Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713926090

On Poiseuille flow of liquid crystals

M. Carme Calderer; Bagisa Mukherjee

Online publication date: 06 August 2010

To cite this Article Calderer, M. Carme and Mukherjee, Bagisa(1997) 'On Poiseuille flow of liquid crystals', Liquid Crystals, 22: 2, 121 — 135

To link to this Article: DOI: 10.1080/026782997209487

URL: http://dx.doi.org/10.1080/026782997209487

LIQUID CRYSTALS, 1997, VOL. 22, NO. 2, 121–135

On Poiseuille flow of liquid crystals†

by M. CARME CALDERER* and BAGISA MUKHERJEE
Department of Mathematics, The Pennsylvania State University, University Park, Pennsylvania 16802, U.S.A.

(*Received 15 November 1995; in final form 15 June 1996; accepted 15 July 1996*)

We consider Poiseuille flow of polymeric liquid crystals corresponding to large values of the velocity gradient. The model employed [Ericksen, 1991] proposes governing equations for the velocity field, $\mathbf{v}$, the pressure p, the director $\mathbf{n}$, and the order parameter s. The constitutive functions for the Leslie coefficients α_i derived from the molecular theory of Doi [1981] play a crucial role in the modelling. In addition to the Ericksen number, E, the present model exhibits a new non-dimensional parameter $\mathscr{I}$, that represents the contribution of the elastic free energy of non-gradient type with respect to Frank–Oseen's elasticity. One of the goals of the analysis was to examine the role of s in describing singularities as well as in obtaining regimes which are not predicted by the previous Leslie–Ericksen model. In particular, solutions are obtained that correspond to domain structures parallel to the flow. Such domains are separated by singular lines across which the director experiences jumps of, approximately, ± 45 degrees with respect to the flow direction. A condition on the size of $\mathscr{I}$ is required in order to support such layered structures. The contribution of the energy associated with $\mathscr{I}$ turns out to play the role of an elastic surface energy which is, otherwise, neglected in the present model.

1. Introduction

In this article we study modelling as well as mathematical aspects of plane Poiseuille flows of uniaxially nematic liquid crystals corresponding to high values of the velocity gradient. The model employed is that due to Ericksen for liquid crystals with variable degree of orientation [1]. The constitutive equations for the Leslie coefficients as derived by Doi and Kuzuu [2] and Marrucci [3], play an essential role in the analysis. The present work addresses some aspects of the non-Newtonian flow behaviour of rod-like polymeric fluids and their relationship with the presence of defects and texture in the material.

In addition to the Ericksen number, E, associated with the Leslie–Ericksen equations, an additional non-dimensional quantity, $\mathscr{I}$, plays a fundamental role in the present modelling context. We find that such a quantity is associated with the presence in the model of an elastic energy of non-gradient type, which in turn, allows for the presence of internal layers parallel to the flow direction. The analysis reveals two types of such layers, *isotropic* as well as those associated with *stress jumps*. The former may correspond to disclinations in the flow region whereas the latter ones may be related with spatially rapid changes of stress. We consider boundary value problems for Poiseuille flow and study solutions with singularities along the flow direction.

The present theory assigns to the order parameter values $s \in (-1/2, 1)$, with $s=1$ corresponding to perfect alignment along the director, $s=-1/2$ corresponds to the molecules being placed on a plane perpendicular to the director and $s=0$ is defined as the *isotropic* state with randomly oriented molecules. The director is not defined at points where $s=0$. This introduces some difficulties in the analysis such as the governing equation for the director becoming singular at the isotropic state.

One of the goals of the present paper is to highlight the role of the order parameter in the model. From one point of view, it enhances the elastic mechanisms of the model as it introduces a higher degree of non-linearity in the equations. On the other hand, it allows us to give a rather detailed study of singularities. We also point out that the present model yields solutions that do not arise in the Leslie–Ericksen theory. We also emphasize how configurations with defects arise naturally in the present context.

Experimental observations indicate that uniformly aligned flows of polymers with ratio $\alpha_2/\alpha_3 \geqslant 0$ might not be maintained at high rates of shear and, phenomena analogous to that of the case with negative ratio may actually occur [4–6]. In general, there is evidence that shearing at high rates produces disclinations in configurations with well-defined orientation (for example, [7] and [8], §5·1).

*Author for correspondence.
†Supported by NSF Grant no. DMS-9403915.

In the present work, we consider regimes that fulfil the alignment condition $\alpha_2/\alpha_3 \geqslant 0$, and show that, in some appropriately defined limit of (high) shear rate gradients, solutions exhibiting disclinations in the flow region can be found. Moreover we show that across the singular lines, the director experiences jump discontinuities of approximately ± 45 degrees to the direction of flow. The analysis also shows that solutions with disclinations occur in the limit of validity of the alignment condition.

It results from the analysis that the boundary conditions on $\mathbf{n}$ and s are only felt in a narrow layer near the boundary. This is consistent with the behaviour of flows with large velocity gradients [8A].

In § 2, we introduce the model and establish a list of constitutive properties, in part, by combining results of [1], stemming from the continuum mechanics approach, with those from molecular theories as described in [2–4]. In particular, we adopt the approximate forms of Leslie coefficients derived by Marrucci to guide our assumptions.

The molecular theory for polymeric liquid crystals developed by Doi [9] employs as the relevant quantity, the distribution function $f_0(\mathbf{u})$. This denotes the probability that the axis of an arbitrarily chosen molecule is in the direction of the vector $\mathbf{u}$. This theory consists of two equations, a kinetic equation for the evolution of f_0 and another one that expresses the stress tensor in terms of the orientational distribution function. In [10], it is shown that the Leslie–Ericksen equations follow from the microscopic model under special assumptions: *(a)* f_0 is a first order perturbation of equilibrium and *(b)* the flow regime produces alignment. The latter is consistent with considering *weak velocity gradients.*

The Helmholtz free energy consistent with the current framework is presented in § 2. In particular, we adopt a simplified version of the more general and physically realistic one described in the Appendix, where we also give a justification for our simpler choice. The present form has been widely used in various analyses involving Ericksen's model.

In order to render the notion of *high gradient or fast flow* rigorous, in § 3, we carry out the non-dimensionalization of the governing equations and introduce the relevant dimensionless parameter groups of the model. This suggests interpreting such conditions in terms of the large Ericksen number, i.e., $\mathrm{E} \gg 1$. The equations governing static solutions of shear flow regimes in plane geometries are derived in § 3. We point out that the choice of plane flow configuration meets the purpose of showing that the present model is capable of predicting very complex flow structure and physical phenomenology even for the simplest flow geometries.

The analysis of solutions corresponding to constant gradient is carried out in § 4. No boundary conditions are taken into account within the context of that section. The multiple uniform solutions corresponding to a prescribed value of the shear rate are interpreted in terms of the sign of the first normal stress difference. Conditions referring to the latter are related to those stemming from stability considerations. In particular, we point out that uniformly aligned flows corresponding to negative values of the normal stress difference are unstable. The solutions obtained in this section are the building blocks of more complex flows described later. Boundary-value problems for the governing equations are formulated in § 5.

In § 6, we study solutions corresponding to Poiseuille flow geometries for large values of E. Since the equations exhibit a singular dependence on the parameter $\mu \equiv \mathrm{E}^{-1}$, we seek solutions $\{s(x, \mu), \phi(x, \mu)\}$, $x \in (-1, 1)$, that admit an asymptotic expansion with respect to μ. Solutions with a single disclination along the line $x = 0$ are, in fact analogous to those predicted by the Leslie–Ericksen theory. In such case, the present analysis would provide a more detailed description of the flow configuration.

The construction of solutions with one or more singularities in the flow region (in addition to that in $x = 0$) is based on the idea of properly connecting, at a given point, branches as those of § 4. The connection is achieved with an internal layer. If branches with opposite sign of the order parameter are brought together, then the connecting layer approximates a disclination. Even in the case that there is no change of sign of the order parameter the rapid variations of the fields $\mathbf{n}$ and s across such layers is consistent with the analogous behaviour of the components of the stress. This, in turn, may be interpreted as an indication of *melt-fracture.* Experimental observations of such *stress jumps* are found in some of the chemical engineering literature, for example, [11, 12].

In order to understand how the non-dimensional parameters allow for such structures, we make the following observations. The mathematical mechanism in the equations permitting the matching construction of solutions is associated with the Ericksen number being large. Existence of solution branches as in § 4 depends on the ratio $\mathrm{E}/\mathscr{I}$, whereas the requirement of $\mathscr{I}$ to be sufficiently large allows for internal layers.

The latter condition can also be found in analogous problems related to existence of phase boundaries in elastic solids, as illustrated in the article by [13]. In both situations, it accounts for surface energy that it is not explicitly present in the model.

2. Modelling and constitutive equations

In order to describe flows of uniaxially nematic liquid crystals employing the model proposed by Ericksen [1], we need to introduce the vector fields

$$\mathbf{v}=(v_1, v_2, v_3) \quad (1)$$

$$\mathbf{n}=(n_1, n_2, n_3). \quad (2)$$

They represent the *velocity* of the fluid and the *director,* respectively, at a point $\mathbf{x}\in\Omega$ of the flow region, at time $t\geqslant 0$. Moreover, we let the scalar field

$$s=s(\mathbf{x}, t) \quad (3)$$

denote the *order parameter.* We suppose that

$$\nabla\cdot\mathbf{v}=0 \quad \text{and} \quad \mathbf{n}\cdot\mathbf{n}=1, \quad (4)$$

hold, for all $\mathbf{x}\in\Omega$. The first equation is a consequence of the incompressibility assumption on the material and the second one expresses the condition of the director being a unit vector field. Here s and $\mathbf{n}$ correspond to the common eigenvalue and to the distinct eigenvector, respectively, of the *order tensor, Q,* for optically uniaxial materials.

We assume that the *Helmholtz free energy,* $\mathscr{F}$, and the Cauchy stress tensor, σ, are of the form

$$\mathscr{F}=\mathscr{F}(s, \nabla\mathbf{n}, \nabla s)=k_1|\nabla s|^2+k_2 s^2|\nabla\mathbf{n}|^2+\nu f(s) \quad (5)$$

$$\sigma=-pI-\nabla\mathbf{n}^T\frac{\partial\mathscr{F}}{\partial\nabla\mathbf{n}}-\nabla s\otimes\frac{\partial\mathscr{F}}{\partial\nabla s}+\hat{\sigma}, \quad (6)$$

respectively. Here k_1, k_2 and ν denote positive constants. $f(s)$ denotes the scalar contribution to the free energy.

The expression given in (5) is a simplified version of the more general and physically realistic free energy functional given in the Appendix. There we justify the simpler choice made here.

$\hat{\sigma}$ denotes the viscous part of the stress tensor which we will assume to be linear on the velocity gradient:

$$\hat{\sigma}=(\beta_1\dot{s}+\alpha_1\mathbf{n}\cdot\mathbf{A}\mathbf{n})\mathbf{n}\otimes\mathbf{n}+\alpha_2\mathbf{N}\otimes\mathbf{n} + \alpha_3\mathbf{n}\otimes\mathbf{N}+\alpha_4\mathbf{A}+\alpha_5\mathbf{A}\mathbf{n}\otimes\mathbf{n}+\alpha_6\mathbf{n}\otimes\mathbf{A}\mathbf{n}, \quad (7)$$

with

$$2\mathbf{A}=\nabla\mathbf{v}+(\nabla\mathbf{v})^T, \quad 2\Omega=\nabla\mathbf{v}-(\nabla\mathbf{v})^T \quad (8)$$

and

$$\mathbf{N}=\dot{\mathbf{n}}-\Omega\mathbf{n}. \quad (9)$$

$p(\mathbf{x}, t)$ denotes the pressure.

The balance laws associated with the dependent variables $\mathbf{v}$, $\mathbf{n}$ and s are given by

$$\rho\dot{\mathbf{v}}=\nabla\cdot\sigma, \quad (10)$$

$$\beta_2(s)\dot{s}=\nabla\cdot\left(\frac{\partial\mathscr{F}}{\partial\nabla s}\right)-\frac{\partial\mathscr{F}}{\partial s}-\beta_3(s)\mathbf{n}\cdot\mathbf{A}\mathbf{n} \quad (11)$$

and

$$\gamma_1(s)\dot{\mathbf{n}}\times\mathbf{n}=\nabla\cdot\left(\frac{\partial\mathscr{F}}{\partial\nabla s}\right)\times\mathbf{n}-\frac{\partial\mathscr{F}}{\partial\mathbf{n}}\times\mathbf{n} + \gamma_1(s)\Omega\mathbf{n}\times\mathbf{n}-\gamma_2(s)\mathbf{A}\mathbf{n}\times\mathbf{n}. \quad (12)$$

The constant $\rho>0$ denotes the density and $\alpha_i(s)$, $\beta_i(s)$ and $\gamma_i(s)$ are constitutive functions. They correspond to the Leslie coefficients in the Leslie–Ericksen theory. Restrictions on them will be discussed later in the section. We assume that they are continuous functions of s on the interval $(-1/2\,1)$.

The second law of thermodynamics in the form of the Clausius–Duhem inequality implies that the coefficients satisfy the following relations, cf [17], chapter 3:

$$\alpha_4>0, \quad (13)$$

$$\alpha_1+\frac{3}{2}\alpha_4+\alpha_5+\alpha_6-\frac{\beta_1^2}{\beta_2}>0, \quad (14)$$

$$2\alpha_4+\alpha_5+\alpha_6-\frac{\gamma_2^2}{\gamma_1}>0, \quad (15)$$

$$\beta_2>0, \quad (16)$$

$$\gamma_1=\alpha_3-\alpha_2>0, \quad (17)$$

$$\gamma_2=\alpha_6-\alpha_5. \quad (18)$$

Ericksen's theory also requires the stress coefficients to satisfy

$$\alpha_6-\alpha_5=\alpha_2+\alpha_3, \quad (19)$$

and

$$\beta_1=\beta_3. \quad (20)$$

The former corresponds to Parodi's relation and it is predicted by molecular theory arguments. However similar justifications do not appear to lead to the second relation.

We conclude the first part of this section by listing additional hypotheses to be placed on the Leslie coefficients. Their motivation lies on the properties of the approximation formulas for such coefficients as obtained from the molecular theory of lyotropic liquid crystals developed by Kuzuu and Doi [10]. We outline their derivation in the next subsection and we now complete the list of assumptions as follows:

$$\left|\frac{\gamma_1}{\gamma_2}(s)\right|\leqslant 1, \quad \text{for all } s\in\left(-\frac{1}{2}, 1\right), \quad (21)$$

$$\lim_{s\to 0}\frac{\gamma_1}{\gamma_2}(s)=0, \quad \gamma_1(0)=0=\gamma_2(0), \quad (22)$$

$$\lim_{s\to 1-}\frac{\gamma_1}{\gamma_2}(s)=-1, \quad (23)$$

$$\lim_{s \to -\frac{1}{2}^+} \frac{\gamma_1}{\gamma_2}(s) = 1, \tag{24}$$

$$\beta_1(s) < 0, \quad s\gamma_2(s) \leqslant 0, \quad s \in \left(-\frac{1}{2}, 1\right). \tag{25}$$

We observe that (21) together with (17)–(19) is equivalent to the inequality

$$\frac{\alpha_2}{\alpha_3}(s) \geqslant 0, \quad \text{for all } s \in \left(-\frac{1}{2}, 1\right). \tag{26}$$

This is in turn consistent with the study of aligning flow regimes.

2.1.1. *Remarks*

(1) Inequality (21) should be regarded as a restriction on the flow regimes to be analysed. It was studied by Leslie [14] in the modelling of aligning regimes of the Leslie–Ericksen equations. In the present work, we relate the degeneracy of such a ratio with the presence of defects.

(2) The limiting conditions (22)–(24) express growth hypotheses on the coefficients. They account for the observed angles of alignment of the director with the flow at the corresponding limits.

(3) Inequalities (25) are related to the mechanism of the flow that cause the director to align.

2.1.2. *The Leslie coecients*

The continuum theory alone does not provide sufficient information on the viscosity coefficients. Here we explore the joint approaches of Kuzuu and Doi [2] and that of Ericksen [1] to gain the needed information on α_i.

The derivation of such coefficients carried out by Kuzuu and Doi proceeds by comparing the Leslie–Ericksen equations with the molecular theory that they previously developed for lyotropic liquid crystals [10]. Such a derivation is based on the following assumptions:

(1) The flows under consideration correspond to aligning regimes.

(2) The order tensor takes on equilibrium values only.

The aforementioned authors proceed to obtain expressions of the Leslie coefficients involving the viscosity of the isotropic state η^*, a dimensionless concentration C and order parameters

$$S_2 = \langle P_2(\mathbf{u} \cdot \mathbf{n}) \rangle, \quad S_4 = \langle P_4(\mathbf{u} \cdot \mathbf{n}) \rangle.$$

P_2, P_4 denote Legendre polynomials of second and fourth order, respectively, and $\langle \cdots \rangle$ denotes the average with respect to the distribution function $f_0(\mathbf{u})$. The function $f_0(\mathbf{u})$ is the minimizer of the microscopic free energy $\mathscr{A}$ proposed by Onsager. (We note that S_2 corresponds to the order parameter s of the continuum theory.)

They point out that no closed forms of the equilibrium distribution function $f_0(\mathbf{u})$ can be obtained by the minimization of $\mathscr{A}$, and therefore, the method does not yield explicit forms of the Leslie coefficients. The approximation schemes to minimize $\mathscr{A}$ developed by [2–4], yield

$$\alpha_i(s) = k(s) A_i(s), \quad 1 \leqslant i \leqslant 6, \quad \text{where} \qquad k(s) = \eta_0 (1 - s^2)^2. \tag{27}$$

The quantity η_0 depends on C, η^* as well as on the molecular weight and the length of the rod of the molecular theory model. $\{A_i(s)\}$ denote dimensionless polynomials.

The type of approximation involved in calculating the orientation distribution function determines the form of the functions $A_i(\cdot)$. Although the aforementioned approaches yield distinct forms of the functions $A_i(\cdot)$, they all predict the limiting properties (22)–(24) as well as inequalities (25). Here we present the simpler expressions derived by Marrucci [3]:

$$\left.\begin{aligned} \alpha_1/k &\quad -s^2, \\ \alpha_2/k &\quad -s(1+2s)/(2+s), \\ \alpha_3/k &\quad -s(1-s)/(2+s), \\ \alpha_4/k &\quad (1-s)/3, \\ \alpha_5/k &\quad s, \\ \alpha_6/k &\quad 0. \end{aligned}\right\} \tag{28}$$

While (28) give a positive ratio α_2/α_3 (and therefore, satisfy inequality (21)), for those given by Berry, such quotient changes sign at $s = 1/4$. One can see that α_2/α_3 becomes degenerate at $s = 0$. This turns out to be a very relevant property in the modelling of line defects within the present order parameter model. In general, $\alpha_6 \neq 0$ (the vanishing of α_6 is due to simplifications made on the derivation of (28)). Our analysis does hold in the more general case.

We observe that (17) and (18) combined with (28) give

$$\left.\begin{aligned} \gamma_1(s) &= k(s)\frac{3s^2}{2+s}, \\ \gamma_2(s) &= -k(s)s. \end{aligned}\right\} \tag{29}$$

However, neither of the approaches previously discussed provides information on the coefficients β_i. For this, we make use of the following results.

Ericksen [1] derives expressions that approximate the coefficients α_i, β_i, and γ_i near $s = 0$. They are obtained as consistency conditions between the *dissipation function*, Δ, expressed as a quadratic function of $\dot{s}$, $\mathbf{N}$ and $\mathbf{A}$, i.e.,

$$\Delta = \alpha_4 \mathbf{A} \cdot \mathbf{A} + (\alpha_5 + \alpha_6)\mathbf{n} \cdot \mathbf{A}^2\mathbf{n} + \alpha_1(\mathbf{n} \cdot \mathbf{A}\mathbf{n})^2 + \gamma_1|\mathbf{N}|^2 + 2\gamma_2\mathbf{N} \cdot \mathbf{A}\mathbf{n} + \beta_2\dot{s}^2 + 2\beta_1\dot{s}\mathbf{n} \cdot \mathbf{A}\mathbf{n},$$

and the analogous function written in terms of **A** and Q, the co-rotational time derivative of Q,

$$\mathring{Q} = \dot{Q} - \Omega Q + Q\Omega.$$

This yields the following approximate relations,

$$2\gamma_2 = s(2A_0 + A_1 s + 4A_2 s^2 + A_3 s^3 + 2A_4 s^4)\eta_0 \quad (30)$$

$$2\beta_1 = (A_0 + A_1 s + 2A_2 s^2 + A_3 s^3 + A_4 s^4)\eta_0, \quad (31)$$

where A_0, A_1, A_2, A_3 and A_4 are constants. In order to determine them, we now identify the second equation in (29) with (30). This gives

$$A_0 = -1 = A_4, \quad A_1 = 0 = A_3, \quad A_2 = 1,$$

and, consequently,

$$\beta_1 = -\frac{1}{2}k(s). \quad (32)$$

We let

$$\beta(s) \equiv -\beta_1(s) = -\beta_3(s), \quad (33)$$

and point out the positivity of β.

2.1.3. *The scalar energy f(s)*

The presence of such a term in the free energy originates with Frank's idea of representing $\mathscr{F}$ as a truncated Taylor expansion of the gradients of the fields, with $f(s)$ corresponding to the zero order term. (The rotational invariance of $\mathscr{F}$ excludes the dependence of f on **n**.) The inclusion of the term $f(s)$ seems to be relevant to the modelling of polymeric behaviour [9, 15], and, in general it has the form of a double-well potential (with the single-well case as a special one).

In general $f(s)$ and ν depend on the temperature or the concentration. However, we regard such variables as parameters and consider, instead, a family of functions $f(s)$ parameterized by them. Of course, different shapes of the graphs of $f(s)$ result from variations of either of such parameters.

Letting the *prime* notation in the constitutive functions denote derivative with respect to s, i.e.,

$$f'(s) = \frac{\mathrm{d}f}{\mathrm{d}s}(s),$$

we place the following assumptions on $f(s)$:

(1) It is a smooth function of s on the interval $(-1/2, 1))$.

(2) $\lim_{s\to -1/2,1} f(s) = +\infty$.

(3) There exist real numbers $s_1, s_2, s_3 \in (-1/2, 1)$, $s_3 \geqslant 0$, $s_1 \leqslant s_2 \leqslant s_3$, $s_1 s_2 = 0$ and such that $f'(s_i) = 0$, $f''(s_i) \neq 0$, $i = 1, 2, 3$.

These hypotheses hold for a very general class of functions $f(s)$. In particular, it includes the case of a single-well potential located at $s_1 = 0 = s_2 = s_3$. In the case that all values s_i, $i = 1, 2, 3$ are distinct $f(s)$ correspond to a double-well potential with minimum points $s = s_1$ and $s = s_3$, respectively, separated by a maximum point $s = s_2$. The nearly isotropic transition is a special case of the latter and corresponds to $f(s_1) \approx f(s_3)$, with $s_1 = 0$ and $s_1 \neq s_3$.

Functions $f(s)$ with $s_2 = 0$ are associated with high values of the concentration (for lyotropic liquid crystals) as well as to low temperatures (for thermotropic ones). Such conditions correspond to prevailing nematic configurations at equilibrium over unstable isotropic ones.

The growth conditions on $f(s)$ express the fact that highly aligned nematic configurations are rarely observed and, likewise, configuration with $s = -1/2$.

3. Governing equations

In order to make rigorous comparisons between the elastic and viscous mechanisms of liquid crystal flows, it is necessary to write the governing equations in dimensionless form. First of all, we will discuss the main non-dimensional groups of parameters involved in the study of flow problems. We conclude the section with the derivation of the governing equations of plane shear flow regimes.

We first introduce the dimensionless form $\bar{\mathbf{x}}$, $\bar{t}$, of the independent variables

$$\mathbf{x} = L\bar{\mathbf{x}}, \quad t = \frac{L}{V}\bar{t}. \quad (34)$$

V, L and ρ denote a characteristic speed, length and the density of the system, respectively. We introduce the following scaling of the dependent variables:

$$\left.\begin{aligned} \mathbf{v}(\mathbf{x}, t) &= V\bar{\mathbf{v}}(\bar{\mathbf{x}}, \bar{t}), & p &= \rho V^2 \bar{p}, \\ s(\mathbf{x}, t) &= \bar{s}(\bar{\mathbf{x}}, \bar{t}), & \mathbf{n}(\mathbf{x}, t) &= \bar{\mathbf{n}}(\bar{\mathbf{x}}, \bar{t}), \end{aligned}\right\} \quad (35)$$

The resulting equations for the new scaled variables have the same form as those in (10)–(12) after setting the coefficient of $\dot{\mathbf{v}}$ on the left-hand side of (10) equal to one, and replacing the constitutive functions α_i, β_i, γ_i, k_i and ν, respectively, with $\bar{\alpha}_i$, $\bar{\beta}_i$, $\bar{\gamma}_i$ and $\bar{\nu}$. The latter are defined as follows:

$$\left.\begin{aligned} \bar{\alpha}_i &= \frac{1}{\rho V L}\alpha_i \\ \bar{\beta}_i &= \frac{1}{\rho V L}\beta_i \\ \bar{\gamma}_i &= \frac{1}{\rho V L}\gamma_i \\ \bar{k}_i &= \frac{1}{\rho V^2 L^2}k_i \\ \bar{\nu} &= \frac{1}{\rho V^2}\nu. \end{aligned}\right\} \quad (36)$$

In particular, the previous relations indicate that to obtain the correct scaling of the special coefficients α_i and γ_i given in §2, one should make the following replacement in (27):

$$\eta_0 \to \eta_0 = \frac{1}{\rho V L} \eta_0. \quad (37)$$

Next, we introduce the non-dimensional groups commonly employed to characterize flow regimes. We let η, ν and K denote typical viscosity and elasticity coefficients (specific choices for them depend on the problem at hand).

(1) Ericksen number:

$$\mathrm{E} = \eta \frac{VL}{K}. \quad (38)$$

(2) Reynolds number:

$$\mathcal{R} = \frac{\rho L V}{\eta}. \quad (39)$$

Moreover the scalar quantity

$$\mathcal{I} = L^2 \frac{\nu}{K}, \quad (40)$$

where ν is as in (5), plays a significant role in flows with either internal or boundary layers. $\bar{\eta}$, $\bar{\nu}$ and $\bar{K}$ employed next represent the scaled versions of η, ν and K, respectively. In terms of such quantities, (38)–(40) adopt the following form:

$$\left.\begin{aligned} &\mathrm{E} = \bar{\eta}/K, \\ &\mathcal{R} = 1/\bar{\eta}, \quad \mathcal{I} = \bar{\nu}/K. \end{aligned}\right\} \quad (41)$$

E gives a measure of the relative size of the viscous contributions with respect to the elastic ones whereas $\mathcal{I}$ measures the scalar contribution to the free energy with respect to the gradient one. An interpretation of such quantity is given next. Since the current model does not include a surface energy term, $\mathcal{I}$ takes on such a role: its contribution becomes relevant whenever the solution presents an interface. In particular, conditions ensuring the stability of boundary layers are formulated in terms of the quantity [16]

$$\mathcal{T} = \frac{\mathrm{E}}{\mathcal{I}}. \quad (42)$$

Since ∇v appears in the governing equations multiplying a coefficient of the form α_i, β_i or γ_i, when assuming ∇v *large*, we may instead take the corresponding viscosity coefficient to be *large* holding ∇v fixed.

We adopt the convention that, unless otherwise stated, all quantities encountered from now on have been scaled according to the previous criteria. However, in order to simplify the notation, we will drop the superimposed *bar* previously introduced.

We now consider the class of steady state flows in a domain $\Omega = (-1, 1) \times \mathbb{R}^2$ such that

$$\left.\begin{aligned} &\mathbf{v} = (0, 0, v_3), \quad p = p(x, y, z), \\ &n_1 = \sin\phi, \quad n_2 = 0, \quad n_3 = \cos\phi, \quad (x, y, z) \in \Omega. \end{aligned}\right\} \quad (43)$$

We let

$$v_3 = v(x), \quad \phi = \phi(x), \quad s = s(x), \quad (44)$$

$x \in (-1, 1)$. We denote derivative with respect to x with a prime. Substituting (43) and (44) into the governing equations (5)–(12), the following equations for the new fields v, p, ϕ are obtained:

$$0 = \left\{ p + 2k_2 s^2 \phi'^2 + \left(\alpha_1 \sin^3\phi\cos\phi + \frac{1}{2}\left(\alpha_2 + \alpha_3 + \alpha_5 + \alpha_6\right)\right) v' \sin\phi\cos\phi \right\}' + 2k_1\{(s')^2\}', \quad (45)$$

$$0 = -\partial p/\partial y, \quad (46)$$

$$0 = -\frac{\partial p}{\partial z} + \left\{ \left(\frac{1}{2}\alpha_4 + \alpha_1 \sin^2\phi\cos^2\phi + \frac{1}{2}(\alpha_5 - \alpha_2)\sin^2\phi \right) v' \right\} + \left\{ \frac{1}{2}\cos^2\phi\, v'(\alpha_3 + \alpha_6) \right\}', \quad (47)$$

$$0 = \left(\frac{\gamma_2 - \gamma_1}{2}\sin^2\phi - \frac{\gamma_1 + \gamma_2}{2}\cos^2\phi \right) v' + 2k_2 (s^2\phi')' \quad (48)$$

and

$$0 = 2k_1 s'' - \nu f'(s) - 2k_2 s\phi'^2 - \beta_3 v' \sin\phi\cos\phi. \quad (49)$$

4. Shear flow with constant gradient

In this section we consider plane, homogeneous shear flow with constant velocity gradient. We let

$$v(x) = x, \quad \phi = \text{constant}, \quad s = \text{constant}, \quad p = \text{constant}.$$

Employing equation (33) we write (49) for the previously given fields

$$0 = \beta(s)\cos\phi\sin\phi - \nu f'(s).$$

We divide the latter equation through by K and recast it in the form

$$f'(s) = \mathcal{T}\,\omega(s)\sin 2\phi, \quad (50)$$

where

$$\omega(s) = \frac{1}{2}\eta^{-1}\beta(s),$$

with η and K as in equations (41) and (42). Likewise, we rewrite equation (48),

$$E\left\{-\frac{1}{2}(\gamma_1+\gamma_2)\cos^2\phi+\frac{1}{2}(\gamma_2-\gamma_1)\sin^2\phi\right\}=0. \tag{51}$$

Constant solutions of (50) and (51) give homogeneous aligning regimes.

We now show existence of multiple aligning flows corresponding to given parameter values E and $\mathscr{I}$. For this, we discuss the solvability of equations (50) and (51), in view of the constitutive properties of § 2.

4.1. *Proposition 1*

We assume that the constitutive equations satisfy relations (13)–(20) and (21)–(25). Let $f(s)$ be as in § 2.

(1) If $E=0$, then $s=0$ solves equations (50) and (51). Moreover, in such case ϕ is undetermined.

(2) Solutions of (50) and (51) with $s\neq 0$ satisfy the algebraic equations

$$f'(s)=e\mathscr{T}\omega(s)\left(1-\frac{\gamma_1^2}{\gamma_2^2}(s)\right)^{1/2} \tag{52}$$

with

$$e=\pm 1.$$

Furthermore, for each $s\in(-1/2, 1)$ satisfying (52)

$$\cos 2\phi=-\gamma_1(s)/\gamma_2(s). \tag{53}$$

Part (1) follows as a consequence of the fact that $f'(0)=0$. We point out that the above proposition is valid independently of whether $f(s)$ is a single or a double-well potential.

In order to study the solvability of equation (52), we introduce the following notation.

$$h(s)=\left(1-\frac{\gamma_1^2}{\gamma_2^2}(s)\right)^{1/2} \tag{54}$$

$$H(s,\mathscr{T})=\mathscr{T}\omega(s)h(s). \tag{55}$$

We observe that,

$$\lim_{s\to 0}h(s)=1 \quad\text{and}\quad \lim_{s\to 0}h(s)=0=\lim_{s\to -1/2}h(s), \tag{56}$$

hold. In particular, for α_i as in (28), expression (54) becomes

$$h(s)=2(2+s)^{-1}[(1+2s)(1-s)]^{1/2}. \tag{57}$$

Employing the previous notation, we rewrite equation (52) as

$$f'(s)=eH(s,\mathscr{T}). \tag{58}$$

For $f(s)$ non-convex, let $c_1<c_2$ denote the critical points of $f'(s)$. Without loss of generality we assume that

$$f'(c_1)>|f'(c_2)|.$$

The solvability of equation (58) can now be summarized in *Proposition 2*. For this, we observe that $\lim_{s\to 0}H(s,\mathscr{T})>0$ as a result of (25), (33) and (56).

4.2. *Proposition 2*

Let $f(s)$, $\alpha_i(s)$, $\beta_i(s)$ be as in *Proposition 1* and such that $s_1<s_2<s_3$ holds. Suppose that the following growth conditions are satisfied:

$$\lim_{s\to\{1-,-1/2+\}}\frac{\beta(s)h(s)}{f'(s)}=0,$$

then for a given value of the ratio $\mathscr{T}$ such that:

Case 1.

$$H(s,\mathscr{T})\leqslant|f'(c_2)|,\quad \text{for all } s\in[c_1,c_2], \tag{59}$$

there are solutions S_i^+, S_i^-, $1\leqslant i\leqslant 3$, corresponding to $e=+1$ and $e=-1$, respectively, satisfying $S_1^-<S_1^+<S_2^+<S_2^-<S_3^-<S_3^+$, $S_1^-<0$.

Case 2.

$$f'(c_1)>H(s,\mathscr{T})>|f'(c_2)|,\quad \text{for all } s\in[c_1,c_2], \tag{60}$$

there exist solutions satisfying $S_1^-<S_1^+<S_2^+<S_3^+$.

Case 3.

$$f'(c_1)<H(s,\mathscr{T}),\quad \text{for all } s\in[c_1,c_2], \tag{61}$$

there exist two solutions such that $S_1^-<S_3^+$ and $S_1^-<0$. Moreover,

$$S_1^-\to-\frac{1}{2}\quad\text{and}\quad S_3^+\to 1,\quad \text{as } \mathscr{T}\to\infty. \tag{62}$$

In the latter limiting situation,

$$\phi\to\left\{\frac{\pi}{2},0\right\}, \tag{63}$$

respectively, hold (see figure 1).

4.3. *Remarks*

(1) The second limiting statements in (62) and (63) establish that, in the limit of high shear rate, the molecules tend to follow a perfectly aligned configuration with the director becoming parallel to the flow direction.

(2) We point out that condition (59) is satisfied for $\mathscr{T}$ sufficiently small. Likewise, inequality (61) holds for large values of such ratio.

(3) In the case that $s_1=0=s_2=s_3$, i.e., $f(s)$ is a single-well potential, *Proposition 2* guarantees the existence of two solutions: $S_1^+>0$ and $S_1^-<0$, corresponding to the upper and lower regions of the graph, $e=1$ and $e=-1$, respectively.

We conclude this section giving an interpretation of the previously obtained solution branches in terms of the sign of the first normal stress difference, $\sigma_N\equiv\sigma_{33}-\sigma_{11}$. This can be summarized as follows [16]:

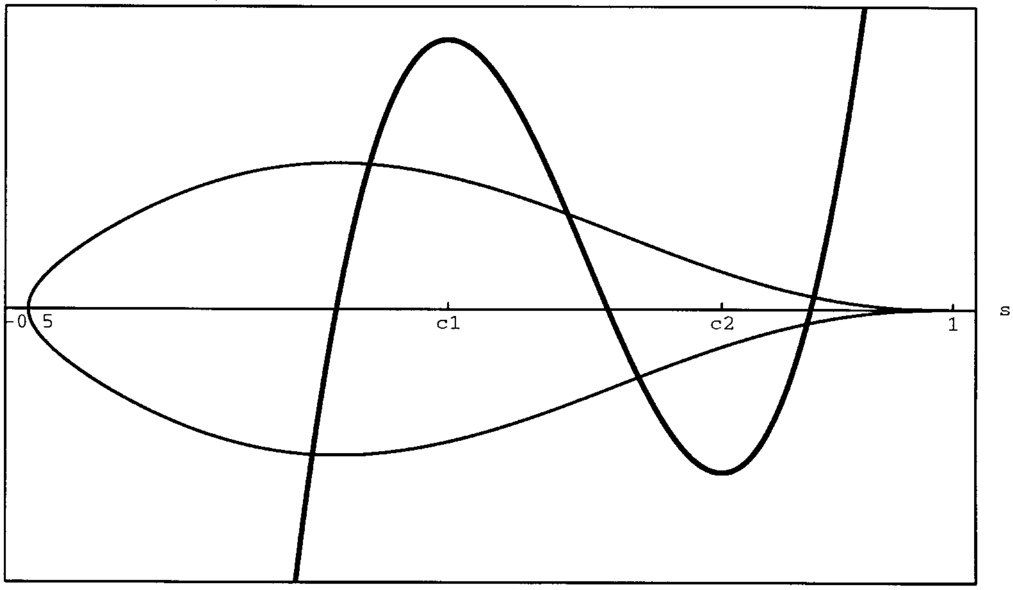

Figure 1. The graph of $f'(s)$ (thick line) together with those of $\pm H(s, \mathcal{T})$. The upper part of the diagram shows the two points of intersection, S_i^+, $i=1,2,3$, of $f'(s)$ with $H(s, \mathcal{T})$. Likewise, the lower part shows the points S_i^-, $i=1,2,3$.

(1) If $s_1=0$ then solutions such that $s=S_i^+$, $1\leqslant i\leqslant 3$, $s=S_1^-$ satisfy

$$\sigma_N > 0. \tag{64}$$

Otherwise, $\sigma_N < 0$ holds.

(2) If $s_2=0$ then solutions such that $s=S_1^-, S_3^+$ also satisfy (64), whereas the remaining solutions satisfy $\sigma_N < 0$.

Furthermore, it turns out that $\sigma_N > 0$ is a necessary condition for the stability of the previously obtained flows with respect to time-dependent perturbations.

5. Plane Poiseuille flow fields

From now on, we will consider boundary-value problems for the dimensionless equations (44)–(49). We prescribe boundary conditions for the flow fields as in plane Poiseuille geometry,

$$\frac{\partial p}{\partial z}=1, \quad v(-1)=0=v(1). \tag{65}$$

The choice of one as a prescribed gradient of pressure is made keeping in mind the non-dimensional character of the variables of the problem.

In addition to (65), we also prescribe boundary conditions for the optic fields. Given constants $s_a, s_b \in (-1/2, 1)$ and $\phi_a, \phi_b \in [-\pi/2, \pi/2]$, we seek solutions satisfying

$$s(-1)=s_a, \quad s(1)=s_b \tag{66}$$

$$\phi(-1)=\phi_a, \quad \phi(1)=\phi_b. \tag{67}$$

Throughout this section, we will assume that $s(\cdot)\in(-1/2,1)$, $\phi(\cdot)\in[-\pi/2,\pi/2]$ are prescribed.

Integration of equation (47) taking (45) into account gives

$$\partial p/\partial z=\mathcal{K}, \tag{68}$$

$$v'(x)g(s,\phi)=\mathcal{K}x+\mathcal{K}_0 \tag{69}$$

where $\mathcal{K}$ and $\mathcal{K}_0$ are constant, and

$$g(s,\phi)=\frac{1}{2}\alpha_4+\alpha_1\sin^2\phi\cos^2\phi + \frac{1}{2}(\alpha_5-\alpha_2)\sin^2\phi+\frac{1}{2}(\alpha_3+\alpha_6)\cos^2\phi. \tag{70}$$

5.1. *Remark*

Observe that $g(c,\phi)$ (with $-1/2<c<1$ a constant) appears in Leslie's derivation of the equations of shear flow in the Leslie–Ericksen model. As in that case, it follows from the *dissipation inequalities* (13)–(15) that

$$g(s,\phi)>0, \quad \text{for all } s\in\left(-\frac{1}{2},1\right), \quad \phi\in[-\pi/2,\pi/2]. \tag{71}$$

It vanishes at the limits $s=1$ and $s=-1/2$ which does not pose a difficulty since such values are never reached within the present model. Integration of (69) with respect to x gives

$$v(x)=\int_{-1}^{x} g^{-1}(s,\phi)(\mathcal{K}x+\mathcal{K}_0)\,dx+C, \tag{72}$$

with C an arbitrary constant.

We now give families of flows associated with the boundary conditions (65). The non-slip conditions on the boundary give the following relation:

$$\int_{-1}^{1} g^{-1}(s, \phi)x\,\mathrm{d}x + \mathscr{K}_0 \int_{-1}^{1} g^{-1}(s, \phi)\mathrm{d}x = 0, \qquad (73)$$

from which

$$v'(x) = g^{-1}(s, \phi)x - g^{-1}(s, \phi)\left\{\int_{-1}^{1} g^{-1}(s, \phi)\mathrm{d}x\right\}^{-1} \times \left\{\int_{-1}^{1} g^{-1}(s, \phi)x\,\mathrm{d}x\right\}, \qquad (74)$$

follows. This reduces to

$$v'(x) = g^{-1}(s, \phi)x, \qquad (75)$$

in the case that $s(\cdot)$ is even and $\phi(\cdot)$ is either even or odd.

6. Flows with high shear rates: plane Poiseuille geometry

In this section we consider flow regimes with large Ericksen number. This corresponds to configurations with the viscosity effects being predominant over the elastic ones. Within the non-dimensional framework that we present here, this may provide a mathematical interpretation to the ansatz of a large velocity gradient.

The goal is to construct solutions with one or more line defects parallel to the velocity field. The first type of solutions that we obtain exhibit a line defect in the centre of the region. The second class present one or more *isotropic internal layers* away from the centre. The order parameter takes the value zero across such layers while the director experiences a jump discontinuity of the order ± 45 degrees. While the first type correspond to those already predicted from the Leslie–Ericksen theory [14], the second ones seem to be a novelty of modelling flow problems with the inclusion of additional optic variables.

We set

$$\left.\begin{aligned} \mu &= \frac{2K_0}{\eta_0}, \quad \text{with} \\ K_0 &= \max\{k_1, k_2\}, \end{aligned}\right\} \qquad (76)$$

and η_0 as in (37). We observe that μ is, in fact, (twice) the inverse of the Ericksen number given in (41).

We consider the boundary value problem (45)–(49) and (65)–(67). After integrating equation (47) as previously described, and dividing the remaining equations through by η_0, the governing equations become

$$0 = \frac{\mu}{K_0}(k_1 s'' - k_2 s(\phi')^2) - \mathscr{T}^{-1} f'(s) - g_3(s)v' \sin\phi\cos\phi \qquad (77)$$

and

$$0 = (g_1(s)\sin^2\phi - g_2(s)\cos^2\phi)v' + \mu\frac{k_2}{K_0}(s^2\phi')', \qquad (78)$$

together with (45), (66), (67) and (75). Here,

$$\left.\begin{aligned} g_1(s) &= \frac{1}{2\eta_0}(-\gamma_1 + \gamma_2), \quad g_2(s) = \frac{1}{2\eta_0}(\gamma_1 + \gamma_2) \\ \text{and} \quad g_3(s) &= \frac{\beta_3}{\eta_0}. \end{aligned}\right\} \qquad (79)$$

In particular, for γ_i as in (29) we obtain

$$\left.\begin{aligned} g_1(s) &= \frac{-(1-s^2)^2}{2+s}(2s^2 + s), \\ g_2(s) &= \frac{-s(1-s)}{2+s}(1-s^2)^2 \\ \text{and} \quad g_3(s) &= -\frac{1}{2}(1-s^2)^2. \end{aligned}\right\} \qquad (80)$$

We observe that g_1, g_2 and g_3 are independent of η_0. From now on we assume that

$$0 < \mu \ll 1. \qquad (81)$$

We seek solutions such that, away from the boundary of the flow region, admit the following asymptotic expansions,

$$s(x, \mu) = \sum_{n=0}^{N} s_n(x)\mu^n + \mathscr{O}(\mu^{N+1}) \qquad (82)$$

$$\phi(x, \mu) = \sum_{n=0}^{N} \phi_n(x)\mu^n + \mathscr{O}(\mu^{N+1}). \qquad (83)$$

In order to simplify the notation, we let

$$S = s_0 \quad \text{and} \quad \Phi = \phi_0, \qquad (84)$$

denote the leading terms. Later in the section, we will modify the asymptotic expansions in (82) and (83) to account for internal layer contributions.

6.1. *Governing equations for the leading terms*

We consider equations (77) and (78) after setting $\mu = 0$:

$$0 = f'(S(x)) - \frac{1}{2}\mathscr{T}|g_3(S(x))| v'(x)\sin 2\Phi(x) \qquad (85)$$

$$0 = g_1(S(x))v'(x)\sin^2\Phi(x) - g_2(S(x))v'(x)\cos^2\Phi(x). \qquad (86)$$

Next we discuss the solvability of equations (85) and (86), for $v'(x)$ as in (74). We make use of relations (22).

We observe that equation (86) is identically satisfied for

$$Sv'(x)=0.$$

On the other hand, for points $x\in(-1,1)$ such that $Sv'(x)\neq 0$, we have

$$\cos 2\Phi(x)=-\frac{\gamma_1}{\gamma_2}(S(x)),\quad \text{or, equivalently,} \tag{87 a}$$

$$\sin 2\Phi(x)=eh(S(x)),\quad e=\pm 1,\quad \text{where } S \text{ satisfies,} \tag{87 b}$$

$$0=f'(S(x))-\frac{e}{2}\mathcal{T}\,|g_3((S(x)))|\,v'(x)h(S(x)), \tag{88}$$

with $h(s)$ as in (54). Equation (85) holds identically at points $x\in(-1,1)$ such that $S(x)=0$ and $v'(x)=0$. Equation (87 b) defines functions

$$\Phi=\Phi(S). \tag{89}$$

We denote

$$G(s)=g(s,\Phi(s)). \tag{90}$$

Taking into account that $\Phi(\cdot)$ satisfies

$$\sin^2\Phi=\frac{1}{2}\left(1+\frac{\gamma_1}{\gamma_2}\right) \quad\text{and}\quad \cos^2\Phi=\frac{1}{2}\left(1-\frac{\gamma_1}{\gamma_2}\right),$$

one can rewrite (90) as

$$4G(s)=2\alpha_4+\alpha_1\left(1-\frac{\gamma_1^2}{\gamma_2^2}\right)+(\alpha_5-\alpha_2)\left(1+\frac{\gamma_1}{\gamma_2}\right)$$
$$+(\alpha_3+\alpha_6)\left(1-\frac{\gamma_1}{\gamma_2}\right).$$

Since the right-hand side of (70) depends on ϕ through combinations of $\sin^2\phi$ and $\cos^2\phi$ only, $G(s)$ is well defined and independent of the sign chosen in (87 b).

In particular, employing the approximation given in (29) the previous relation becomes

$$G(s)=\eta_0(1-s)^2\frac{(2s+1)}{3(s+2)^2}(3s+2)(1-s^2)^2. \tag{91}$$

To study the solvability of the governing system for the leading terms S and Φ, we first examine the question of existence of solutions of equations (88) and (74). Subsequent substitution of S into (87) gives then the angle of alignment. Before proceeding with such a scheme, the following observations are in place:

(1) The solutions expected to follow from such method, in general, will not satisfy the boundary conditions. This requires to supplement the asymptotic expansions (82) and (83) with boundary layer ones. The goal is to satisfy the boundary conditions as well as ultimately achieve convergence of the previous expansions. Such issues will be treated in forthcoming work.

(2) When discussing the solvability of (88) special emphasis will be placed on configurations with defects. Equations (29) suggest that the only mechanism for loosing plane alignment in the present context is by reaching $s=0$ in some points of the domain.

We seek solutions such that

$$\left.\begin{aligned} &s(\cdot,\mu)\ \text{ is even, and}\\ &\phi(\cdot,\mu)\ \text{ is either even or odd,}\end{aligned}\right\} \tag{92}$$

in which case, expression (74) reduces to (75). Consequently, we will further restrict the choice of boundary conditions so as to satisfy either of the following,

$$s_a=s_b,\quad\text{and}\quad \phi_a=\pm\phi_b. \tag{93}$$

Substitution of $v'(x)$ as in equation (75) into (88) reduces the latter to the following,

$$0=-f'(S(x))+e\mathcal{T}F(S(x))x, \tag{94}$$

where

$$F(s)=\frac{|g_3(s)|}{2}G^{-1}(s)h(s). \tag{95}$$

We observe that

$$F(0)>0.$$

In particular, for $g_3(s)$ as in (80), $h(s)$ as in (56) and $G(s)$ as in (91), we have

$$F(s)=\frac{3(2+s)}{2(2s+1)^{1/2}(3s+2)(1-s)^{3/2}}. \tag{96}$$

Moreover

$$F(s)\approx\frac{3}{10}(3)^{1/2}(1-s)^{-3/2}\quad\text{and}\quad \approx(6)^{1/2}(2s+1)^{-1/2} \tag{97}$$

hold, for s close to 1 and $-1/2$, respectively.

In general, for the constitutive properties of *Proposition 1*, the following limiting properties hold:

$$\lim_{s\to 1-}F(s)=+\infty,\qquad \lim_{s\to -1/2+}F(s)=+\infty. \tag{98}$$

Taking such properties into account, we can now study the solvability of equations (94) and (87).

6.2. *Solutions with a disclination in the symmetry line of the flow region*

The next proposition shows the construction of two solutions, $(S^+(x),\Phi^+(x))$ and $(S^-(x),\Phi^-(x))$, that present a line defect at $x=0$. Although for simplicity we assume

$f(s)$ to be a single-well potential, the results also hold if the function $f(s)$ is non-convex.

6.2.1. *Proposition 3*

Suppose that $\alpha_i, \beta_i, \gamma_i$ are as in *Proposition 1*. Let $f(s)$ be such that $s_1 = s_2 = s_3 = 0$. Then:

(1) There exist $\alpha > 0$ such that (94) has two continuous solutions $S = S^+(x)$ and $S = S^-(x)$, $x \in (-\alpha, \alpha)$. They are both even on $(-\alpha, \alpha)$ and monotonic on the subintervals $(0, \alpha)$ and $(-\alpha, 0)$.

(2) $S^+(x) \geqslant 0$, $S^-(x) \leqslant 0$ and satisfy $S^+(0) = 0 = S^-(0)$.

(3) $S^+(\cdot)$ and $S^-(\cdot)$ satisfy the boundary conditions (66) and (93) provided s_a solves equation (94) for $x = -1$.

(4) The solutions $\Phi^+(\cdot)$ and $\Phi^-(\cdot)$ associated with $S^+(\cdot)$ and $S^-(\cdot)$, respectively, are discontinuous at $x = 0$ and satisfy

$$\Phi^{\pm}(x) = -\Phi^{\pm}(-x), \quad x \in (-\alpha, \alpha), \tag{99}$$

$$0 \leqslant \Phi^+(x) < \frac{\pi}{4}, \quad -\frac{\pi}{4} < \Phi^-(x) < 0, \quad x \in (0, \alpha), \tag{100}$$

$$\lim_{x \to 0+} \Phi^+(x) = \frac{\pi}{4} = \lim_{x \to 0-} \Phi^-(x), \tag{101}$$

$$\lim_{x \to 0-} \Phi^+(x) = -\frac{\pi}{4} = \lim_{x \to 0+} \Phi^-(x). \tag{102}$$

Proof. The existence of α, $1 \geqslant \alpha > 0$, with the previously established properties follows from the hypothesis $f'(0) = 0$ together with the continuity of the constitutive functions at $s = 0$. Without loss of generality, we construct the solution $S^+(x)$, $x \in (-\alpha, \alpha)$ as follows.

(1) For $x \in (0, \alpha)$, we let $S^+(x)$ be the solution of $f'(s) = \mathscr{T} F(s) x$.

(2) For $x \in (-\alpha, 0)$, we let $S^+(x)$ be the solution of $f'(s) = -\mathscr{T} F(s) x$.

Since $f'(s) = \mathscr{T} F(s)|x|$, for $x \in (-\alpha, \alpha)$, then $S^+(x) = S^+(-x) \geqslant 0$.

Likewise, we construct $S^-(\cdot)$ as the solution of

$$f'(s) = -\mathscr{T} F(s) x, \quad x \in (0, \alpha),$$
$$f'(s) = \mathscr{T} F(s) x, \quad x \in (-\alpha, 0).$$

Part (2) follows from the property $f'(0) = 0$ and part (3) is a consequence of the intermediate value theorem for continuous functions.

Finally, the oddness property (99) of $\Phi^{\pm}(x)$, $x \in (-\alpha, \alpha)$, follows from the construction in part (1), together with (87). In deriving (101) and (102) we also employ relations (22) and the first one of (87).

6.2.2. *Remark*

For $\alpha = 1$ to hold the additional hypothesis on the growth of $f'(s)$ near $s = 1$ has to be made:

$$f'(s) = \mathcal{O}(F(s)), \tag{103}$$

i.e. $f'(s)$ needs to grow faster that $F(s)$ as s approaches 1. The analogous condition should also hold for $s \approx -1/2$ in the case of the solution $S^-(x)$.

If $\alpha < 1$, then the fields on the intervals $(\alpha, 1)$ as well as $(-1, -\alpha)$ do not correspond to solutions of the form (43). In particular, the director may come out of the plane there. We point out that both $S^+(\cdot)$ and $S^-(\cdot)$ give positive values of the first normal stress difference. A further selection criteria between them should involve minimization of the dissipation function [16].

6.3. *Solutions with disclinations away from the centre of the flow region*

For a given $0 < X < 1$, we investigate whether the governing equations admit the following type of solution: $s(x) = S_l^+$, $x \in (0, X)$, $s(x) = S_l^-$, $x \in [X, 1]$, $s(x) = s(-x)$, $x \leqslant 0$, $\phi(x)$ satisfies equation (58), for $x \in (0, 1)$, and

$$\phi(x) = -\phi(-x), \quad \text{for } x < 0. \tag{104}$$

Here $S_l^{\pm}$ denote solution branches as in §4. In particular, the field s as constructed in (104) changes sign at $x = X$ and, therefore, a defect may be present there.

It is easy to check, however, that (104) does not solve the governing equations. (In particular, the σ_{13} component of the stress tensor corresponding to such construction is not continuous.) The presence of an internal layer around X matching both branches, S_l^+ and S_l^-, respectively, becomes necessary for the governing equations to be satisfied at $x = X$. For this, we rewrite the asymptotic expansions (82) and (83) accordingly. For a given integer $N \geqslant 0$, we seek solutions that for $\mu > 0$ sufficiently small can be expressed as follows:

$$s(x, \mu) = \sum_{n=0}^{N} s_n(x)\mu^n + \sum_{n=0}^{N} IS_n(\lambda)\mu^n + \mathrm{o}(\mu^N), \tag{105}$$

$$\phi(x, \mu) = \sum_{n=0}^{N} \phi_n(x)\mu^n + \sum_{n=0}^{N} I\Phi_n(\lambda)\mu^n + o(\mu^N), \tag{106}$$

$$\lambda = \frac{1}{\varepsilon}(x - X), \quad \text{with } \mu = \varepsilon^2. \tag{107}$$

The term IS_n and $I\Phi_n$, $n \geqslant 0$, represent internal layer contributions around $x = X$. We introduce the notation

$$IS \equiv IS_0, \quad I\Phi \equiv I\Phi_0. \tag{108}$$

To derive equations for the leading terms of such expansions, we substitute (105) and (106) into the governing equations (77) and (78) and neglect higher order terms in μ. This yields

$$0=\mu a_1(S''+IS'')-\frac{1}{\mathscr{T}}f'(S+IS)$$
$$-\mu a_2(S+IS)(\Phi'+I\Phi')^2$$
$$-g_3(S+IS)v'(x)\sin(\Phi+I\Phi)\cos(\Phi+I\Phi), \qquad (109)$$
$$0=\mu a_2 S^2(\Phi''+I\Phi'')$$
$$+v'(x)((g_1(S+IS)\sin^2(\Phi+I\Phi)$$
$$-g_2(S+IS)\cos^2(\Phi+I\Phi))$$
$$+2\mu a_2(S+IS)(S'+IS')(\Phi'+I\Phi'). \qquad (110)$$

6.3.1. *Solution in the interior of the domain*

In order to determine the fields away from the layer $x=X$ and the boundaries $x=\pm 1$, we let $\mu\to 0$ in the previous equations while holding $x\in(0,1)$, $x\neq X$ fixed. This gives equations (85), (86) together with (75). With the analogous solvability arguments leading to *Proposition 3*, we can now state the following result.

6.3.1.1. *Proposition 4*

Suppose that the hypotheses of *Proposition 1* hold. We assume that $f(s)$ satisfies growth conditions at $s=-1/2, 1$, i.e.

$$\lim_{s\to(-1/2,1)}\frac{F(s)}{|f'(s)|}=0. \qquad (111)$$

Then:

(1) There exists an even solution $S=S(x)$, $x\in(-1,1)$ that is discontinuous at $x=\pm X$. Moreover, it is monotonic on the subintervals $(0,X)$, $(X,1)$, $(-1,-X)$ and $(-X,0)$. It satisfies $S(0)=0$.
(2) $\Phi(\cdot)$ is odd, discontinuous at $x=\pm X$ and satisfies

$$\left.\begin{aligned} &0\leqslant\Phi(x)<\frac{\pi}{4}, \quad x\in(-X,0)\cup(X,1) \quad \text{and} \\ &-\frac{\pi}{4}<\Phi(x)<0, \quad x\in(-1,-X)\cup(0,X). \end{aligned}\right\} \qquad (112)$$

Moreover,

$$\lim_{x\to 0+}\Phi(x)=-\frac{\pi}{4} \quad \text{and} \quad \lim_{x\to 0-}\Phi(x)=\frac{\pi}{4}. \qquad (113)$$

Proof. We construct $S(x)$ as the solution of equation (94) with the following properties:

(1) for $x\in(-1,-X)\cup(0,X)$ let $e=-1$ in (94), and
(2) for $x\in(-X,0)\cup(X,1)$, let $e=1$.

For a given $X\in(0,1)$, the existence of such a solution follows from the continuity of $f'(s)$ and $F(s)$, for $s\neq 0$, together with the growth condition (111). The corresponding $\Phi(x)$ is calculated from equations (87 *b*), taking

(1) $e=-1$, for $x\in(-1,-X)\cup(0,X)$, and
(2) $e=+1$, for $x\in(-X,0)\cup(X,1)$.

Since

$$f'(s)=-\mathscr{T}F(s)|x|, \quad \text{for } x\in(-X,X), \quad \text{and}$$
$$f'(s)=+\mathscr{T}F(s)|x|, \quad \text{for } x\in(-1,-X)\cup(X,1),$$

then

$$S(x)=S(-x), \quad x\in(-1,1). \qquad (114)$$

Moreover,

$$\Phi(x)=-\Phi(-x), \quad \text{for } x\in(-1,1).$$

In deriving (114), we employ relations (22). We denote

$$\left.\begin{aligned} &S_-(x)=S(x), \quad x\in(0,X) \\ \text{and} \quad &S_+(x)=S(x), \quad x\in(X,1), \end{aligned}\right\} \qquad (115)$$

and likewise for $\Phi_\pm(x)$.

6.3.1.2. *Remarks*

(1) The growth conditions (111) are analogous to those of *Proposition 2*. As in the former case, they play the role of ensuring the solvability of (91) and (92) on the entire interval $(-1,1)$. Without such conditions, the solvability can only be guaranteed on an interval $(-\alpha,\alpha)$, $1>\alpha>0$. (This is a consequence of the property $f'(0)=0$ together with a continuity argument.) The type of structures constructed here would then be restricted to the smaller interval with $X\in(-\alpha,\alpha)$.

(2) The analogous construction in the case that $f(s)$ is non-convex allows the coexistence of distinct solution branches in the region such as S_1^+ and S_3^+ of §4 (instead of the matching of S_1^+ and S_1^- carried out here). We observe that matching of such branches does not involve passing through the isotropic state, $s=0$. This fact is exploited in forthcoming work in order to model phenomena such as *melt-fracture* and *stress jumps* [11, 12].

6.3.2. *Internal layer regions*

We start introducing the following notation. For a given function $\omega(\lambda)$, $\lambda\in(-\infty,\infty)$ differentiable, we denote

$$\frac{d\omega}{d\lambda}\equiv\dot{\omega}.$$

We now set $\mu=0$ in equations (109) and (110) while holding λ fixed. This gives the governing system for

$\{IS(\lambda), I\Phi(\lambda)\}$, $\lambda \in (-\infty, \infty)$:

$$0 = a_1(IS) - \left(\frac{1}{\mathcal{T}} f''(S) + \frac{1}{2} g_3'(S) v'(X) \sin(2\Phi)\right)(IS) - g_3(S) v'(X) \cos 2\Phi (I\Phi) + q_1(IS, I\Phi), \quad (116)$$

$$0 = \frac{1}{2}(g_1(S) + g_2(S)) v'(X) \sin 2\Phi \sin 2(I\Phi) + (g_1'(S)\sin^2\Phi - g_2'(S)\cos^2\Phi) v'(X)(IS) + a_2 S^2 (I\Phi) + q_2(IS, I\Phi), \quad (117)$$

where

$$S = S_-(X), \quad \Phi = \Phi_-(X), \quad \text{whenever } \lambda < 0, \quad (118)$$

$$S = S_+(X), \quad \Phi = \Phi_+(X), \quad \text{whenever } \lambda > 0. \quad (119)$$

$q_1(IS, I\Phi)$, $q_2(IS, I\Phi)$ denote the non-linear terms of the equations. We note that the coefficients of $(IS, I\Phi)$ in equations (116) and (117) are discontinuous at $\lambda = 0$.

We seek solutions $(IS(\lambda), I\Phi(\lambda))$, $\lambda \in (-\infty, \infty)$ of (116) and (117) satisfying the following conditions:

$$\left.\begin{aligned} &\lim_{\lambda \to 0+} IS(\lambda) = -S_+(X), \\ &\lim_{\lambda \to 0-} IS(\lambda) = -S_-(X), \\ &\lim_{\lambda \to 0+} I\Phi(\lambda) = \frac{\pi}{4} - \Phi_+(X), \\ &\lim_{\lambda \to 0-} I\Phi(\lambda) = -\frac{\pi}{4} - \Phi_-(X), \end{aligned}\right\} \quad (120)$$

and

$$\lim_{\lambda \to \pm\infty} IS(\lambda) = 0, \quad \lim_{\lambda \to \pm\infty} I\Phi(\lambda) = 0. \quad (121)$$

6.3.2.1. *Remark*

The first two limiting conditions in (120) establish the singularity of the line $x = X$ and the last two state that the director jumps from $\pi/4$ to $-\pi/4$ across such line. The limits in (121) are the standard ones in the theory of singular perturbations for Ordinary Differential Equations and express the condition that, away from the boundary layer region, the boundary layer contribution becomes negligible.

Existence of solutions of the problem (116)–(121) follow under the assumptions of *Proposition 3* together with the additional condition

$$\mathcal{I} \gg 1. \quad (122)$$

The proof is presented in [16].

6.3.3. *Multistripe solutions and selection of points X*

For a given integer $M > 0$, we consider points X_i, $1 \leqslant i \leqslant M$, such that $0 < X_i < 1$, $X_i < X_{i+1}$. We then construct a $2M$-layered solution following the method developed in this section. We point out that the method previously shown does not determine M as well as some of the points X. In fact, for the functions that we construct to be approximations of solutions of the boundary value problem (77) and (78), the data M and X_i cannot be arbitrarily prescribed but must be determined from μ.

There are two mechanisms of selection of the layer position X that reveal the different nature of such points. First of all, let us assume that $f(\cdot)$ is non-convex and $0 < c_1 < c_2 < 1$ denote the critical points of $f'(\cdot)$ as in §4. Let $x_1 > 0$ denote the point such that $s(x_1) = c_1$. Then for $\mathcal{T} > 0$ such that $c_1 \mathcal{T} < 1$, we take $X = x_1$.

Moreover for such a choice of X, we observe that another solution construction is available by letting

$$s(x) = S_3^+, \quad x \in [X, 1),$$

instead of S_I^- in (104). Out of both such solutions, we select the one that minimizes the rate of dissipation.

The second mechanism is associated with the fact that the first term of the right hand side of (78) changes sign at $s = 0$ and, consequently, the forcing term of the equation becomes oscillatory. (Moreover, points where s vanishes are associated with infinite values of $|\phi'|$.) In forthcoming work, we develop an algorithm to get numerical approximations to such points. We also provide a qualitative argument based on phase-plane analysis of a related second order nonlinear differential equation.

7. Conclusions

In this article we have illustrated how new mathematical mechanisms arise in the equations when the order parameter is included in the model. The new mechanisms extend those of the Leslie–Ericksen theory and help towards the study of local effects not modelled by the former. In particular, we have shown that the energy associated with the order parameter introduces a mechanism of surface energy which accounts for the presence of defects in the form of singular internal layers or stress jumps.

The contribution to the model of the latter mechanism is quantified by the dimensionless parameter $\mathcal{I}$, the interface number, which together with E give a characterization of stationary flow regimes.

The work presented in this paper seems to outline material properties and mathematical methods useful in describing regimes with large E well beyond the scope of the model and geometry presented here.

From the modelling point of view, it reinforces the idea that tools from Continuum Mechanics combined with other physical theories (for example, molecular theory) provide a systematic procedure to obtain systems of governing equations amenable to mathematical analysis and computing. Whereas the former establishes guidelines on obtaining balance laws and relating kinematic fields with dynamic ones, the latter give invaluable information on material properties.

References

[1] ERICKSEN, J. L., 1991, Liquid crystals with variable degree of orientation, *Arch. Rational Mech. Anal.,* **113,** 97.

[2] KUZUU, N., and DOI, M., 1984, Constitutive equation for nematic liquid crystals under weak velocity gradient derived from a molecular kinetic equation. II, *J. Phys. Soc. Japan,* **53,** 1031.

[3] MARRUCCI, G., 1981, Prediction of Leslie coefficients for rod-like polymer nematics, *Mol. Cryst. liq. Cryst.,* **72,** 153.

[4] BERRY, G. C., 1988, Rheological properties of nematic solutions of rod-like polymers, *Mol. Cryst. liq. Cryst.,* **165,** 333.

[5] LARSON, R. G., and MEAD, D. W., 1992, Development of orientation and texture during shearing of liquid-crystalline polymers, *Liq. Crystals,* **12,** 751.

[6] WISSBRUN, K. F., 1981, Rheology of rod-like polymers in the liquid crystalline state, *J. Rheol.,* **25,** 619.

[7] WAHL, J., and FISCHER, F., 1973, Elastic and viscosity constants of nematic liquid crystals from a new optical method, *Mol. Cryst. liq. Cryst.,* **22,** 359.

[8] DE GENNES, P. G., 1974, *The Physics of Liquid Crystals* (Oxford Univ. Press, Clarendon, London and New York).

[8A] ERICKSEN, J. L., 1969, A boundary-layer effect in viscosity of liquid crystals, *Trans. Soc. Rheol.,* **13, 9.**

[9] DOI, M., 1981, Molecular dynamics and rheological properties of concentrated solutions of rod-like polymers in isotropic and liquid crystalline phases, *J. Polym. Sci. Polym. Phys. Ed.,* **19,** 229.

[10] KUZUU, N., and DOI, M., 1983, Constitutive equation for nematic liquid crystals under weak velocity gradient derived from a molecular kinetic equation, *J. Phys. Soc. Japan,* **52,** 3486.

[11] GOTSIS, A. D., and BAIRD, D. G., 1986, Primary normal-stress difference for two liquid crystalline copolyesters, *Rheol. Acta,* **25,** 275.

[12] VIOLA, G. G., BAIRD, D. G., and WILKES, G. L., 1985, The development of molecular orientation and morphological texture in thermotropic copolyesters, *Polym. Eng. Sci.,* **25,** 888.

[13] FONSECA, I., and TARTAR, L., 1989, The gradient theory of phase transitions for systems with two potential wells, *Proc. Roy. Soc. Edinburgh,* **111A,** 89.

[14] LESLIE, F. M., 1979, Theory of flow phenomena in liquid crystals, *Adv. Liq. Crystals,* **4,** 1.

[15] LONGA, L., MONSELESAN, D., and TREBIN, H. R., 1987, An extension of the Landau–Ginsburg–de Gennes theory for liquid crystals, *Liq. Crystals,* **2,** 769.

[16] CALDERER, M. C., and MUKHERJEE, B., 1996, Chevron pattern in liquid crystal flows, *Physica D,* **1350,** 1.

[17] CHANDRASEKHAR, S., 1992, *Liquid Crystals,* Second Edition (Cambridge University Press, Cambridge, New York and Oakleigh).

Appendix: The Helmholtz free energy

The purpose of this appendix is to provide a justification for the use of the simpler form of the free energy (5) instead of the more physically realistic one given below. First of all, the function shown in (5), even though it depends on s, it does not exhibit all the terms of the Oseen–Frank free energy expression. In addition, no coupling between $\mathbf{n}$ and s is taken into account in the simplified form. Here, as in [1], we propose the following form:

$$\mathscr{F} = W_0 + W_2,$$

with

$$\begin{aligned} 2W_2 = {} & K_1(\nabla\cdot\mathbf{n})^2 + K_2(\mathbf{n}\cdot\nabla\times\mathbf{n})^2 + K_3|\mathbf{n}\times\nabla\times\mathbf{n}|^2 \\ & + (K_2+K_4)(\operatorname{tr}(\nabla\mathbf{n})^2 - (\nabla\cdot\mathbf{n})^2) + L_1|\nabla s|^2 \\ & + L_2(\nabla s\cdot\mathbf{n})^2 + L_3\nabla\cdot\mathbf{n}(\nabla s\cdot\mathbf{n}) + L_4\nabla s\cdot(\nabla\mathbf{n}\mathbf{n}). \end{aligned} \tag{A 1}$$

We let K_1, K_2, K_3, K_4, L_1, L_2, L_3 and L_4 denote functions of s. In general, they should be regarded as functions of the temperature or the concentration as well, but in the present context, we take the latter as parameters.

Restrictions on such functions stem from the requirement that the total energy is bounded below. A reorganization of terms in (A 1) gives

$$\left.\begin{aligned} &\bar{K}_1>0, \quad K_2>|K_4|, \quad \bar{K}_3>0, \quad 2\bar{K}_1-K_2-K_4>0, \\ &\qquad K_5, \quad K_6>0, \end{aligned}\right\} \tag{A 2}$$

for all $s\in(-1/2, 1)$, with

$$\left.\begin{aligned} \bar{K}_1 &= K_1 - \frac{L_3^2}{4(L_1+L_2)}, \\ \bar{K}_3 &= K_3 - \frac{L_4^2}{4L_1} \\ K_5 &= L_1, \\ K_6 &= L_1+L_2. \end{aligned}\right\} \tag{A 3}$$

The remaining task is to determine suitable expressions for K_i, L_j. Assuming that they are polynomials in s, Ericksen proceeds to compare the free energy given by (A 1) with expressions of the form $W_2(Q, \nabla Q)$ corresponding to Landau–Ginzburg–de Gennes models [15]. Specifically, we write

$$W_2(Q, \nabla Q) = W_2^0(Q, \nabla Q) + W_2^1(Q, \nabla Q),$$

where $W_2^0(Q, \nabla Q)$ denotes a quadratic function of ∇Q with coefficients independent of Q whereas $W_2^1(Q, \nabla Q)$ corresponds to coefficients that are of the first order with respect to Q. Such comparison gives the following expressions of the coefficients,

$$\left.\begin{aligned} &\frac{K_1}{2}=\frac{K_3}{2}+cs^3,\\ &\frac{K_2}{2}=as^2+bs^3=\frac{K_3}{2},\\ &\frac{K_4}{2}=ms^2+cs^3,\\ &\frac{L_1}{2}=n, \quad \frac{L_2}{2}=qs, \quad L_3=-ms=-L_4, \end{aligned}\right\} \quad \text{(A 4)}$$

where a, b, c, m, n, q are constants whose choice is restricted by inequalities (A 2). Finally we derive the governing equations for fields $\mathbf{v}$, $\mathbf{n}$ and s as given in § 3. First of all, in such case the free energy becomes

$$\begin{aligned} 2W_2 = &(K_1\cos^2\phi + K_3\sin^2\phi)(\phi')^2\\ &+(L_1+L_2\sin^2\phi)(s')^2. \end{aligned} \quad \text{(A 5)}$$

The governing equations in dimensional form become

$$\left.\begin{aligned} 0 = &(2(n+qs\sin^2\phi)s')' - (2as+3(b+c\cos^2\phi)s^2)(\phi')^2\\ &-q\sin^2\phi(s')^2 - W_0'(s) - \beta_3\sin\phi\cos\phi v',\\ 0 = &(as^2+(b+c\cos^2\phi)s^3\phi')' + cs^3\sin\phi\cos\phi(\phi')^2\\ &-\frac{1}{4}(\gamma_1+\gamma_2\cos 2\phi)v',\\ 0 = &\frac{\partial(-p-A+\hat{\sigma}_{11})}{\partial x}, \end{aligned}\right\} \quad \text{(A 6)}$$

with

$$A = 2(as^2+(b+c\cos^2\phi)s^3)(\phi')^2 + 2(n+qs\sin^2\phi)(s')^2, \quad \text{(A 7)}$$

together with equations (45) and (46).

After carrying out the non-dimensionalization of the previous system as done in § 3, we observe that the results of § 4, 5 and 6 apply directly to them. The new terms exhibited by the governing system (A 5)–(A 7) become relevant only in analyses concerning low and intermediate values of E.