in the general situation. A classical example from finite-dimensional mechanics when the system has no minimum at an equilibrium but this equilibrium is stable may be

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found in [7] (see also [8, 9]). In continuum mechanics the situation is much more complicated and, as was pointed out in [10–12], it is always necessary to prove the corresponding proposition (the converse Lagrange theorem).

The major aims of the paper are: (i) to prove, in the linear approximation, the converse Lagrange theorem for general equilibria of nematic liquid crystals, our consideration being restricted to a simple case of equilibria without external electro-magnetic fields; (ii) to obtain the lower and upper bounds for the growing solutions of the corresponding linearized problem and to identify a perturbation with the maximal growth rate.

For simple geometries of a domain containing a nematic it is possible to show the instability (under the condition of the converse Lagrange theorem) by the usual normal mode technique [13]. In the general situation of an arbitrary domain this is, however, impossible. We therefore adopt a more general technique – the direct Lyapunov method, which allows us to treat the problem in a general formulation (without even solving the equations of motion). The main idea of the method (e.g. see [8, 9]) is to construct a positive definite (with respect to perturbations) functional that changes monotonically with time by virtue of the equations governing the evolution of perturbations (a non-increasing functional will prove stability and an increasing functional will prove instability). To construct such a functional, we exploit some general ideas recently developed in hydrodynamic stability theory [10–12].

We start with the formulation of the basic equations of nematodynamics in §2 and identify the basic equilibrium state as an exact solution of these equations. In §3 we formulate the linearized stability problem and discuss the (direct) Lagrange theorem. Then, in §4, we construct the Lyapunov functional. The result of §4 is the basic inequality (4.5) that gives an exponential decrease of an energy-type functional, this inequality being true for any equilibrium configuration of nematic. In §5 we use this inequality to obtain the lower bound (5.7) for the growing solutions of the linearized problem. This lower bound is the central result of the paper. It states that the perturbations increase exponentially with time, the growth rate being given by an explicit formula. Finally, in §6 we obtain the upper bound for the growing perturbations to identify the most unstable mode (the perturbation with the maximum value of the growth rate).

2 Basic equations

Let τ be a three-dimensional domain entirely filled with a nematic liquid crystal. The boundary $\partial\tau$ of the domain τ is fixed; $\mathbf{x} \equiv (x_1, x_2, x_3)$ are Cartesian coordinates. The state of a nematic at every point is described by density ρ, pressure p, velocity $\mathbf{u} = (u_1, u_2, u_3)$ and a vector $\mathbf{n} = (n_1, n_2, n_3)$ (called the 'director'), normalized so that

$$\mathbf{n}^2 = 1, \tag{2.1}$$

which characterizes the orientation of the molecular axes in space. We consider an incompressible nematic $\rho \equiv const$. Equations of motion are taken in a form proposed first by the Harvard group [14] (see also [1, §5.1]):

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$$\rho(\partial_t u_i + u_k \partial_k u_i) = \partial_k\{\sigma^e_{ik} + \sigma^s_{ik} + \tfrac{1}{2}(n_i h^\perp_k - n_k h^\perp_i)\}, \quad \partial_k u_k = 0, \tag{2.2}$$

$$\partial_t n_i = -u_k \partial_k n_i + \Omega_{ki} n_k + \lambda(\delta_{il} - n_i n_l) n_k A_{kl} + \frac{1}{\gamma} h^\perp_i, \tag{2.3}$$

where

$$\partial_t \equiv \partial/\partial t, \quad \partial_k \equiv \partial/\partial x_k, \quad \Omega_{ik} \equiv \tfrac{1}{2}(\partial_i u_k - \partial_k u_i), \tag{2.4a}$$

$$A_{ik} \equiv \tfrac{1}{2}(\partial_i u_k + \partial_k u_i), \quad \sigma^e_{ik} = -p\delta_{ik} - \pi_{kl}\partial_i n_l, \tag{2.4b}$$

$$\sigma^s_{ik} = 2\nu_2 A_{ik} + 2(\nu_3 - \nu_2)(n_i n_l A_{kl} + n_k n_l A_{il}) + 2(\nu_1 + \nu_2 - 2\nu_3) n_i n_k n_l n_m A_{lm} - \frac{\lambda}{2}(n_i h^\perp_k + n_k h^\perp_i), \tag{2.4c}$$

$$\mathbf{h}^\perp = \mathbf{h} - \mathbf{n}(\mathbf{n}\cdot\mathbf{h}), \quad h_i = \partial_k \pi_{ki} - \partial F_d/\partial n_i, \quad \pi_{ki} \equiv \partial F_d/\partial(\partial_k n_i), \tag{2.4d}$$

$$F_d = \frac{k_1}{2}(\operatorname{div}\mathbf{n})^2 + \frac{k_2}{2}(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 + \frac{k_3}{2}(\mathbf{n}\times\operatorname{curl}\mathbf{n})^2. \tag{2.4e}$$

In equations (2.2)–(2.4) we use the notations and terminology introduced by de Gennes [1]. The summation convention is used, σ^e_{ik} is the Ericksen (equilibrium) stress, σ^s_{ik} is the symmetric part of the viscous stress, $\mathbf{h}$ is the molecular field, F_d is the free energy (per unit volume of nematic) due to the distortion of $\mathbf{n}$, k_1, k_2, k_3 are the Frank elastic constants†, λ is the 'reactive parameter', $\gamma, \nu_1, \nu_2, \nu_3$ are the dissipation coefficients. Note that the constants $\lambda, \gamma, \nu_1, \nu_2, \nu_3$ are related to the Leslie coefficients $\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_6$ by the equations [1]:

$$2\nu_1 = \alpha_1 + \alpha_4 + \alpha_5 + \alpha_6, \quad 2\nu_2 = \alpha_4, \quad \gamma = \alpha_3 - \alpha_2,$$
$$2\nu_3 = \alpha_4 + \alpha_6 + \lambda\alpha_3, \quad \lambda = -(\alpha_2 + \alpha_3)/\gamma = -(\alpha_6 - \alpha_5)/\gamma.$$

The boundary conditions are taken in the simplest form, namely the director $\mathbf{n}$ on $\partial\tau$ has a prescribed, fixed orientation (a strong anchoring condition) and the velocity is zero (no-slip condition):

$$\mathbf{n}(\mathbf{x}) = \mathbf{n}_b(\mathbf{x}), \quad \mathbf{u} = 0 \quad \text{on} \quad \partial\tau. \tag{2.5}$$

An equilibrium state of a nematic liquid crystal

$$\mathbf{n}(\mathbf{x}) = \mathbf{n}^0(\mathbf{x}), \quad \mathbf{n} = 0, \quad p = p(\mathbf{x}) \tag{2.6}$$

is described by equations that are consistent with (2.2):

$$p(\mathbf{x}) = \text{const} - F_d(\mathbf{x}), \quad \mathbf{h}^\perp = 0. \tag{2.7}$$

The first of equations (2.7) expresses the balance of forces in the equilibrium, the second represents the balance of moments [1, 3].

3 The stability problem

In this section we shall formulate the stability problem for the equilibrium (2.6) as well as briefly discussing the (direct) Lagrange theorem for nematic liquid crystals.

† Note that the Frank elastic constants k_1, k_2, k_3 must be positive to provide the stability of a homogeneous state $\mathbf{n} = \text{const}$.

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Consider an infinitesimal perturbation of the basic equilibrium state (2.6) in the form

$$\mathbf{n}(\mathbf{x},t)=\mathbf{n}^0(\mathbf{x})+\tilde{\mathbf{n}}(\mathbf{x},t),\quad \mathbf{u}(\mathbf{x},t)=0+\tilde{\mathbf{u}}(\mathbf{x},t),\quad \mathbf{h}(\mathbf{x},t)=\mathbf{h}^0(\mathbf{x})+\tilde{\mathbf{h}}(\mathbf{x},t),\quad \text{etc.}$$

where $\tilde{\mathbf{n}}(\mathbf{x},t)$ is the disturbance director, $\tilde{\mathbf{u}}(\mathbf{x},t)$ is the disturbance velocity, $\tilde{\mathbf{h}}(\mathbf{x},t)$ is the disturbance molecular field, etc. On substituting these expressions into equations (2.2), (2.3), neglecting all terms quadratic in disturbances and then dropping 'tildes' to simplify the notation, we obtain the linearized equations of motion

$$\rho\partial_t u_i=\partial_k\{\sigma^e_{ik}+\sigma^s_{ik}+\tfrac{1}{2}(n^0_i h^\perp_k-n^0_k h^\perp_i)\},\quad \partial_k u_k=0, \tag{3.1}$$

$$\partial_t n_i=-u_k\partial_k n^0_i+\Omega_{ki}n^0_k+\lambda(\delta_{il}-n^0_i n^0_l)n^0_k A_{kl}+\frac{1}{\gamma}h^\perp_i. \tag{3.2}$$

From here on, $\mathbf{u}$, $\mathbf{n}$, Ω_{ik}, A_{ik}, σ^e_{ik}, σ^s_{ik}, $\mathbf{h}^\perp$ etc. denote the infinitesimal disturbances of the corresponding equilibrium quantities, e.g. $\sigma^e_{ik}=-p\delta_{ik}-\pi^0_{kl}\partial_i n_l-\pi_{kl}\partial_i n^0_l$.

The linearized version of (2.1) is

$$\mathbf{n}\cdot\mathbf{n}^0=0. \tag{3.3}$$

The boundary conditions for perturbations are

$$\mathbf{u}=\mathbf{0},\quad \mathbf{n}=\mathbf{0}\quad \text{on}\quad \partial\tau. \tag{3.4}$$

Equations (3.1), (3.2) with boundary conditions (3.4) completely describe the evolution of small perturbations of the basic state (2.6). (In spite of the considerable simplification resulting from linearization, a general analysis of these equations has never been done. To a certain extent we shall do this in the present paper.)

It may be shown (see Appendix A) that the equation expressing energy dissipation for the linearized problem (3.1)–(3.4) is

$$\dot{E}\equiv\partial_t E=-D \tag{3.5a}$$

where

$$E=K+\Pi_2,\quad K\equiv\frac{1}{2}\int_\tau \rho u_i u_i\,d\tau, \tag{3.5b}$$

$$\Pi_2\equiv\frac{1}{2}\int_\tau (k_1(\operatorname{div}\mathbf{n})^2+k_2(\mathbf{n}^0\cdot\boldsymbol{\zeta}+\mathbf{n}\cdot\boldsymbol{\zeta}^0)^2+2k_2(\mathbf{n}^0\cdot\boldsymbol{\zeta}^0)(\mathbf{n}\cdot\boldsymbol{\zeta})$$
$$+k_3(\mathbf{n}^0\times\boldsymbol{\zeta}+\mathbf{n}\times\boldsymbol{\zeta}^0)^2+2k_3(\mathbf{n}^0\times\boldsymbol{\zeta}^0)(\mathbf{n}\times\boldsymbol{\zeta})+(\mathbf{n}^0\cdot\mathbf{h}^0)\mathbf{n}^2)\,d\tau, \tag{3.5c}$$

$$D\equiv\int_\tau\left(d_{ik}A_{ik}+\frac{1}{\gamma}h^\perp_k h^\perp_k\right)d\tau,\quad \boldsymbol{\zeta}\equiv\operatorname{curl}\mathbf{n},\quad \boldsymbol{\zeta}^0\equiv\operatorname{curl}\mathbf{n}^0, \tag{3.5d}$$

$$d_{ik}\equiv\sigma^s_{ik}+\frac{\lambda}{2}(n^0_i h^\perp_k+n^0_k h^\perp_i)=\mu_1 A_{ik}$$
$$+\mu_2(n^0_i n^0_l A_{kl}+n^0_k n^0_l A_{il})+\mu_3 n^0_i n^0_k n^0_l n^0_m A_{lm}. \tag{3.5e}$$

In (3.5e) we have used the notations $\mu_1\equiv 2\nu_2$, $\mu_2\equiv 2(\nu_3-\nu_2)$, $\mu_3\equiv 2(\nu_1+\nu_2-2\nu_3)$. The functionals E, K, Π_2 and D can be treated as the total, kinetic, potential energies and the

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energy dissipation for the linearized problem. According to their definitions, the functionals K and D are positive definite while the functional Π_2 can be either positive definite or indefinite in sign for various equilibria.

There is an important connection between the properties of the functional Π_2 and the stability properties of the corresponding equilibrium state. Indeed, if Π_2 is a positive definite functional, i.e.

$$\Pi_2 > 0 \quad \text{for all} \quad \mathbf{n}(\mathbf{x}) \not\equiv 0, \tag{3.6}$$

then the total energy E is also positive definite, and E, which is quadratic in perturbations, may therefore be taken as a norm to measure the deviation of a perturbed state of nematic from an unperturbed one. The energy equality (3.5a) and the fact that D is a positive definite functional then give the estimate

$$E(t) \leqslant E(0), \tag{3.7}$$

so that the norm of a perturbation at any time t is bounded by the norm of this perturbation at initial instant $t = 0$, and the corresponding equilibrium is therefore linearly stable (in the sense of Lyapunov).

Here we are interested in an opposite situation when the functional Π_2 is indefinite in sign. In this case, there exists such a set $\mathcal{Q}$ of functions $\mathbf{n}(\mathbf{x})$ that:

$$\Pi_2 < 0 \quad \text{for} \quad \mathbf{n}(\mathbf{x}) \in \mathcal{Q}, \tag{3.8a}$$

$$\Pi_2 \geqslant 0 \quad \text{for} \quad \mathbf{n}(\mathbf{x}) \notin \mathcal{Q}, \tag{3.8b}$$

One of our major aims here is to show that an equilibrium state is unstable provided Π_2 is indefinite in sign (i.e. the set $\mathcal{Q}$ defined by (3.8) is not empty).

The properties of the functional Π_2 (and, as a consequence, the stability properties of the equilibrium (2.6)) have, in turn, a close connection with the properties of the potential energy of distortion:

$$\Pi_d \equiv \int_\tau F_d \, d\tau. \tag{3.9}$$

It may be shown that on the set of smooth functions $\mathbf{n}(\mathbf{x})$ that are subject to the constraint (2.1) and that satisfy the boundary condition (2.5) the functional Π_d has a critical point at the equilibrium $\mathbf{n}^0(\mathbf{x})$, i.e. the first variation of the functional

$$\Pi \equiv \Pi_d + \frac{1}{2}\int_\tau \alpha \, \mathbf{n}^2 \, d\tau \tag{3.10}$$

is equal to zero:

$$\delta\Pi = 0. \tag{3.11}$$

In equation (3.10), α is the Lagrange multiplier for the constraint (2.1). In fact, the variational principle (3.11) is the usual way to obtain the equilibrium equations (2.6) [1, 3]. The local properties of the functional Π (in the vicinity of a critical point) are determined by its second variation $\delta^2\Pi$. The functional Π has a local minimum at $\mathbf{n}^0(\mathbf{x})$ (2.6) if the second variation $\delta^2\Pi$ is positive definite. Accordingly, Π had has a local 'saddle point' at (2.6) if it is indefinite in sign.

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In our case, the second variation is given by the equation

$$\delta^2 \Pi = \frac{1}{2}\int_\tau \left(\frac{\partial^2 F_d}{\partial n_i \partial n_j}\delta n_i \delta n_j + 2\frac{\partial^2 F_d}{\partial n_i \partial(\partial_k n_j)}\delta n_i \partial_k \delta n_j + \frac{\partial^2 F_d}{\partial(\partial_i n_j)\partial(\partial_k n_l)}\partial_i \delta n_j \partial_k \delta n_l + (\mathbf{n}^0 \cdot \mathbf{h}^0)\,\delta n_i \delta n_i \right) d\tau, \tag{3.12}$$

which after substitution of equation (2.4e), and some manipulations, can be written as

$$\delta^2 \Pi = \frac{1}{2}\int_\tau (k_1(\operatorname{div}\delta\mathbf{n})^2 + k_2(\mathbf{n}^0 \cdot \delta\boldsymbol{\zeta} + \delta\mathbf{n}\cdot\boldsymbol{\zeta}^0)^2 + 2k_2(\mathbf{n}^0\cdot\boldsymbol{\zeta}^0)(\delta\mathbf{n}\cdot\delta\boldsymbol{\zeta}) + k_3(\mathbf{n}^0\times\delta\boldsymbol{\zeta} + \delta\mathbf{n}\times\boldsymbol{\zeta}^0)^2 + 2k_3(\mathbf{n}^0\times\boldsymbol{\zeta}^0)(\delta\mathbf{n}\times\delta\boldsymbol{\zeta}) + (\mathbf{n}^0\cdot\mathbf{h}^0)\,\delta\mathbf{n}^2)\,\mathrm{d}\tau, \tag{3.13}$$

where $\delta\boldsymbol{\zeta} \equiv \operatorname{curl}\delta\mathbf{n}$.

Comparing this with equation (3.5c), one can see that up to the change of notation $\mathbf{n} \to \delta\mathbf{n}$ the functional Π_2 is the same as the second variation $\delta^2\Pi$. Therefore, the case of a positive definite functional Π_2 corresponds to a positive definite $\delta^2\Pi$, and hence to a local minimum of Π, so that the above conclusion about stability may be formulated as the (direct) Langrange theorem: the equilibrium (2.6) is linearly stable if the free energy of distortion has a local minimum at this equilibrium. Accordingly, the converse Lagrange theorem whose proof will be given in §§4–5 states that the equilibrium (2.6) is linearly unstable if the free energy of distortion has a local 'saddle point' at this equilibrium.

4 Basic inequality

In this section, we shall establish an equality that gives a basis for obtaining lower and upper bounds for the solutions of the linearized problem (3.1)–(3.4) in §§5–6.

Let us introduce the Lagrangian displacements of fluid particles $\boldsymbol{\xi}(\mathbf{x}, t)$ defined by the equation

$$\partial_t \boldsymbol{\xi} = \mathbf{u} \quad \text{in} \quad \tau$$

with boundary condition $\boldsymbol{\xi} = 0$ on $\partial\tau$. $\boldsymbol{\xi}(\mathbf{x}, t)$ describes the displacement of a fluid element in the perturbed flow relative to its location $\mathbf{x}$ in the unperturbed state (2.6). Then formal integration of equation (3.2) over time gives the relation between fields $\boldsymbol{\xi}$ and $\mathbf{n}$:

$$n_i = -\xi_k \partial_k n_i^0 + \tfrac{1}{2}(\partial_k \xi_i - \partial_i \xi_k) n_k^0 + \lambda(\delta_{il} - n_i^0 n_l^0) n_k^0 \xi_{kl} + \frac{1}{\gamma}\hat{h}_i, \tag{4.1a}$$

where

$$\xi_{ik} \equiv \tfrac{1}{2}(\partial_i \xi_k + \partial_k \xi_i), \quad \hat{\mathbf{h}} \equiv \int_0^t \mathbf{h}^\perp(\mathbf{x}, t')\,dt' + \mathbf{f}(\mathbf{x}),$$

and $\mathbf{f}(\mathbf{x})$ is an arbitrary function. Note that, according to (4.1a), the relation between initial values $\boldsymbol{\xi}(\mathbf{x}, 0)$, $\mathbf{n}(\mathbf{x}, 0)$ and $\hat{\mathbf{h}}(\mathbf{x}, 0)$ is given by

$$\frac{1}{\gamma}\hat{h}_i(0) = n_i(0) + \xi_k(0)\,\partial_k n_i^0 - \tfrac{1}{2}(\partial_k \xi_i(0) - \partial_i \xi_k(0))\, n_k^0 - \lambda(\delta_{il} - n_i^0 n_l^0)\, n_k^0 \xi_{kl}(0). \tag{4.1b}$$

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Let us now consider the functionals first introduced in [11]:

$$M \equiv \int_\tau \rho\, \xi_i\, \xi_k\, d\tau, \quad \dot{M} \equiv 2 \int_\tau \rho \xi_i\, u_i\, d\tau, \tag{4.2a}$$

$$G \equiv \int_\tau \left(\hat{d}_{ik}\, \xi_{ik} + \frac{1}{\gamma} \hat{h}_i\, \hat{h}_i \right) d\tau, \quad X \equiv \dot{M} + G, \tag{4.2b}$$

$$\hat{d}_{ik} \equiv \mu_1\, \xi_{ik} + \mu_2 (n_i^0\, n_l^0\, \xi_{kl} + n_k^0\, n_l^0\, \xi_{il}) + \mu_3\, n_i^0\, n_k^0\, n_l^0\, n_m^0\, \xi_{lm}. \tag{4.2c}$$

By differentiating the functional X with respect to time and subsequent transformations, it may be shown that (see Appendix B)

$$\dot{X} = 4(K - \Pi_2) = 8K - 4E. \tag{4.3}$$

Equation (4.3) is called the 'generalized virial equality' [11] (the reason for this is that $\dot{M}$ (4.2a) is an analogue of the virial of classical finite-dimensional mechanics).

Multiplying equation (4.3) by a constant factor $(-s/2)$ and adding the result to equation (3.5a) we find

$$\dot{E}_s = 2s\, E_s - 4s\, K_s - D_s, \tag{4.4a}$$

where

$$E_s = K_s + \Pi_s, \quad 2\Pi_s \equiv 2\Pi_2 + sG + s^2 M, \tag{4.4b}$$

$$2K_s \equiv 2K - s\dot{M} + s^2\, M = \int_\tau \rho(\mathbf{u} - s\boldsymbol{\xi})^2\, d\tau, \tag{4.4c}$$

$$\begin{aligned} D_s &\equiv D - s\dot{G} + s^2 G \\ &= \int_\tau \left(\frac{1}{\gamma} (\mathbf{h}^\perp - s\hat{\mathbf{h}})^2 + \mu_1\, a_{ik}\, a_{ik} + 2\mu_2\, n_k^0\, n_l^0\, a_{ik}\, a_{il} + \mu_3 (n_k^0\, n_l^0\, a_{kl})^2 \right) d\tau, \end{aligned} \tag{4.4d}$$

$$a_{ik} \equiv A_{ik} - s\xi_{ik}.$$

Let $s > 0$. Then, since K_s and D_s cannot be negative, it follows from (4.4a) that

$$E_s \leqslant 2s\, E_s.$$

Integration of this inequality over time gives

$$E_s(t) \leqslant E_s(0) \exp(2st). \tag{4.5}$$

Note that (4.5) holds true for any solutions of the problem (3.1)–(3.4) and for any positive values of s. Note also that so far we have not placed any restriction on the form of the potential energy functional Π_2.

The inequality (4.5) will play an essential role in the subsequent analysis; all the results that follow will be obtained using this inequality.

5 Lower bound

In this section, we shall demonstrate that under the condition (3.8a) of no potential energy minimum at a given equilibrium $\mathbf{n}^0(\mathbf{x})$ there exist solutions of the linearized problem (3.1)–(3.4) that grow with time, and we shall obtain a lower bound for these solutions.

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Suppose that the condition (3.8a) is satisfied. This means that we can take the initial data for $\mathbf{n}(\mathbf{x}, t)$ such that

$$\mathbf{n}(\mathbf{x}, 0) \in \mathcal{Q},$$

and therefore,

$$\Pi_2(0) < 0. \tag{5.1}$$

Let us show that under condition (5.1) it is always possible to choose $E_s(0) < 0$ (if it is so then exponential growth of perturbations follows directly from inequality (4.5)). According to equations (4.4) we have

$$E_s(0) = s^2 M(0) + sA(0) + E(0), \quad A(0) \equiv \tfrac{1}{2}(G(0) - \dot{M}(0)).$$

We choose the initial data $\mathbf{u}(\mathbf{x}, 0)$ for the velocity field such that $K(0) < |\Pi_2(0)|$, and hence $E(0) < 0$. Then $E_s(0)$ is a quadratic polynomial in s with a positive coefficient $M(0)$ of s^2 and with a negative constant term $E(0)$. Therefore the conditions $s > 0$ and $E_s(0) < 0$ determine the interval of admissible values of s:

$$0 < s < S_1, \tag{5.2a}$$

where

$$S_1 \equiv -\frac{A(0)}{2M(0)} + \left[\left(\frac{A(0)}{2M(0)}\right)^2 - \frac{E(0)}{M(0)}\right]^{\frac{1}{2}}. \tag{5.2b}$$

It is obvious that $S_1 > 0$ for any initial data which are consistent with condition $E(0) < 0$.

We now show that $E_s(0) < 0$ implies exponential growth with time of the solutions of the problem (3.1)–(3.4). From the fact that $K_s \geqslant 0$ and from the definition of Π_s, it follows that

$$E_s(t) \equiv K_s(t) + \Pi_s(t) > \Pi_2(t).$$

This and equation (4.5) give

$$\Pi_2(t) < E_s(0) \exp(2st). \tag{5.3}$$

For any s from the interval defined by equations (5.2) this inequality means that the potential energy $\Pi_2(t)$ is exponentially decreasing with time from its negative initial value $\Pi_2(0)$, so that, in absolute value, Π_2 is growing. The expression (3.5c) for Π_2 is quite complicated. To extract the part of Π_2 which is really growing with time we need to transform (3.5c) to more convenient form.

Consider now the functional $\Pi_2(t)$. By using the identities

$$2(\mathbf{n}^0 \cdot \zeta^0)(\mathbf{n} \cdot \zeta) = (\mathbf{n} \times \zeta^0 - \mathbf{n}^0 \times \zeta)^2 - (\mathbf{n} \times \zeta^0)^2 - (\mathbf{n}^0 \times \zeta)^2,$$
$$2(\mathbf{n}^0 \times \zeta^0)(\mathbf{n} \times \zeta) = (\mathbf{n} \cdot \zeta^0 - \mathbf{n}^0 \cdot \zeta)^2 - (\mathbf{n} \cdot \zeta^0)^2 - (\mathbf{n}^0 \cdot \zeta)^2,$$

this functional may be written in the form

$$\begin{aligned}\Pi_2 = \frac{1}{2}\int_\tau \Big\{ & k_1(\operatorname{div}\mathbf{n})^2 + k_2[(\mathbf{n}^0 \cdot \zeta + \mathbf{n} \cdot \zeta^0)^2 + (\mathbf{n} \times \zeta^0 - \mathbf{n}^0 \times \zeta)^2 \\ & - (\mathbf{n} \times \zeta^0)^2 - (\mathbf{n}^0 \times \zeta)^2] + k_3[(\mathbf{n}^0 \times \zeta + \mathbf{n} \times \zeta^0)^2 \\ & + (\mathbf{n} \cdot \zeta^0 - \mathbf{n}^0 \cdot \zeta)^2 - (\mathbf{n} \cdot \zeta^0)^2 - (\mathbf{n}_0 \cdot \zeta)^2] + (\mathbf{n}^0 \cdot \mathbf{h}^0)\mathbf{n}^2 \Big\} d\tau.\end{aligned} \tag{5.4}$$

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From equation (5.4), it follows that

$$\Pi_2 \geqslant -I, \tag{5.5}$$

where

$$I(t) \equiv \frac{1}{2}\int_\tau (k_2(\mathbf{n}^0\times\boldsymbol{\zeta})^2 + k_2(\mathbf{n}\times\boldsymbol{\zeta}^0)^2 + k_3(\mathbf{n}^0\cdot\boldsymbol{\zeta})^2 + k_3(\mathbf{n}\cdot\boldsymbol{\zeta}^0)^2 + |\mathbf{n}^0\cdot\mathbf{h}^0|\,\mathbf{n}^2)\,d\tau. \tag{5.6}$$

Since the integrand in (5.6) is a positive definite quadratic form of the perturbation of the director and its spatial derivatives, it may therefore be taken as a norm to measure the difference between perturbed and unperturbed states. The inequalities (5.3), (5.5) give the estimate

$$I(t) > |E_s(0)|\exp(2st) \tag{5.7}$$

with any s from the interval (5.2). Inequality (5.7) gives the lower bound for the solutions of the linearized problem. This means that small deviations of the director from its equilibrium orientation grow exponentially with time, and this fact, in turn, implies linear instability of the equilibrium state. Thus, we have proved the converse Lagrange theorem for nematic liquid crystals.

It also follows from equation (5.7) that the lower bound for growth rate of the solutions of the problem (3.6)–(3.9) is given by the constant $S_1-\delta$, where δ is any number from the interval (5.2); in particular, δ may be an arbitrarily small number. Note that S_1 is completely determined by the initial data for perturbations. The upper limit for the growth rate corresponds to the maximum value of the parameter S_1 for all possible initial fields $\mathbf{n}(\mathbf{x},0)$, $\boldsymbol{\xi}(\mathbf{x},0)$ and $\mathbf{u}(\mathbf{x},0)$. The problem of maximizing S_1 is quite complicated. It may however be considerably simplified by considering a particular class of the solutions that, as will be clear later, corresponds to the maximal growth rate.

Consider such a class of solutions of the problem (3.1)–(3.4) for which the initial values of velocity and Lagrangian displacements of fluid particles are related by the equation

$$\mathbf{u}(\mathbf{x},0) = s\boldsymbol{\xi}(\mathbf{x},0). \tag{5.8}$$

It follows from (4.4c), (5.8) that

$$K_s(0) = 0, \quad E_s(0) = \Pi_s(0). \tag{5.9}$$

Since

$$2\Pi_s(0) \equiv 2\Pi_2(0) + sG(0) + s^2M(0),$$

both conditions $s>0$, $E_s(0)<0$ are equivalent to choosing s from the interval

$$0 < s < S_2, \tag{5.10a}$$

where

$$S_2 \equiv -\frac{G(0)}{2M(0)} + \left[\left(\frac{G(0)}{2M(0)}\right)^2 - \frac{2\Pi_2(0)}{M(0)}\right]^{\frac{1}{2}}. \tag{5.10b}$$

Since $\Pi_2(0)<0$, the parameter S_2 is always positive. Note also that S_2 depends only on $\boldsymbol{\xi}(\mathbf{x},0)$, $\mathbf{n}(\mathbf{x},0)$, while S_1 depends on $\boldsymbol{\xi}(\mathbf{x},0)$, $\mathbf{n}(\mathbf{x},0)$ and $\mathbf{u}(\mathbf{x},0)$). The dependence of S_2 (and S_1 as well) upon $\hat{\mathbf{h}}(\mathbf{x},0)$ is supposed to have been eliminated by using the relationship (4.1b).

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From (4.5), (5.5), (5.9), we easily obtain the inequality

$$I(t) > |\Pi_{S_2-\delta}(0)| \exp[2(S_2-\delta)\, t], \tag{5.11}$$

which holds for any δ from the interval (5.10a). Inequality (5.11) shows that $S_2-\delta$ (δ may be arbitrarily small) gives the lower bound for the growth rate of the solutions of the problem (3.6)–(3.9) from the class defined by equation (5.8).

Let us show now that

$$S_2\{\mathbf{n}(\mathbf{x},0), \boldsymbol{\xi}(\mathbf{x},0)\} \geqslant S_1\{\mathbf{n}(\mathbf{x},0), \boldsymbol{\xi}(\mathbf{x},0), \mathbf{u}(\mathbf{x},0)\} \tag{5.12}$$

for any field $\mathbf{u}(\mathbf{x},0)$ compatible with the condition $E(0) < 0$. To do this, it is sufficient to show that any s from the interval (5.2) is also in the interval (5.10). Suppose that s^* is such that $0 < s^* < S_1$. This means that $E_{s^*}(0) < 0$. On the other hand, since $E_{s^*}(0) \equiv K_{s^*}(0) + \Pi_{s^*}(0) \geqslant \Pi_{s^*}(0)$, we have: $E_{s^*}(0) < 0 \Rightarrow \Pi_{s^*}(0) < 0$. Hence, $0 < s^* < S_2$. We have thus proved that $s^* \in (0, S_1) \Rightarrow s^* \in (0, S_2)$ and, therefore, $S_1 \leqslant S_2$.

In the next section it will be shown that the perturbations from the class (5.8) are the most unstable ones because the greatest growth rate corresponds to the disturbance for which the quantity S_2 is maximal.

6 Upper bound

The upper bound for the growing perturbations also follows from the basic inequality (4.5). To obtain the upper bound we have to find a value of s for which the functional Π_s is positive definite for all admissible fields $\boldsymbol{\xi}$ and $\mathbf{n}$. Then E_s will be also positive definite and, as a consequence, the basic inequality (4.5) will give the upper bound for the growing perturbations. Let

$$S^* \equiv \sup_{\boldsymbol{\xi}, \mathbf{n}} S_2, \tag{6.1}$$

where $\sup S_2$ is calculated on the set of smooth functions $\boldsymbol{\xi}(\mathbf{x},0)$ satisfying the conditions $\operatorname{div}\boldsymbol{\xi} = 0$ in τ, $\boldsymbol{\xi} = 0$ on $\partial\tau$, and on the set $\mathcal{Q}$ (defined by (3.8)) of functions $\mathbf{n}(\mathbf{x},0)$.

Now let $s > S^*$. Then for all $\mathbf{n}(\mathbf{x},0) \in \mathcal{Q}$ we have $\Pi_s(0) > 0$. On the other hand, for all $\mathbf{n}(\mathbf{x},0) \notin \mathcal{Q}$, $\Pi(0) \geqslant 0$ and hence $\Pi_s(0) \geqslant 0$. The functional $\Pi_s(0)$ is thus positive definite for *all* admissible fields $\mathbf{n}(\mathbf{x},0), \boldsymbol{\xi}(\mathbf{x},0)$. Equations (4.4b, c) then show that $E_s(0)$ is also positive definite for all fields $\mathbf{n}(\mathbf{x},0)$, $\boldsymbol{\xi}(\mathbf{x},0)$ and $\mathbf{u}(\mathbf{x},0)$. Obviously, the same conclusion is valid for $E_s(t)$. Therefore, from (4.5) we obtain the following inequality:

$$E_{S^*+\epsilon}(t) \leqslant E_{S^*+\epsilon}(0) \exp[2(S^*+\epsilon)\, t] \tag{6.2}$$

for any $\epsilon > 0$. Since E_s is a positive definite quadratic functional of the perturbations, this inequality gives the upper bound for the growing solutions of the problem (3.1)–(3.4).

According to equation (5.11), the growth rate of a perturbation may be greater than $S^*-\delta$ with arbitrarily small δ. On the other hand, according to (6.2), it must be less than $S^*+\epsilon$ with arbitrarily small ϵ. We therefore identify S^* as the growth rate of the most unstable perturbation.

7 Concluding remarks

In this paper, we have applied the direct Lyapunov method to prove the converse Lagrange theorem for nematic liquid crystals. The theorem states that an equilibrium alignment of a nematic is unstable (in linear approximation) if the free energy of distortion has no

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minimum at this equilibrium. We supposed that a nematic was confined in a three-dimensional domain of an arbitrary form and that on the boundary of the domain the director had a prescribed, fixed orientation.

Using the techniques recently developed in the hydrodynamic stability theory [10–12] we have constructed a Lyapunov functional and have obtained the lower bound for growing solutions of the linearized problem, the latter ensured an exponential growth of small perturbations of the basic equilibrium state. We have then obtained the upper bound for these solutions with the aim of identifying the most unstable perturbation.

Much remains to be done in this area, particularly the problem of calculating the maximal growth rate (6.1) (it involves maximizing the functional S_2 (5.10b) on all admissible fields $\boldsymbol{\xi}$ and $\mathbf{n}$ and is quite complicated; it may be solved numerically at least in the case of a simple geometry of the domain). This is the subject of a continuing investigation.

The results of this paper can be generalized to the case of nematic equilibria in an external electro-magnetic field. In this case, estimates analogous to (5.11), (6.2) may give an approach for evaluating the growth rate of perturbations and eventually may lead to a prediction of the time interval needed for switching between configurations of different energy by using electric fields. This will also be the subject of a future communication.

Similar theories can be developed for other types of liquid crystals such as cholesterics and smectics.

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Appendix A. Derivation of the energy equation (3.5a)

It is convenient to rewrite the disturbance energy (3.5b) in the form

$$E = \int_\tau \mathscr{E}\, d\tau, \quad \mathscr{E} \equiv \tfrac{1}{2}\rho u_i u_i + F_2 + \tfrac{1}{2}(\mathbf{n}^0 \cdot \mathbf{h}^0) n_i n_i, \tag{A 1}$$

where

$$2F_2 \equiv \frac{\partial^2 F_d}{\partial n_i^0 \partial n_j^0} n_i n_j + 2\frac{\partial^2 F_d}{\partial n_i^0 \partial(\partial_k n_j^0)} n_i \partial_k n_j + \frac{\partial^2 F_d}{\partial(\partial_i n_j^0)\partial(\partial_k n_l^0)} \partial_i n_j \partial_k n_l + (\mathbf{n}^0 \cdot \mathbf{h}^0) n_i n_i, \tag{A 2}$$

so that F_2 represents the second term in the expansion of the distortion energy $F_d(n_i, \partial_k n_i)$ (2.4e) in the Taylor series at the point $(n_i^0, \partial_k n_i^0)$.

It may be shown that

$$\pi_{ki} \equiv \frac{\partial \pi_{ki}^0}{\partial n_j^0} n_j + \frac{\partial \pi_{ki}^0}{\partial(\partial_l n_j^0)} \partial_l n_j = \frac{\partial F_2}{\partial(\partial_k n_i)}$$

and that

$$\frac{\partial^2 F_d}{\partial n_i^0 \partial n_j^0} n_j + \frac{\partial^2 F_d}{\partial n_i^0 \partial(\partial_l n_j^0)} \partial_l n_j = \frac{\partial F_2}{\partial n_i}.$$

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Therefore, the disturbance molecular field $\mathbf{h}$ can be presented in the form

$$h_i = \partial_k \pi_{ki} - \partial F_2/\partial n_i, \quad \pi_{ki} = \partial F_2/\partial(\partial_k n_i). \tag{A 3}$$

Note also that the linear (in disturbances) part of the transverse component of the molecular field is given by

$$\mathbf{h}^\perp = \mathbf{h} - \mathbf{n}(\mathbf{n}^0 \cdot \mathbf{h}^0) - \mathbf{n}^0(\mathbf{n}^0 \cdot \mathbf{h}). \tag{A 4}$$

In deriving this equation we have used equation (3.3) and the fact that $\mathbf{h}^0$ has no transverse component.

We now calculate the derivative of $\mathscr{E}$ with respect to time. Observe first that

$$\begin{aligned}\partial_t F_2 &= \frac{\partial F_2}{\partial n_i}\partial_t n_i + \frac{\partial F_2}{\partial(\partial_k n_i)}\partial_t(\partial_k n_i) = \frac{\partial F_2}{\partial n_i}\partial_t n_i + \pi_{ki}\partial_t(\partial_k n_i) \\ &= \frac{\partial F_2}{\partial n_i}\partial_t n_i - \partial_k \pi_{ki}\partial_t n_i + \partial_k(\pi_{ki}\partial_t n_i) = -h_i \partial_t n_i + \partial_k(\pi_{ki}\partial_t n_i).\end{aligned} \tag{A 5}$$

Using this equation and equations (A 4) and (3.3), we immediately obtain

$$\partial_t(F_2 + \tfrac{1}{2}(\mathbf{n}^0 \cdot \mathbf{h}^0) n_i n_i) = -h_i^\perp \partial_t n_i + \partial_k(\pi_{ki}\partial_t n_i). \tag{A 6}$$

It can be shown from equation (3.2) that

$$h_i^\perp \partial_t n_i = -h_i^\perp u_k \partial_k n_i^0 + \frac{1}{\gamma}(\mathbf{h}^\perp)^2 + \tfrac{1}{2}\partial_k u_i(h_i^\perp n_k^0 - h_k^\perp n_i^0) + \frac{\lambda}{2}(h_i^\perp n_k^0 + h_k^\perp n_i^0). \tag{A 7}$$

From (3.1), after simple manipulations, we obtain

$$\begin{aligned}\partial_t(\tfrac{1}{2}\rho \mathbf{u}^2) = &-\tfrac{1}{2}\partial_k u_i(n_i^0 h_k^\perp - n_k^0 h_i^\perp) + \frac{\lambda}{2}(n_i^0 h_k^\perp + n_k^0 h_i^\perp) \\ &- d_{ik} A_{ik} - u_i \partial_k B_{ik} + \partial_k[u_i(-p\delta_{ik} + \tfrac{1}{2}(n_i^0 h_k^\perp - n_k^0 h_i^\perp) + \sigma_{ik}^s)],\end{aligned} \tag{A 8}$$

where d_{ik} is defined by equation (3.5e) and

$$B_{ik} \equiv \pi_{kl}^0 \partial_i n_l + \pi_{kl}\partial_i n_l^0.$$

Then equations (A 6), (A 7), (A 8) give

$$\begin{aligned}\partial_t \mathscr{E} = \partial_t(\tfrac{1}{2}\rho u_i u_i + F_2 + \tfrac{1}{2}(\mathbf{n}^0 \cdot \mathbf{h}^0) n_i n_i) = &h_i^\perp u_k \partial_k n_i^0 - u_i \partial_k B_{ik} \\ &- \frac{1}{\gamma}(\mathbf{h}^\perp)^2 - d_{ik} A_{ik} + \partial_k[\pi_{ki}\partial_t n_i + u_i(-p\delta_{ik} + \tfrac{1}{2}(n_i^0 h_k^\perp - n_k^0 h_i^\perp) + \sigma_{ik}^s)].\end{aligned} \tag{A 9}$$

By standard manipulations it can be shown that

$$\partial_k B_{ik} = h_k^\perp \partial_i n_k + \partial_i F_1, \tag{A 10}$$

where F_1 is linear in the disturbances part of the distortion energy F_d:

$$F_1 \equiv \frac{\partial F_d}{\partial n_l^0} n_l + \frac{\partial F_d}{\partial(\partial_k n_l^0)}\partial_k n_l.$$

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Finally, substituting (A 10) into (A 9) gives the equation

$$\partial_t \mathscr{E} = -\frac{1}{\gamma}(\mathbf{h}^{\perp})^2 - d_{ik} A_{ik} + \partial_k X_{ik}, \tag{A 11}$$

where

$$X_{ik} \equiv \pi_{ki} \partial_t n_i + u_i(-(p+F_1)\delta_{ik} + \tfrac{1}{2}(n_i^0 h_k^{\perp} - n_k^0 h_i^{\perp}) + \sigma_{ik}^s).$$

Integrating (A 11) over τ and using boundary condition (3.9) results in the energy equation (3.5a).

Appendix B. Derivation of the 'generalized virial equation' (4.3)

Using the definition of the field $\boldsymbol{\xi}$ and equations (3.1) and (4.2), we obtain

$$\ddot{M}/2 = \int_\tau \left\{ \rho u_i u_i + \xi_i \left(-\partial_i p - \partial_k B_{ik} + \tfrac{1}{2}\partial_k (n_i^0 h_k^{\perp} - n_k^0 h_i^{\perp}) - \frac{\lambda}{2}\partial_k (n_i^0 h_k^{\perp} + n_k^0 h_i^{\perp}) + \partial_k d_{ik} \right) \right\} d\tau.$$

After integrating by parts and using boundary condition $\boldsymbol{\xi} = 0$ on $\partial\tau$ we find

$$\ddot{M}/2 = 2K + \int_\tau \left\{ -\xi_i \partial_k B_{ik} - \xi_{ik} d_{ik} - \tfrac{1}{2}\partial_k \xi_i (n_i^0 h_k^{\perp} - n_k^0 h_i^{\perp}) + \frac{\lambda}{2}\partial_k \xi_i (n_i^0 h_k^{\perp} + n_k^0 h_i^{\perp}) \right\} d\tau. \tag{B 1}$$

It follows from (4.1a) that

$$h_i^{\perp} n_i = -\xi_k h_i^{\perp} \partial_k n_i^0 - \tfrac{1}{2}\partial_k \xi_i (n_i^0 h_k^{\perp} - n_k^0 h_i^{\perp}) + \frac{\lambda}{2}\partial_k \xi_i (n_i^0 h_k^{\perp} + n_k^0 h_i^{\perp}) + \frac{1}{\gamma} h_i^{\perp} \hat{h}_i. \tag{B 2}$$

Taking account of (B 2) we can rewrite equation (B 1) in the form

$$\ddot{M}/2 = 2K + \int_\tau \left\{ -\xi_i \partial_k B_{ik} - \xi_{ik} d_{ik} + \xi_k h_i^{\perp} \partial_k n_i^0 + h_i^{\perp} n_i - \frac{1}{\gamma} h_i^{\perp} \hat{h}_i \right\} d\tau. \tag{B 3}$$

Using equation (A 10), we immediately obtain

$$\ddot{M}/2 = 2K + \int_\tau \left\{ h_i^{\perp} n_i - \xi_{ik} d_{ik} - \frac{1}{\gamma} h_i^{\perp} \hat{h}_i \right\} d\tau. \tag{B 4}$$

It may be shown by standard calculations that the 'potential energy' Π_2 given the equation (3.5c) can also be written as

$$\Pi_2 = -\frac{1}{2}\int_\tau h_i^{\perp} n_i \, d\tau. \tag{B 5}$$

After using equation (B 5) and the definition of the functional G from (4.2b), equation (B 4) takes the form

$$\ddot{M} = 4(K - \Pi_2) - \dot{G},$$

which, in view of the definition of X in (4.2b), coincides with equation (4.3).

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