

Home Search Collections Journals About Contact us My IOPscience

Geometry and dynamics of a nematic liquid crystal in a uniform shear flow

This article has been downloaded from IOPscience. Please scroll down to see the full text article. 2001 J. Phys. A: Math. Gen. 34 1393 (http://iopscience.iop.org/0305-4470/34/7/312)

View the table of contents for this issue, or go to the journal homepage for more

Download details: IP Address: 171.66.16.101 The article was downloaded on 02/06/2010 at 09:50

Please note that terms and conditions apply.

J. Phys. A: Math. Gen. 34 (2001) 1393-1404

www.iop.org/Journals/ja PII: S0305-4470(01)16970-2

# Geometry and dynamics of a nematic liquid crystal in a uniform shear flow

# D R J Chillingworth, E Vicente Alonso and A A Wheeler

Department of Mathematics, University of Southampton, Southampton SO17 1BJ, UK

Received 8 September 2000, in final form 23 December 2000

#### Abstract

We study the dynamics of a nematic liquid crystal in a shear flow by employing the gradient of the Landau–de Gennes free-energy function on second-rank tensors, modified by constant and rotational terms. We predict configurations of equilibria and periodic solutions found in numerical simulations and explain certain anomalous nongeneric continua of equilibria. The existence of these continua shows that the model is structurally unstable.

PACS numbers: 0240, 4720, 6130

## 1. Introduction

In this paper we derive some mathematically rigorous results using geometric techniques concerning a Landau–de Gennes model of a liquid crystal in a uniform shear flow and prompted by a detailed study carried out by Vicente Alonso [20].

Olmsted and Goldbart [14] investigated a Landau–de Gennes model for this situation. Subsequently Vicente Alonso [20] conducted a more thorough investigation and extended the work of Olmsted and Goldbart by using a combination of analytical and numerical techniques based on bifurcation theory. She has been able to elucidate systematically the complicated solution structure of this problem in both two and three dimensions, identify time-dependent tumbling and wagging modes and discover a Takens–Bogdanov bifurcation point associated with this dynamical behaviour.

This problem has also been considered by other researchers using different physical models. Larson [10] employed a Doi model [2] and demonstrated that the system exhibits a complex variety of behaviour including tumbling and wagging. Subsequently Maffettone and co-workers [5, 11, 12] examined the Doi model using techniques of numerical bifurcation theory to reveal systematically the underlying solution structure. Numerical bifurcation theory has also been employed by Rey and co-workers [6,7,16,18,19] on a hybrid model that marries to the Doi model or the Leslie–Ericksen theory in different limits.

The degree of coherence of alignments of molecules in a nematic liquid crystal is often represented by a field of symmetric  $3 \times 3$  tensors Q(x),  $x \in \mathbb{R}^3$  with tr(Q) = 0 (the *tensor* order parameter or Saupe ordering matrix) [17]. In a spatially uniform system the matrix Q is independent of  $x \in \mathbb{R}^3$ . When Q = 0 the system is said to be isotropic, with the molecules not aligned in any particular direction. The configuration space for the dynamical study of such systems is thus the five-dimensional linear space V of traceless real symmetric  $3 \times 3$  matrices. In the absence of external influence (such as an electric or magnetic field or a fluid flow) the governing equations are invariant under rigid rotations and reflections in  $\mathbb{R}^3$  and hence under the conjugacy action of the orthogonal group O(3) on V.

Equilibrium states of a bulk liquid crystal are taken to be critical points of a smooth *free-energy* function

$$F: V \to \mathbf{R}$$

for which the O(3)-invariance is expressed by the fact (see e.g. [1]) that F(Q) is composed of sums and products of the two basic functions  $tr(Q^2)$  and  $tr(Q^3)$  (or  $tr(Q^2)$  and det(Q)since  $tr(Q^3) = 3 det(Q)$  when tr(Q) = 0). The simplest such model that gives realistic stable equilibria (local minima of F) is the Landau–de Gennes model [3]

$$F(Q) = \frac{1}{2}\tau \operatorname{tr}(Q^2) - \frac{1}{3}B\operatorname{tr}(Q^3) + \frac{1}{4}C(\operatorname{tr}(Q^2))^2$$
(1.1)

in which B, C > 0 are constants of the material and  $\tau$  represents deviation from a critical temperature. Equilibria are fixed points of the flow generated by grad F on V, the gradient being defined using the standard inner product  $\langle Q, R \rangle = tr(Q^T R) = tr(QR)$  for  $Q, R \in V$ .

The governing equations in the presence of a shear flow have been derived [8, 13–15] using this free-energy function enhanced with additional gradient energy terms to account for elastic effects. We assume that the nematic liquid crystal is both isothermal and incompressible. Standard procedures from nonequilibrium thermodynamics requiring positive energy production and conservation of momentum and mass yield a rate equation for the order tensor together with a momentum equation for a divergence-free velocity field.

In this paper we focus on a simple model where the shear flow is confined to the (x, y)-plane. In particular we assume the velocity field is v(y, 0, 0), where v is the shear rate. In this situation the momentum equation is automatically satisfied and the rate equation for the order tensor may be expressed as

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = \delta P(Q) - \operatorname{grad} F(Q) \tag{1.2}$$

where  $\delta$  is the dimensionless shear rate and where

$$P(Q) = [W, Q] + \beta D \tag{1.3}$$

in which

$$W = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad D = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$
(1.4)

and  $\beta > 0$  is a constant.

We study the system (1.2), first in the case when all configurations are constrained to lie in the plane of the shear flow (the *in-plane* case) and then when arbitrary configurations are allowed (*out of plane*). As we show, there are in fact *no* out-of-plane equilibria with the exception of an anomalous continuum (ellipse) of equilibria that exists only for parameter values ( $\tau$ ,  $\delta$ ) lying on a circle in  $\mathbb{R}^2$ , a phenomenon first discovered numerically [20]. We conclude from this that the model is not structurally stable, and thus not fully adequate as a representation of observable physical phenomena.

#### 2. The in-plane case without flow

This case has been well studied previously: see for example [4]. In the absence of flow we have  $\delta = 0$  and (1.2) gives

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = -\mathrm{grad}F(Q). \tag{2.1}$$

We restrict our attention to configurations which are symmetric with respect to reflection in the x-, y-plane, so that molecules are aligned either in that plane or in the direction of the z-axis. Without loss of generality we may express Q in the form

$$Q = \begin{pmatrix} \eta + \sqrt{3}\mu & \sqrt{3}\nu & 0\\ \sqrt{3}\nu & \eta - \sqrt{3}\mu & 0\\ 0 & 0 & -2\eta \end{pmatrix} = \eta E + \sqrt{3}\rho R(\alpha)$$
(2.2)

with  $\mu, \nu, \eta \in \mathbf{R}$ , where  $\mu + i\nu = \rho e^{i\alpha}$  and

$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \qquad R(\alpha) = \begin{pmatrix} \cos \alpha & \sin \alpha & 0 \\ \sin \alpha & -\cos \alpha & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$
 (2.3)

In these coordinates

$$tr(Q^2) = 6(\rho^2 + \eta^2)$$
(2.4)

$$tr(Q^3) = 6\eta(3\rho^2 - \eta^2) = 6 \operatorname{Im}(\rho + i\eta)^3.$$
(2.5)

Let  $U \cong \mathbb{R}^3$  denote the space of all  $3 \times 3$  matrices of the form (2.2). The free-energy function *F* restricted to *U* is clearly invariant with respect to the symmetries:

- (i) rotation about the  $\eta$ -axis;
- (ii)  $D_3$  in the  $(\rho, \eta)$ -plane

where  $D_3$  is the group of symmetries of an equilateral triangle, generated by rotation by  $2\pi/3$  and reflection in the  $\eta$ -axis. This immediately gives:

**Proposition 2.1.** The critical points of F restricted to U occur either as circles about the  $\eta$ -axis or as points on the  $\eta$ -axis. The set of critical points meets any plane in U containing the  $\eta$ -axis in a  $D_3$ -symmetric configuration.

See figure 1 as a schematic indication of this geometry.

By first considering the restriction of F to the  $\eta$ -axis and then exploiting symmetry it is straightforward to deduce the following description of equilibria for the system  $\dot{Q} = -\text{grad}F(Q)$ :

$$\tau > \tau_0 > 0$$
:  $Q = 0$  stable

$\tau_0 > \tau > 0$ :	Q = 0	stable
	$Q = Q_i = \eta_i E,  i = 1, 2,  \eta_1 < \eta_2 < 0$	
	$Q = \tilde{Q}_i(\alpha) = -\frac{1}{2}\eta_i(E + 3R(\alpha)),  0 \le \alpha < 2\pi$	
	i = 1: stable, $i = 2$ : unstable	

$$\begin{array}{ll} 0 > \tau \colon & Q = 0 & \text{unstable} \\ & Q = Q_1, \, \tilde{Q}_1(\alpha), \quad \eta_1 < 0 & \text{stable} \\ & Q = Q_2, \, \tilde{Q}_2(\alpha), \quad \eta_2 > 0 & \text{unstable} \end{array}$$

As  $\tau$  decreases through  $\tau_0 = B^2/24C$  there are simultaneous saddle-node creations of pairs of equilibria at  $(\rho, \eta) = (0, \eta_0)$  and  $(\pm \rho_0, -\frac{1}{2}\eta_0)$  where  $\rho_0 = \frac{\sqrt{3}}{2}\eta_0$  and  $\eta_0 = -2\tau_0/B$ ;



Figure 2. Bifurcation diagram for critical points of F on U. Bold Figure 1. Sketch of symmetries of F on curves represent stable equilibria.

subsequently the innermost equilibria approach the origin and coalesce at a degenerate critical point there as  $\tau$  decreases to 0, emerging on the other side as  $\tau$  becomes negative. See figures 2, 3.

The physical interpretation is that in the absence of a velocity field for  $\tau > \tau_0$  the only stable state is the isotropic (Q = 0) state, while for  $\tau < \tau_0$  there are further stable states with molecules aligned in the z-direction or (for the same free energy) with molecules aligned in some direction in the (x, y)-plane; all directions have equal likelihood. The isotropic state loses stability when  $\tau$  becomes negative.

## 3. Nonzero shear: the in-plane case

We now consider the dynamical system (1.2), (1.3) with W, D nonzero but still restricted to the space U of in-plane configurations. The first step is an elementary but crucial observation.

**Proposition 3.1.** Since F is invariant under rotation about the  $\eta$ -axis, the  $(\mu, \nu)$  component of grad F is radial. Hence equilibria for (1.2) can occur only where the  $(\mu, \nu)$  component of P is radial.

Later we generalize this to the full out-of-plane context. Meanwhile, it is easily checked that for the in-plane case the vector field P is given in  $(\mu, \nu, \eta)$ -coordinates by

$$P(\mu, \nu, \eta) = \left(2\nu, -2\mu + \frac{1}{\sqrt{3}}\beta, 0\right)$$
(3.1)

for which the integral flow is rotation about the point  $(\frac{1}{2\sqrt{3}}\beta, 0, \eta)$  in each plane  $\eta = \text{constant}$ . Elementary geometry shows that this flow is radial in  $(\mu, \nu)$  at precisely those points where  $(\mu, \nu)$  lies on the circle *C* with diameter the interval  $[0, \frac{1}{2\sqrt{3}}\beta]$  on the  $\mu$ -axis: see figure 4.

If  $\tilde{C}$  denotes the cylinder that is the product of C with the  $\eta$ -axis we then have:

U.



**Figure 3.** Phase portraits for  $\dot{Q} = -\text{grad}F(Q)$  (schematic).



Figure 4. Circle *C* where *P* is radial.

**Proposition 3.2.** All in-plane equilibria for (1.2), (1.3) lie on  $\tilde{C}$ .

The behaviour of equilibria as  $\tau$ ,  $\delta$  are varied has been fully investigated by analytical and numerical methods by Vicente Alonso [20]. Some of these results can be recovered qualitatively by geometric arguments, which we do not pursue here.



**Figure 5.** Bifurcation diagram showing equilibria coalescing at a saddle-node to become a tumbling orbit when  $\delta > 0$ .

## 4. Some dynamics for the in-plane case

When  $\delta = 0$  the equilibria (critical points of *F*) which are not on the  $\eta$ -axis occur in circles about the  $\eta$ -axis, and for  $\tau \neq 0$ ,  $\tau_0$  these circles are *normally hyperbolic*: the eigenvalues of the local linearization of grad *F* in the  $(\rho, \eta)$ -plane are nonzero. Since there is zero flow along the circles themselves they are thus *r*-normally hyperbolic [9] for all r > 0. The invariant manifold theorem [9] therefore implies that they persist as  $C^{\infty}$  invariant manifolds for sufficiently small  $C^{\infty}$  perturbations of the flow. More specifically:

**Proposition 4.1.** Let  $\tau \neq 0$ ,  $\tau_0$  and let *S* be a circle of critical points of *F* restricted to *U*. Then for sufficiently small  $\delta > 0$  (depending on  $\tau$ ) there is a  $C^{\infty}$  closed curve *S'* close to *S* which is invariant under the flow of the non-gradient system (1.2).

**Corollary 4.2.** The only points of S' which can be equilibria are those of  $S' \cap \tilde{C}$ ; for sufficiently small  $\delta > 0$  there are at most two such points.

Since the radii of the circles *S* tend to  $+\infty$  as  $\tau \to -\infty$  and the cylinder  $\tilde{C}$  is fixed it follows that for sufficiently small  $\delta > 0$  the solution branches representing circles *S* for  $\delta = 0$  become pairs of branches of equilibria that mutually annihilate at a saddle-node for some  $\tau < 0$ . This can be clearly seen in the study of equilibrium paths in [20], from which figure 5 is taken as an illustration.

**Corollary 4.3.** Suppose  $\tau$  is sufficiently large and negative so that S is disjoint from (i.e. encircles)  $\tilde{C}$ . Then for sufficiently small  $\delta > 0$  the loop S' is a periodic orbit of (1.2).

Such periodic orbits necessarily encircle the  $\eta$ -axis and hence represent so-called *tumbling* motion of the molecules [20]. Only those arising from S corresponding to  $\tilde{Q}_1$  (see section 2) will be stable.

There is a useful extension to proposition 3.2. Any periodic orbit of (1.2) which cuts  $\tilde{C}$  must do so in a radial direction as both *P* and grad *F* are radial there. This is nicely illustrated by



Figure 6. Wagging orbits created at a Hopf bifurcation becoming larger-amplitude tumbling orbits.

the family of periodic orbits created by a Hopf bifurcation at a point of  $\tilde{C}$  as shown numerically in figure 6. These orbits initially do not encircle the  $\eta$ -axis and represent wagging motion.

There are more complicated bifurcations that occur, including a Takens–Bogdanov bifurcation. For further details see [20].

### 5. Out-of-plane equilibria

Finally we turn to out-of-plane equilibria, that is equilibrium states in which molecules are oriented neither in nor orthogonal to the plane of the shear flow. Numerical evidence [20] suggests that there exist in general *no* out-of-plane equilibrium states for the system (1.2). The curious exception is that for sufficiently small  $\delta > 0$  there are apparently two values  $\tau = \tau_1, \tau_2$  (depending on  $\delta$ ) for which there exists a *continuum* of equilibria: see figure 7.

The aim in this section is to give the geometric explanation for this highly nongeneric behaviour. On this basis we make some comments on the robustness of the dynamical model (1.2).

We begin by formulating the analogue of proposition 3.1 for the full out-of-plane system.

For  $Q \in V$  consider the orbit  $\Gamma Q$  of Q under the action of the group  $\Gamma = O(3)$  on V. For typical Q the orbit is a smooth 3-manifold, while for nonzero Q with two equal eigenvalues it is a 2-manifold (projective plane). The tangent space to  $\Gamma Q$  at Q is the linear subspace  $T_Q$  of V given by

$$T_O = \{ [\tilde{W}, Q] : \tilde{W} \in \text{Skew} \}$$

where Skew denotes the set of  $3 \times 3$  real skew-symmetric matrices (the Lie algebra of the group O(3)). Since the free-energy function F is  $\Gamma$ -invariant it is constant on each  $\Gamma$ -orbit and so grad F(Q) is orthogonal to  $T_Q$  for every  $Q \in V$ . We can now generalize proposition 3.1.

**Proposition 5.1.** Equilibria for (1.2) on V can occur only where P(Q) is orthogonal to  $T_Q$ .

This orthogonality can be neatly characterized.

**Proposition 5.2.** The matrix P = P(Q) is orthogonal to  $T_Q$  if and only if P commutes with Q.



**Figure 7.** The ellipses  $E_1$ ,  $E_2$  of out-of-plane equilibria. Here p, t are respectively a diagonal and off-diagonal component of the matrix Q: see (5.1).

**Proof.** Since  $\langle P, [\tilde{W}, Q] \rangle = \langle [Q, P], \tilde{W} \rangle$  we see that *P* is orthogonal to  $T_Q$  precisely when [Q, P] is orthogonal to every  $\tilde{W} \in$  Skew, that is [Q, P] is symmetric. However, since Q, P are symmetric the matrix [Q, P] is in any case skew-symmetric and so symmetric if and only if it is zero, that is QP = PQ.

Defining the *normality locus*  $\mathcal{N} \subset V$  by

 $\mathcal{N} = \{ Q \in V : P(Q) \text{ commutes with } Q \}$ 

we thus have:

**Corollary 5.3.** All equilibria for (1.2) in V lie on  $\mathcal{N}$ .

**Remark.** An equilibrium state Q satisfies  $\delta P(Q) = \text{grad}F(Q)$ , which automatically commutes with Q, so proposition 5.2 follows immediately from this. However, we later wish to exploit the geometry behind this algebraic conclusion.

The equations for  $\mathcal{N}$  are easy to write down. Taking

$$Q = \begin{pmatrix} p & u & t \\ u & q & s \\ t & s & r \end{pmatrix} \qquad p + q + r = 0 \tag{5.1}$$

gives

$$[W, Q] = \begin{pmatrix} 2u & q-p & s \\ q-p & -2u & -t \\ s & -t & 0 \end{pmatrix}$$

and the three equations requiring that the skew-symmetric matrix [P(Q), Q] be zero are

$$(q-p)^{2} + s^{2} + t^{2} + 4u^{2} = -\beta(q-p)$$
(5.2)

$$3(ut - ps) = -\beta s \tag{5.3}$$

$$3(qt - us) = -\beta t. \tag{5.4}$$

Note that setting s = t = 0 leaves the single equation

$$(q-p)^2 + \beta(q-p) + 4u^2 = 0$$

which in  $(\mu, \nu, \eta)$ -coordinates is the cylinder  $\tilde{C}$  from section 4.

Let  $\tilde{\mathcal{N}}$  denote  $\mathcal{N} \setminus \tilde{C}$ , that is the out-of-plane part of  $\mathcal{N}$ , corresponding to  $(s, t) \neq (0, 0)$ .

**Proposition 5.4.** The set  $\tilde{\mathcal{N}}$  lies on the sphere in V with centre the origin and radius  $\sqrt{\frac{2}{3}}\beta$ .

**Proof.** Rewrite the equations (5.2)–(5.4) as

$$\frac{1}{2}|Q|^2 + 3(u^2 - pq) = \beta(p - q)$$
(5.5)

$$ut = ps - \frac{1}{3}\beta s \tag{5.6}$$

$$us = qt + \frac{1}{3}\beta t \tag{5.7}$$

recalling that  $|Q|^2 = tr(Q^2)$ . Multiplying (5.6) and (5.7) gives when  $st \neq 0$ 

$$u^{2} = (p - \frac{1}{3}\beta)(q + \frac{1}{3}\beta)$$
(5.8)

and substitution into (5.5) gives  $\frac{1}{2}|Q|^2 = \frac{1}{3}\beta^2$ . If s = 0 and  $t \neq 0$  then u = 0,  $q = -\frac{1}{3}\beta$  and again (5.5) gives  $\frac{1}{2}|Q|^2 = \frac{1}{3}\beta^2$ ; similarly if  $s \neq 0$ , t = 0.

**Corollary 5.5.** For fixed  $\beta$  and B, C the out-of-plane equilibrium states for (1.2) remain bounded (and hence also the free energy remains bounded) regardless of the values of  $\tau$  and  $\delta$ .

In fact, as we see below, such equilibria exist only for  $(\tau, \delta)$  in a bounded region of the parameter space. This contrasts with in-plane equilibria which exist for arbitrarily large  $|\tau|$  and  $\delta$ .

Now replacing  $|Q|^2$  by  $\frac{2}{3}\beta^2$  in the expression

$$\operatorname{grad} F(Q) = \tau Q - B(Q^2 - \frac{1}{3}|Q|^2 I) + C|Q|^2 Q$$
(5.9)

for the gradient of F on V we obtain the following simplification of the problem:

**Corollary 5.6.** The out-of-plane equilibria of (1.2) coincide with the zeros on  $\tilde{N}$  of the vector field

$$\tilde{X}(Q) = \delta P(Q) - Z(Q) \tag{5.10}$$

where

$$Z(Q) = \frac{2}{9}\beta^2 BI + \tau_* Q - BQ^2$$
(5.11)

with  $\tau_* = \tau + \frac{2}{3}\beta^2 C$ .

Let K denote the orthogonal complement of U in V; thus K consists of the matrices of the form

$$M(s,t) = \begin{pmatrix} 0 & 0 & t \\ 0 & 0 & s \\ t & s & 0 \end{pmatrix}$$
(5.12)

for  $s, t \in \mathbf{R}$ . We identify M(s, t) with  $(s, t) \in \mathbf{R}^2$ . If  $\pi : V \to K \cong \mathbf{R}^2$  denotes orthogonal projection then out-of-plane equilibria Q are precisely those with  $\pi(Q) \neq (0, 0)$ .

The following calculation is elementary, given tr(Q) = p + q + r = 0.

**Proposition 5.7.** If  $Q \in \mathcal{N}$  and  $\pi(Q) = (s, t)$  then  $\pi(Q^2) = a(-s, t)$  where  $a = \frac{1}{3}\beta$ ; thus

$$\pi(Z(Q)) = ((\tau_* + aB)s, (\tau_* - aB)t).$$
(5.13)

**Corollary 5.8.** For  $Q \in \tilde{\mathcal{N}}$  the projected vector field  $\pi(\tilde{X}(Q))$  is linear and given by  $\pi(\tilde{X}(Q)) = H\pi(Q)$  where H is the  $2 \times 2$  matrix

$$H = \begin{pmatrix} -\tau_* - aB & -\delta \\ \delta & -\tau_* + aB \end{pmatrix}.$$
(5.14)

**Corollary 5.9.** If  $\tilde{X}(Q) = 0 \in V$  with  $\pi(Q) \neq (0,0) \in K \cong \mathbb{R}^2$  then det H = 0 and  $\pi(Q) \in \ker H$ . Thus out-of-plane solutions to (1.2) exist only if

$$\tau_*^2 + \delta^2 = a^2 B^2. \tag{5.15}$$

Such solutions Q have  $\pi(Q) = (s, t)$  with s = kt where

$$k = \delta^{-1}(\tau_* + aB) = -\delta(\tau_* - aB)^{-1}$$
(5.16)

for  $\delta \neq 0$ . When  $\delta = 0$  the solutions have t = 0 or s = 0 for  $\tau_* = aB$  or  $\tau_* = -aB$  respectively.

Putting these results together gives:

**Theorem 5.10.** For  $0 < \delta < aB$  there are two values  $\tau_1, \tau_2$  of  $\tau$  for which out-of-plane equilibria can exist. Such equilibria lie on the ellipse  $E_i = \tilde{N} \cap \mathcal{H}_i$ , i = 1, 2 where  $\mathcal{H}_i$  is the hyperplane s = kt of V with k as in (5.16) for  $\tau_* = \tau_i + \frac{2}{3}\beta^2 C$ . For  $\delta = aB$  there can be out-of-plane equilibria only when  $\tau = -\frac{2}{3}\beta^2 C$ , and for  $\delta > aB$  there are no out-of-plane equilibria.

The ellipses  $E_i$ , i = 1, 2 are those discovered numerically in [20], where they appear to consist entirely of equilibria. We next show that this is indeed the case. We need a preliminary algebraic fact. Let  $\mathcal{H} = \mathcal{H}_1 \cup \mathcal{H}_2$ .

**Proposition 5.11.** For every  $Q \in \tilde{\mathcal{N}} \cap \mathcal{H}$  we have  $T_Q \cap K = \{0\}$ .

The proof follows below. From proposition 5.11 we now obtain the result that all points of  $E_1$ ,  $E_2$  are equilibria for (1.2).

**Theorem 5.12.**  $\tilde{X}(Q) = 0$  for all  $Q \in \tilde{\mathcal{N}} \cap \mathcal{H} = E_1 \cup E_2$ .

**Proof.** Since dim  $T_Q = 3$ , dim K = 2 and  $T_Q \cap K = \{0\}$  by proposition 5.11, we deduce that  $V = \text{span}\{T_Q, K\}$ . Now by definition for  $Q \in \tilde{\mathcal{N}}$  the vector  $\tilde{X}(Q)$  has zero  $T_Q$ -component, and for  $Q \in \tilde{\mathcal{N}} \cap \mathcal{H}$  the vector  $\tilde{X}(Q)$  has zero K-component and must therefore be the zero vector. By corollary 5.6 we have that Q is an out-of-plane equilibrium.

**Proof of proposition 5.11.** For  $w = (w_1, w_2, w_3) \in \mathbb{R}^3$  let S(w) denote the skew-symmetric matrix

$$\begin{pmatrix} 0 & w_3 & -w_2 \\ -w_3 & 0 & w_1 \\ w_2 & -w_1 & 0 \end{pmatrix}.$$
 (5.17)

Then the projection of  $T_Q$  into U is spanned by the projections of the three matrices  $[S(e_i), Q]$  where  $e_1, e_2, e_3$  are the standard basis vectors in  $\mathbb{R}^3$ , namely the matrices

$$\begin{pmatrix} 2u & q-p & 0\\ q-p & -2u & 0\\ 0 & 0 & 0 \end{pmatrix} \qquad \begin{pmatrix} -2t & -s & 0\\ -s & 0 & 0\\ 0 & 0 & 2t \end{pmatrix} \qquad \begin{pmatrix} 0 & t & 0\\ t & 2s & 0\\ 0 & 0 & -2s \end{pmatrix}$$
(5.18)

respectively. These are linearly independent, so that  $T_Q \cap K = \{0\}$  as claimed, unless

$$\det \begin{pmatrix} 2u & -2u & q-p \\ -2t & 0 & -s \\ 0 & 2s & t \end{pmatrix} = 4[u(s^2 - t^2) - (q-p)st] = 0.$$
(5.19)

Using (5.5)–(5.7) this condition reduces to st = 0 when  $Q \in \mathcal{N}$ , and hence to s = t = 0 when  $Q \in \mathcal{H}$  with  $k \neq 0, \infty$ . These exceptional cases are where  $\delta = 0, \tau_* = \pm aB$ , and here it is straightforward to check directly that  $\tilde{X}(Q) = 0$  for  $Q \in \tilde{\mathcal{N}} \cap \mathcal{H}$ .

**Remark.** It is reasonable to conjecture that the ellipses  $E_1$ ,  $E_2$  are the remnants of an O(3)-orbit of solutions to grad F(Q) = 0 surviving the addition of the symmetry-breaking term P(Q). This turns out not to be the case, for although tr(Q) and tr( $Q^2$ ) are constant on  $\tilde{\mathcal{N}} \cap \mathcal{H}$  we find that for  $k \neq 0, \infty$ 

$$\det(Q) = 2a^2(a\cos 2\varphi + u\sin 2\varphi)$$

where  $k = \tan \varphi$ , and so the eigenvalues of Q are not constant on  $E_i$ .

## 6. Conclusion

We have given a rigorous geometric derivation of some of the numerical results on the bifurcation of equilibria and periodic motions of a bulk nematic liquid crystal in a shear flow reported in [20]. In particular we have explained anomalous continua of out-of-plane equilibria for certain parameter values, and shown they are not simply artefacts of residual symmetry in the problem. The creation of these continua can be avoided by arbitrarily small perturbations in the equations of motion, and consequently these are not structurally stable. This suggests that the fourth-order Landau–de Gennes free-energy function on the order tensor is an unreliable model for a nematic liquid crystal in a flow environment.

## Acknowledgments

We are grateful to Tim Sluckin for many helpful and instructive conversations on the mathematical physics of liquid crystals. The research reported here is partially supported by EPSRC.

#### References

- Chossat P and Lauterbach R 2000 Methods in Equivariant Bifurcations and Dynamical Systems (Singapore: World Scientific)
- [2] Doi M 1981 J. Polym. Sci. Polym. Phys. Ed. 19 229
- [3] de Gennes P G 1971 Mol. Cryst. Liq. Cryst. 12 193
- [4] de Gennes P G 1974 The Physics of Liquid Crystals (Oxford: Clarendon)
- [5] Faraoni V, Grosso M, Crescitelli S and Maffettone P L 1999 J. Rheol. 43 829
- [6] Farhondi Y and Rey A D 1993 J. Rheol. 37 289
- [7] Han W H and Rey A D 1994 Phys. Rev. E 50 1688
- [8] Hess S 1976 Z. Naturf. A 31 1034
- [9] Hirsch M, Pugh C C and Shub M 1977 Invariant Manifolds (Lecture Notes in Mathematics vol 583) (Berlin: Springer)
- [10] Larson R G 1990 Macromolecules 23 3983
- [11] Maffettone P L and Crescitelli S 1994 J. Rheol. 38 1559
- [12] Maffettone P L and Crescitelli S 1995 J. Non-Newton. Fluid Mech. 59 73

- [13] Olmsted P D 1991 The effect of a shear flow on the isotropic-nematic transition in liquid crystals *PhD Thesis* University of Illinois at Urbana-Champaign
- [14] Olmsted P D and Goldbart P M 1992 Phys. Rev. A 46 4966
- [15] Qian T and Sheng P 1998 Generalized hydrodynamic equations for nematic liquid crystals Phys. Rev. E 58 7475
- [16] Rey A D and Tsuj T 1998 Macromol. Theory Simul. 7 613
- [17] Sluckin T J 2000 The liquid crystal phases: physics and technology Contemp. Phys. 41 37
- [18] Tsuj T and Rey A D 1997 J. Non-Newton. Fluid Mech. 73 127
- [19] Tsuj T and Rey A D 1998 Phys. Rev. E 57 5609
- [20] Vicente Alonso E 2000 PhD Thesis University of Southampton