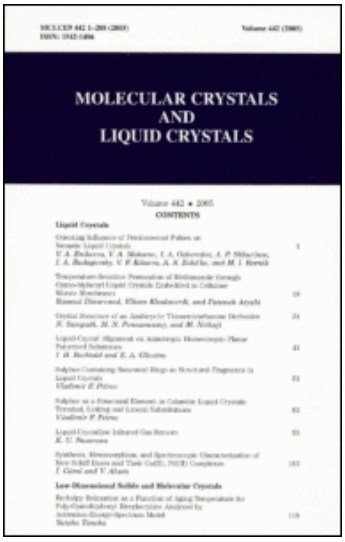

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Bifurcation Analysis of a Mean-Field Model for Biaxial Nematics

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Bifurcation Analysis of a Mean-Field Model for Biaxial Nematics

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The interest for macroscopic biaxiality has been recently revived by the experimental evidence of thermally driven transitions to biaxial phases, promoted by newly synthesized nematogenic molecules. In particular, the interaction model proposed by Straley for molecules endowed with D_{2h} symmetry has been widely reconsidered. We elaborated a mean-field model based on a quadrupolar approximation to the mean torque potential has proven capable of capturing the universal features characterizing all phase diagrams compatible with the interaction model. Moreover, the phase sequences and the order of the transitions are weakly influenced by one of the interaction parameters. Here we show how to we derive the analytical bifurcation equations underlying our numerical analysis, and, subsequently, how these equations are instrumental to the correct resolution of the mean-field model. These bifurcation equations are integrated in a numerical code based on MATCONT, used for bifurcation analysis, which will be made available to the scientific community.

Keywords Biaxial; bifurcation analysis; nematic liquid crystal

1. Introduction

1.1. *Introduction*

Recently, the interest for macroscopic biaxiality in nematic liquid crystals has rised again. In particular, the interaction model proposed by Straley for molecules endowed with D_{2h} symmetry has been widely reconsidered [1]. In fact, several instances of experimental evidence for thermally driven transitions to biaxial phases, promoted by newly synthesised nematogenic molecules, have been reported in the scientific literature (see, for example [2–9]). Nevertheless, this has not gone without controversy, and some results have been long discussed [10–12].

A mean-field model based on a quadrupolar approximation to the mean torque potential was proposed [13]; this model has been elaborated, and has proven capable of capturing the universal features characterising all phase diagrams compatible with the interaction model [14,15]; besides, its predictions are in good ageement with the results obtained by means of Monte-Carlo numerical simulations [16]. In addition to

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that, it has been useful to show that the phase sequences and the order of the transitions are weakly influenced by one of the interaction parameters [17].

To get all the results described above, the model has been implemented in a numerical code, used to perform bifurcation analysis. We think that this code might be useful for the scientific community, to predict the transition temperatures according to the constitutive parameters of the interaction potential, as well as the nature (first- or second-order) of the transition itself. In addition to that, the code might be used to build the profile of the order parameters expected as a function of experimental data simply obtained, namely the ratio of the temperatures for the transition from isotropic to uniaxial nematic phase, and from uniaxial to biaxial nematic phase.

In this short paper we show how the problem can be dealt with, by showing how the bifurcation equation can be derived; a thorough description of the analysis, and of its implementation in the numerical code is given elsewhere [19].

2. The Model

We recall here the main equations characterising the mean-field model adopted; details can be found in several papers [13–18]. Biaxial molecules endowed with D_{2h}-symmetry can be described by the uniaxial and biaxial molecular tensors

$$\mathbf{q} := \boldsymbol{m} \otimes \boldsymbol{m} - \frac{1}{3}\mathbf{I}, \tag{1a}$$

$$\mathbf{b} := \boldsymbol{e} \otimes \boldsymbol{e} - \boldsymbol{e}_\perp \otimes \boldsymbol{e}_\perp. \tag{1b}$$

All condensed phases that an ensemble of biaxial molecules can manifest are represented by the order tensors defined by [13]:

$$\mathbf{Q} := \langle \mathbf{q} \rangle \quad \text{and} \quad \mathbf{B} := \langle \mathbf{b} \rangle, \tag{2}$$

where the ensemble average $\langle \cdots \rangle$ will here be computed within the mean-field approximation [13,14]. Both $\mathbf{Q}$ and $\mathbf{B}$ are symmetric and traceless by construction. In the absence of any external distorting cause that would disrupt their D_{2h} symmetry, they share one and the same eigenframe [20], and so they can be represented as

$$\mathbf{Q} = S\left(\boldsymbol{e}_z \otimes \boldsymbol{e}_z - \frac{1}{3}\mathbf{I}\right) + T\left(\boldsymbol{e}_x \otimes \boldsymbol{e}_x - \boldsymbol{e}_y \otimes \boldsymbol{e}_y\right) \tag{3a}$$

$$\mathbf{B} = S'\left(\mathbf{e}_z \otimes \mathbf{e}_z - \frac{1}{3}\mathbf{I}\right) + T'\left(\mathbf{e}_x \otimes \mathbf{e}_x - \mathbf{e}_y \otimes \mathbf{e}_y\right). \tag{3b}$$

In this representation of a condensed phase, S and S' are uniaxial order parameters, whereas T and T' are biaxial. When these latter vanish, while both S and S' do not, both $\mathbf{Q}$ and $\mathbf{B}$ are uniaxial tensors and so is the phase they describe, even if S and S' have a different meaning, the latter being related to the anisotropy in the distribution of the short molecular axes e and $e_\perp$. Likewise, of the two biaxial parameters T and T', the latter is related to the molecular biaxiality, whilst the former characterizes the lack of rotational symmetry in the distribution of the long molecular axis $\boldsymbol{m}$ [13,18].

The scalar order parameters (S, T, S', T') must obey four consistency conditions, equivalent to the stationarity conditions for the free energy $\mathcal{F}$, which can be written in terms of the prmeters:

$$\mathcal{F} = U_0\left\{\frac{1}{3}S^2 + T^2 + 2\gamma\left(\frac{1}{3}SS' + TT'\right) + \lambda\left(\frac{1}{3}S'^2 + T'^2\right) - \frac{1}{\beta}\ln\left(\frac{Z}{8\pi^2}\right)\right\}, \tag{4}$$

where

$$\frac{1}{\beta} := \frac{k_B t}{U_0} \tag{5}$$

is the dimensionless reciprocal reduced temperature, k_B is the Boltzmann constant and Z is the single particle partition function. (γ, λ) are parameters that describe the potential of the mean torque

$$H = -U_0\{\mathbf{q}_1 \cdot \mathbf{q}_2 + \gamma(\mathbf{q}_1 \cdot \mathbf{b}_2 + \mathbf{b}_1 \cdot \mathbf{q}_2) + \lambda\mathbf{b}_1 \cdot \mathbf{b}_2\}, \tag{6}$$

where $\mathbf{q}$ and $\mathbf{b}$ are the molecular tensors, and the index $i = 1, 2$ identify the two interacting molecules. Although Eq. (6) does not cover all possible instances of a quadrupolar potential, any instance of the potential can be described equivalently by a choice of (γ, λ) in an *essential triangle* in the (γ, λ) plane, defined by the vertices (0, 0), (0, 1/3), (1/2, 0) (more details can be obtained in [13,15]).

2.1. *Order Parameter Profiles*

The order parameter profiles have been obtained from a numerical bifurcation analysis of the equilibrium equations for $\mathcal{F}$, performed with the aid of MATCONT [21], a free software package which integrates into MATLAB [22]. In order to understand the full bifurcation scenario that opens up when solving numerically these equations, we need a detailed mathematical discussion of the problem, in which we re-interpret some results of known bifurcation theories and introduce some useful new results or bifurcations parameters.

3. Symmetries

3.1. *Symmetries in the Order Parameter Set*

It is useful to have a full picture of the symmetries to which the order parameters are subject. If we consider the mean field free energy in an expression indipendent of the representation we are adopting, we write

$$\mathcal{F}(\mathbf{Q}, \mathbf{B}) = \frac{1}{2}(\mathbf{Q} \cdot \mathbf{Q} + 2\gamma\mathbf{Q} \cdot \mathbf{B} + \lambda\mathbf{B} \cdot \mathbf{B}) - \frac{1}{\beta}\ln\frac{Z}{8\pi^2}. \tag{7}$$

When $\gamma = 0$ a further symmetry must be taken into account. For details, see [19].

In the scientific literature there exists a great number of different definitions for the order parameters to describe the nematic phases attainable; the relationship

between these definition variants is well analyzed and discussed in [20]. However, by adopting a normalized representation for the order tensors, many symmetry properties show up:

$$\mathbf{Q} = \widetilde{S}\frac{1}{\sqrt{6}}(3\boldsymbol{e}_z \otimes \boldsymbol{e}_z - \mathbf{I}) + \widetilde{T}\frac{1}{\sqrt{2}}\left(\boldsymbol{e}_x \otimes \boldsymbol{e}_x - \boldsymbol{e}_y \otimes \boldsymbol{e}_y\right) \tag{8a}$$

$$\mathbf{B} \quad = \widetilde{S}'\frac{1}{\sqrt{6}}(3\boldsymbol{e}_z \otimes \boldsymbol{e}_z - \mathbf{I}) + \widetilde{T}'\frac{1}{\sqrt{2}}\left(\boldsymbol{e}_x \otimes \boldsymbol{e}_x - \boldsymbol{e}_y \otimes \boldsymbol{e}_y\right). \tag{8b}$$

The correspondence between the scalar order parameters above and those introduced in Eq. (3) is:

$$\widetilde{S} = \sqrt{\frac{2}{3}}S, \tag{9a}$$

$$\widetilde{S}' = \sqrt{\frac{2}{3}}S', \tag{9b}$$

$$\widetilde{T} = \sqrt{2}T, \tag{9c}$$

$$\widetilde{T}' = \sqrt{2}T'; \tag{9d}$$

with this choice, the free energy assumes a highly symmetric form:

$$\mathcal{F} = \frac{U_0}{2}\left\{\widetilde{S}^2 + \widetilde{T}^2 + 2\gamma(\widetilde{S}\widetilde{S}' + \widetilde{T}\widetilde{T}') + \lambda(\widetilde{S}'^2 + \widetilde{T}'^2) - \frac{1}{\beta}\ln\left(\frac{Z}{8\pi^2}\right)\right\}. \tag{10}$$

Since the structure for both tensors **Q** and **B** is the same, and the permutations in their eigenvalues must be operated simultaneously, we can focus on the former, and the latter will follow consequently. There exist six equivalent permutations of the eigenvalues; the operations that do this can be expressed in terms of a group of order 6 of orthogonal matrices, which is isomorphic to C_{3v}, the symmetry group for an equilateral triangle. For a triangle in the xy-plane, of vertices $(1,0), (-1/2, \sqrt{3}/2)$, $(-1/2, -\sqrt{3}/2)$ the 6 matrices can be assumed as $\{I, R_+, R_-, \sigma_1, \sigma_2, \sigma_3\}$, which are, in order:

1. the identity matrix
2. the clockwise rotation of an angle $2\pi/3$ about z-axis
3. the counterclockwise rotation of an angle $2\pi/3$ about z-axis
4. the reflection across the line $y = 0$ (x-axis)
5. the reflection across the line $y = -\sqrt{3}x$
6. the reflection across the line $y = +\sqrt{3}x$

To get the full symmetry group for the 4 order parameters, we simply have to build 4×4-matrices, having 2 equal diagonal blocks, each one corresponding to one of the above matrices, and 0 elsewhere. With a slight abuse of notation, we use the same letter for these matrices. We will denote by $\mathcal{G}$ the group of order 6

$$\mathcal{G} = \{I, R_+, R_-, \sigma_1, \sigma_2, \sigma_3\} \tag{11}$$

defining the simmetries for the vector $[\widetilde{S}\ \widetilde{T}\ \widetilde{S}'\ \widetilde{T}']^{\mathrm{T}}$, formed by the matrices

$$\begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}, \begin{bmatrix} R_+ & 0 \\ 0 & R_+ \end{bmatrix}, \begin{bmatrix} R_- & 0 \\ 0 & R_- \end{bmatrix}, \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_1 \end{bmatrix}, \begin{bmatrix} \sigma_2 & 0 \\ 0 & \sigma_2 \end{bmatrix}, \begin{bmatrix} \sigma_2 & 0 \\ 0 & \sigma_2 \end{bmatrix}. \tag{12}$$

These symmetry operations transforms equivalent sets of values for the order parameter into one another; the existnece of different equivalent descriptions for the same nematic phase is well known within the model. In particular, for example, the proper subgroups of $\mathcal{G}$ are:

$$\mathcal{G}_1 := \{I, \sigma_1\} \quad \mathcal{G}_2 := \{I, \sigma_2\} \quad \mathcal{G}_3 := \{I, \sigma_3\} \quad \mathcal{G}_R := \{I, R_+, R_-\} \tag{13}$$

(in particular, all σ_i are involutions: $\sigma_i^2 = I$). The fixed-point set under the fourth subgroup correspond to the isotropic phase, whilst the fixed-point set under the first three subgroups to different description of the uniaxial phase.

3.2. *Additional Symmetry for $\gamma = 0$*

When $\gamma = 0$ in Eq. (7), an additional symmetry has to be taken into account; it can be easily seen that the free energy is unvaried if $\mathbf{B} \to -\mathbf{B}$. Indeed, the linear terms in Eq. (7) do not intervene now. Then, it is easily seen that in the integral to obtain the partition function, the change in sign of $\mathbf{B}$, meaning of its eigenvalues, is ineffective. If we denote by $\overline{M}$ the block matrix formed with two 2×2 diagonal blocks, M and $-M$, and zero elsewhere, *i.e.*:

$$\overline{M} = \begin{bmatrix} M & 0 \\ 0 & -M \end{bmatrix}, \tag{14}$$

we obtain a new group, which we call $\overline{\mathcal{G}}$.

$$\overline{\mathcal{G}} = \{I, R_+, R_-, \sigma_1, \sigma_2, \sigma_3, \overline{I}, \overline{R}_+, \overline{R}_-, \overline{\sigma}_1, \overline{\sigma}_2, \overline{\sigma}_3\}. \tag{15}$$

By analyzing the way $\overline{\mathcal{G}}$ has been obtained, we can state this new matrix group is a representation of the direct product of the groups $C_{3v} \times C_{1h}$; in the picture we have given above, $C_{1h} = \{I, \sigma_h\}$ can be described as a simple symmetry group, containing the identity and the reflection across the horizontal plane for a 3D object; this group would be

$$C_{3v} \times C_{1h} \equiv D_{3h} = \{I, R_+, R_-, \sigma_1, \sigma_2, \sigma_3, \sigma_h, \sigma_h R_+, \sigma_h R_-, \sigma_h \sigma_1, \sigma_h \sigma_2, \sigma_h \sigma_3\}. \tag{16}$$

the correspondence to our case is obtained by identifying the action of σ_h with that of $\overline{I}$.

Similar considerations might be carried out for the two lines $3\lambda \pm 2\gamma - 1 = 0$, conjugated to $\gamma = 0$ under the τ_i transformations described in [15].

As done for $\mathcal{G}$, simple matrix algebra would yield the fixed-point sets, which is left to the reader.

4. Definition of the Problem

Here we describe our approach for the bifurcation analysis, adapted to our specific case; for readers interested in this field, a full treatment of related issues can be found in [23,24]. Let $\boldsymbol{G}$: $\mathbb{R}^{n+1} \to \mathbb{R}^n$ be a smooth function; in detail, we will write $\boldsymbol{G} = \boldsymbol{G}(\boldsymbol{x}, \beta)$, and $x = (x_1, x_2, x_3, \ldots, x_n) \in \mathbb{R}^n$ will be the set of variables, and β a continuation parameter. Suppose we want to compute a trajectory (solution curve) $\mathcal{S} = \{\boldsymbol{x}(\beta) \in \mathbb{R}^n : G(x(\beta), \beta)) = 0, \beta \in I\}$ to the equations $\boldsymbol{G}(\boldsymbol{x}, \beta) = 0$, which is parametrized by β under simple non singularity conditions, which we suppose hold in an appropriate interval $I \in \mathbb{R}$. In our example, we will have $x = (S, T, S', T')$, and the equation are obtained as equilibrium equations for the free energy function $F = F(\boldsymbol{x}, \beta)$:

$$\boldsymbol{G}(\boldsymbol{x}, \beta) = \nabla_{\boldsymbol{x}} F(\boldsymbol{x}, \beta) = 0. \tag{17}$$

However, it will be expedient to introduce a different scalar parameter $s \in \mathbb{R}$, which is basically the pseudo-arclength for the solution trajectory; in other word, at least in the neighborhood of a regular point $(\boldsymbol{x}_0, \beta_0) \in \mathcal{S} \times \mathbb{R}$ we will assume both $\boldsymbol{x}$ and β are mapped by $s \in I$, where I is an appropriate interval containing $(\boldsymbol{x}_0, \beta_0)$:

$$s \mapsto \boldsymbol{x}(s), \quad s \mapsto \beta(s) \tag{18}$$

so that the vector tangent to the curve $\boldsymbol{x}(s)$

$$\boldsymbol{t}(s) := \dot{\boldsymbol{x}}(s) \tag{19}$$

is a unit vector, i.e.,

$$\boldsymbol{t}(s) \cdot \boldsymbol{t}(s) = 1 \quad \forall s \in I. \tag{20}$$

An immediate consequence of Eq. (20) is, by differentiating with respect to s:

$$\dot{\boldsymbol{x}}(s) \cdot \boldsymbol{t}(s) = 0 \quad \forall s \in I; \tag{21}$$

this orthogonality condition will be used in the following sections.

The equilibrium equations (17) can be interpreted in terms of a function of s; therefore, we write

$$\widetilde{\boldsymbol{G}}(s) = \nabla_{\boldsymbol{x}} F(\boldsymbol{x}(s), \beta(s)) = 0 \quad \forall s \in I, \tag{22}$$

which yields, upon differentiating with respect to s:

$$\begin{aligned} \dot{\widetilde{\boldsymbol{G}}}(s) :&= \nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}(s), \beta(s)) \dot{\boldsymbol{x}}(s) + \frac{\partial \nabla_{\boldsymbol{x}} F(\boldsymbol{x}(s), \beta(s))}{\partial \beta} \dot{\beta}(s) \\ &= \mathbf{H}(\boldsymbol{x}(s), \beta(s)) \boldsymbol{t}(s) + \dot{\beta}(s) \boldsymbol{b}(s) = \mathbf{0} \quad \forall s \in I, \end{aligned} \tag{23}$$

where $\mathbf{H}(\boldsymbol{x}(s), \beta(s)) := \nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}(s), \beta(s))$ and $\boldsymbol{b}(s) := \frac{\partial}{\partial \beta} \nabla_{\boldsymbol{x}} F(\boldsymbol{x}(s), \beta(s))$.

In general, if the Jacobian of the function $\boldsymbol{G}(\boldsymbol{x}, \beta)$ with respect to x is non singular in $P_0 := (\boldsymbol{x}_0, \beta_0)$, i.e., if $\nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}_0, \beta_0)\, 0$, the implicit function theorem guarantees that a single curve is a solution to Eqs. (17) in proximity of $(\boldsymbol{x}_0, \beta_0)$; in other words, there exist a neighborhood U of $\boldsymbol{x}_0$, a neighborhood V of β_0 and a function $Y: V \to U$

such that Eq. (17) has the unique solution $\boldsymbol{x} = \boldsymbol{Y}(\beta) \in U$, for every $\beta \in V$; explicitly, we might write

$$\boldsymbol{G}(\boldsymbol{Y}(\beta), \beta) \equiv \boldsymbol{0}, \quad \boldsymbol{Y}(\beta_0) = \boldsymbol{x}_0. \tag{24}$$

This justifies the following

Definition 4.1. Let $\boldsymbol{G}$: $\mathbb{R}^{n+1} \to \mathbb{R}^n$ be a C^1-function at least, and let $P_0 = (\boldsymbol{x}_0, \beta_0) \in \mathbb{R}^{n+1}$ be a solution to Eq. (17); let us denote by $\boldsymbol{G}_{\boldsymbol{x}}^0 = \nabla_{\boldsymbol{x}} \boldsymbol{G}(\boldsymbol{x}_0, \beta_0)$ the Jacobian of $\boldsymbol{G}$ in P_0. P_0 is said to be a regular point for the solution trajectory if $\boldsymbol{G}_{\boldsymbol{x}}^0$ is non singular.

Therefore, a necessary condition for bifurcation is the singularity of the Jacobian $\nabla_{\boldsymbol{x}} G(\boldsymbol{x}, \beta)$, i.e., the singularity of the Hessian of $F(\boldsymbol{x}, \beta)$, $\nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}, \beta)$. As we will discuss, this condition is not sufficient.

Definition 4.2. We denote by $\mathcal{K}$ be the kernel of the linear application $\boldsymbol{G}_{\boldsymbol{x}}^0 : \mathbb{R}^n \to \mathbb{R}^n$, or

$$\mathcal{K} := \{\boldsymbol{u} \in \mathbb{R}^n : \boldsymbol{G}_{\boldsymbol{x}}^0 \, \boldsymbol{u} = \boldsymbol{0}\}; \tag{25}$$

furthermore, let m be the dimension of $\mathcal{K}$.

Note 4.1. We recall that $\boldsymbol{G}_{\boldsymbol{x}}^0 = \mathbf{H}(\boldsymbol{x}_0, \beta_0) = \nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}_0, \beta_0)$; therefore, if $F(\boldsymbol{x}_0, \beta_0)$ is at least a C^2–function, $\boldsymbol{G}_{\beta}^0$ is a symmetric linear operator.

Once we have done that, some useful notation correlated to K are introduced:

Definition 4.3. We denote by $\mathcal{K}^{\perp}$ the orthogonal complement of $\mathcal{K}$

$$\mathcal{K}^{\perp} := \{v \in \mathbb{R}^n : \boldsymbol{v} \cdot \boldsymbol{u} = 0 \quad \forall \boldsymbol{u} \in \mathcal{K}\}, \tag{26}$$

we then call global parallel projection tensor the tensor

$$\mathbf{P}_{\mathcal{K}} = \sum_{i=1}^{m} \boldsymbol{u}_i \otimes \boldsymbol{u}_i, \tag{27}$$

where $\{\boldsymbol{u}_1, \ldots \boldsymbol{u}_m\}$ is an orthonormal basis for $\mathcal{K}$. Then we can define the global orthogonal projection tensor as the tensor

$$\mathbf{P}_{\mathcal{K}^{\perp}} = \mathbf{I} - \mathbf{P}_{\mathcal{K}}. \tag{28}$$

We will denote by $()_{\mathcal{K}}$ and $()_{\mathcal{K}^{\perp}}$ the projection of any vector or tensor under these projection tensors; in other words

Definition 4.4. For any vector $\boldsymbol{v} \in \mathbb{R}$ and for any tensor $\mathbf{L}$: $\mathbb{R}^n \to \mathbb{R}^n$ linear, we will call their global parallel component the vector $\boldsymbol{v}_{\mathcal{K}} = \mathbf{P}_{\mathcal{K}} \boldsymbol{v}$ or the tensor $\mathbf{L}_{\mathcal{K}} = \mathbf{P}_{\mathcal{K}} \mathbf{L}$; similarly, we will denominate global orthogonal component the vector $\boldsymbol{v}_{\mathcal{K}^{\perp}} = \mathbf{P}_{\mathcal{K}^{\perp}} \boldsymbol{v}$ or the tensor $\mathbf{L}_{\mathcal{K}^{\perp}} = \mathbf{P}_{\mathcal{K}^{\perp}} \mathbf{L}$.

It is worth pointing out now that in our case both $\mathcal{K}$ and $\mathcal{K}^{\perp}$ have finite dimension, as we have assumed $\boldsymbol{x} \in \mathbb{R}^n$; however, what follows is still applicaple to the case in which $\mathcal{K}^{\perp}$ is infinite dimensional.

We are now in a position to state a fundamental result

Theorem 4.1. *Let $\boldsymbol{G}_{\boldsymbol{x}}^0$ be defined as in Def.*(4.1) *and complying with Eq.* (17); *furthermore, let be $\mathcal{K}$ as in Def* (4.2). *Let $\boldsymbol{b}_0 := \boldsymbol{G}_{\beta}^0 = \frac{\partial}{\partial \beta}\boldsymbol{G}(\boldsymbol{x}_0, \beta_0)$ be the partial derivative of $\boldsymbol{G}(\boldsymbol{x}_0, \beta_0)$ with respect to β in P_0. Suppose P_0 is a non-regular point of the solution trajectory, i.e., $\boldsymbol{G}_{\boldsymbol{x}}^0$ is singular, or, equivalenty dim$(\mathcal{K}) \geq 1$. Then*

1. *If* dim$(\mathcal{K}) = 1$,
   - *If $\boldsymbol{b}_{0\mathcal{K}} \neq \boldsymbol{0}$, P_0 is a* limit point*, and no bifurcation can occur.*
   - *If $\boldsymbol{b}_{0\mathcal{K}} = \boldsymbol{0}$, P_0 is a candidate* bifurcation point*; in other words, a solution curve with a different $t(P_0)$ can be found.*
2. *If* dim$(\mathcal{K}) > 1$,
   - *If $\boldsymbol{b}_{0\mathcal{K}} \neq \boldsymbol{0}$, P_0 is a simple* limit point*, or bifurcations can occur only in non-transverse branches, i.e., the tangent vector $\boldsymbol{t}(P_0)$ is the same for all branches.*
   - *If $\boldsymbol{b}_{0\mathcal{K}} = \boldsymbol{0}$, P_0 is a candidate for a true* bifurcation point*; in other words, a solution curve with a different $\boldsymbol{t}(P_0)$ can be found.*

Detail of the proof can be found in [19].

5. Tangent Vector and Reduced Parallel Projection

We assume now that $\dot{\beta}(s) = 0$ in Eq. (23); as we have seen with Th. (4.1), if $\boldsymbol{b}_{0\mathcal{K}} \neq 0$ this is equivalent to the presence of a limit point. Otherwise, this condition it is not necessary for a generic bifurcation; however, many symmetry breaking bifurcation are characterized by such condition; we are restricting to these case in the following analysis.

We assume that the parameter s for the curves vanishes at P_0. In other words, $P_0 = (\boldsymbol{x}(0), \beta(0))$. Let us denote by $\boldsymbol{t}_0$ the unit vector tangent to the solution curve $\boldsymbol{x}(s)$ in P_0

$$\boldsymbol{t}_0 := \dot{\boldsymbol{x}}(0) \tag{29}$$

From Eq. (23), we know that under the condition we are assuming the candidate direction we are exploring for a bifurcated branch must be in the null space of $\boldsymbol{G}_{\boldsymbol{x}}^0$, that is of the Hessian $\nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}_0, \beta_0)$. We rule out the case in which $\boldsymbol{b}_0 \equiv \boldsymbol{0}$, as this should mean that all equilibrium equations obtained from Eq. (17) are independent of β, which is a non-physical situation.

Under these assumptions, the tangent unit vector is in the null space of the Hessian $\nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}_0, \beta_0)$: $\boldsymbol{t}_0 \in \mathcal{K} = \ker(\boldsymbol{G}_{\boldsymbol{x}_0}) = \ker(\nabla_{\boldsymbol{x}}^2 F(P_0))$. We can now define a *reduced projection tensor* $\mathbf{P}_{\boldsymbol{t}_0}$ acting in $\mathbb{R}^n$ and the *reduced parallel projection* along $\boldsymbol{t}_0$.

Definition 5.1. For any vector $\boldsymbol{v} \in \mathbb{R}^n$ its restricted parallel projection along $\boldsymbol{t}_0$ is

$$\boldsymbol{v}_{\boldsymbol{t}_0} := \mathbf{P}_{\boldsymbol{t}_0} v := (\boldsymbol{t} \otimes \boldsymbol{t})\ \boldsymbol{v}, . \tag{30}$$

The restricted orthogonal projecton is defined accordingly as

$$\boldsymbol{v}_{t_0^\perp} := (\mathbf{I} - \mathbf{P}_{t_0})\boldsymbol{v} := \boldsymbol{v} - \boldsymbol{v}_{t_0}. \tag{31}$$

Note 5.1. From Eq. (21), we know that $\ddot{\boldsymbol{x}}_0 := \ddot{\boldsymbol{x}}(0)$ is orthogonal to $\boldsymbol{t}_0$; if $\dim(\mathcal{K}) = 1$, this implies that $\ddot{\boldsymbol{x}}_{0t_0} = \ddot{\boldsymbol{x}}_{0\mathcal{K}} = \mathbf{0}$, *i.e.*, $\ddot{\boldsymbol{x}}_0 \in \mathcal{K}^\perp$.

This is an immediate consequence of the Defs. (5.1); of course, if $m > 1$ this is not always true, because $\mathbf{P}_{t_0} \neq \mathbf{P}_{\mathcal{K}}$ in this case.

A useful property that applies to $\mathcal{K}$ requires a definition.

Definition 5.2. Let $\mathbf{A}$: $\mathbb{R}^n \to \mathbb{R}^n$ be a linear transformation; we say that $S \subset \mathbb{R}^n$ is $\mathbf{A}-$ invariant if $\forall \boldsymbol{u} \in S$, $\mathbf{A}\boldsymbol{u} \in S$.

A subset $S \subset \mathbb{R}^n$ and its orthogonal complement, $S^\perp = \{u \in \mathbb{R}^n\colon\ \forall \boldsymbol{v} \in S\boldsymbol{u} \cdot \boldsymbol{v} = 0\}$ are easily related. See the following

Theorem 5.1. *If S is $\mathbf{A}-$ invariant, $S^\perp$ is $\mathbf{A}^T-$ invariant.*

Proof. For any $\boldsymbol{u} \in S^\perp$ and for any $\boldsymbol{v} \in S$ we write $\mathbf{A}^{\mathrm{T}}\boldsymbol{u} \cdot \boldsymbol{v} = \boldsymbol{u} \cdot \mathbf{A}\boldsymbol{v}$. Now, by hypothesis S is $\mathbf{A}-$ invariant; therefore, $\mathbf{A}\boldsymbol{v} \in S$, and $\boldsymbol{u}$ is orthogonal to it. Thus, the dot product vanishes, which means $\mathbf{A}^{\mathrm{T}}\boldsymbol{u}$ is orthogonal to any $\boldsymbol{v} \in S$, i.e., $\mathbf{A}^{\mathrm{T}}\boldsymbol{u} \in S^\perp$.

Property 5.1. If $F\colon \mathbb{R}^{n+1} \to \mathbb{R}^n$ is at least a C^2- function in $\boldsymbol{x}$, $\nabla^2_{\boldsymbol{x}} F(P_0)$ is symmetric; this means both $\mathcal{K}$ and $\mathcal{K}^\perp$ are $\nabla^2_{\boldsymbol{x}} F(P_0)$ invariant.

In other words, $\nabla^2_{\boldsymbol{x}} F(P_0)$ never 'mixes' components of vectors in $\mathcal{K}$ with ones in $\mathcal{K}^\perp$, and viceversa. This also holds upon differentiating; consider the following

Theorem 5.2. *Let $\boldsymbol{v}(s) \in \mathbb{R}^n$ be a vector function of a real parameter $s \in I \subseteq \mathbb{R}$, where I is an open interval; if $\forall s \in I$, $\boldsymbol{v}(s) \in \mathcal{K}$, then $\dot{\boldsymbol{v}} \in \mathcal{K}$.*

Proof. Let us suppose $\boldsymbol{v}(s) \notin \mathcal{K}$; this means $\dot{\boldsymbol{v}}(s) \notin \mathcal{K}$ ought to have at least a component in $\mathcal{K}^\perp$, in other words, there ought to exist a unit vector $\boldsymbol{u}$ in the basis of $\mathcal{K}^\perp$ such that $\dot{\boldsymbol{v}}(s) \cdot \boldsymbol{u} \neq 0$. If this was true, for h small enough, we would have $(\boldsymbol{v}(s+h) - \boldsymbol{v}(s)) \cdot \boldsymbol{u} \neq 0$, which is false because, by hypothesis, both $\boldsymbol{v}(s)$ and $\boldsymbol{v}(s+h)$ are in $\mathcal{K}$, and therefore orthogonal to $\boldsymbol{u}$. Thus, $\dot{\boldsymbol{v}}(s) \in \mathcal{K}$. □

We can define an inverse operator for $\nabla^2_{\boldsymbol{x}} F(P_0)$ restricted in $\mathcal{K}^\perp$; we denote this by

$$\overline{\nabla^2_{\boldsymbol{x}} F^{-1}}(P_0) := (\nabla^2_{\boldsymbol{x}} F|_{\mathcal{K}^\perp})^{-1}(P_0); \tag{32}$$

as a consequence of Prop. (5.1), $\forall \boldsymbol{v} \in \mathcal{K}^\perp$, $\overline{\nabla^2_{\boldsymbol{x}} F^{-1}}(P_0)\boldsymbol{v} \in \mathcal{K}^\perp$.

To evaluate the behavior of the solution on the bifurcated branch, we need to know the expansion of $(\boldsymbol{x}(s), \beta(s))$ about $(\boldsymbol{x}_0, \beta_0)$; within our assumptions, the leading term for the continuation parameter is proportional to $\ddot{\beta}(0)$, which cannot be

obtained by Eqs. (23), in any case. We need further differentiation; before doing that, we remind a minor lemma:

Lemma 5.1. *Let* $\mathbf{L}\colon \mathbb{R}^n \to \mathbb{R}^n$ *be a linear symmetric transformation. Then, for any* $\boldsymbol{u}$, $\boldsymbol{v} \in \mathbb{R}^n$, $\mathbf{L}\cdot(\boldsymbol{u}\otimes\boldsymbol{v}) = \mathbf{L}\cdot(\boldsymbol{v}\otimes\boldsymbol{u})$.

Proof. To be convinced of the validity of the thesis, it suffices to write explicitly the quantities in terms of the components:

$$\mathbf{L}\cdot(\boldsymbol{u}\otimes\boldsymbol{v}) = \sum_{i,j,k} S_{ijk}u_j v_k = \sum_{i,j,k} S_{ijk}v_k u_j = \sum_{i,j,k} S_{ikj}v_k u_j = \mathbf{L}\cdot(\boldsymbol{v}\otimes\boldsymbol{u}),$$

where summation is for all indices fro 1 to n, and we have used the symmetry of $\mathbf{L}$.

Upon differentiating Eq. (23) with respect to s we obtain:

$$\begin{aligned}\ddot{\widetilde{\boldsymbol{G}}}(s) = {} & \nabla_{\boldsymbol{x}}^3 F(\boldsymbol{x}(s),\beta(s))\cdot(\dot{\boldsymbol{x}}(s)\otimes\dot{\boldsymbol{x}}(s)) + \nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}(s),\beta(s))\ddot{\boldsymbol{x}}(s)\\ & + 2\dot{\beta}(s)\frac{\partial}{\partial\beta}\nabla_{\boldsymbol{x}}^2 F(x(s),\beta(s))\dot{\boldsymbol{x}}(s) + \ddot{\beta}(s)\frac{\partial}{\partial\beta}\nabla_{\boldsymbol{x}} F(\boldsymbol{x}(s),\beta(s))\\ & + (\dot{\beta}(s))^2\frac{\partial^2}{\partial\beta^2}\nabla_{\boldsymbol{x}} F(\boldsymbol{x}(s),\beta(s)) = \mathbf{0} \quad \forall s\in I,\end{aligned} \tag{33}$$

further differentiation yields, by using Lemma (5.1)

$$\begin{aligned}\dddot{\widetilde{\boldsymbol{G}}}(s) = {} & \nabla_{\boldsymbol{x}}^4 F(\boldsymbol{x}(s),\beta(s))\cdot(\dot{\boldsymbol{x}}(s)\otimes\dot{\boldsymbol{x}}(s)\otimes\dot{\boldsymbol{x}}(s))\\ & + 3\nabla_{\boldsymbol{x}}^3 F(\boldsymbol{x}(s),\beta(s))\cdot(\dot{\boldsymbol{x}}(s)\otimes\ddot{\boldsymbol{x}}(s)) + \nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}(s),\beta(s))\dddot{\boldsymbol{x}}(s)\\ & + 3\dot{\beta}(s)\frac{\partial}{\partial\beta}\nabla_{\boldsymbol{x}}^3 F(\boldsymbol{x}(s),\beta(s))\cdot(\dot{\boldsymbol{x}}(s)\otimes\dot{\boldsymbol{x}}(s))\\ & + 3(\dot{\beta}(s))^2\frac{\partial^2}{\partial\beta^2}\nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}(s),\beta(s))\dot{\boldsymbol{x}}(s)\\ & + 3\frac{\partial}{\partial\beta}\nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}(s),\beta(s))(\ddot{\beta}(s)\dot{\boldsymbol{x}}(s) + \dot{\beta}(s)\ddot{\boldsymbol{x}}(s))\\ & + 3\dot{\beta}(s)\ddot{\beta}(s)\frac{\partial^2}{\partial\beta^2}\nabla_{\boldsymbol{x}} F(\boldsymbol{x}(s),\beta(s))\\ & + (\dot{\beta}(s))^3\frac{\partial^3}{\partial\beta^3}\nabla_{\boldsymbol{x}} F(\boldsymbol{x}(s),\beta(s)) + \dddot{\beta}(s)\frac{\partial}{\partial\beta}\nabla_{\boldsymbol{x}} F(\boldsymbol{x}(s),\beta(s)) = \mathbf{0}\\ & \forall s\in I.\end{aligned} \tag{34}$$

Equations (33,34) are now evaluated at $s=0$, by recalling our assumption requires $\dot{\beta}(0)=0$. Then, we project both equations in $\mathcal{K}$ and Eq. (33) in $\mathcal{K}^{\perp}$; in doing this, we recall the $\nabla_{\boldsymbol{x}}^2 F(P_0)$ – invariance of $\mathcal{K}$, which means $(\nabla_{\boldsymbol{x}}^2 F(P_0)\ddot{\boldsymbol{x}}(0))_{\mathcal{K}} = \nabla_{\boldsymbol{x}}^2 F(P_0)(\ddot{\boldsymbol{x}}(0))_{\mathcal{K}} = 0$. By adopting a subscript 0 to denote evaluation at $(\boldsymbol{x}(0), \beta(0))$, we obtain:

$$[\nabla_{\boldsymbol{x}}^3 F(\boldsymbol{x}_0,\beta_0)\cdot(\boldsymbol{t}_0\otimes\boldsymbol{t}_0)]_{\kappa} + \ddot{\beta}_0\boldsymbol{b}_{0\kappa} = 0 \tag{35a}$$

$$[\nabla_{\boldsymbol{x}}^3 F(\boldsymbol{x}_0, \beta_0) \cdot (\boldsymbol{t}_0 \otimes \boldsymbol{t}_0)]_{\mathcal{K}^\perp} + \nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}_0, \beta_0)\ddot{\boldsymbol{x}}_{0\mathcal{K}^\perp} + \ddot{\beta}_0 \boldsymbol{b}_{0\mathcal{K}^\perp} = 0 \tag{35b}$$

$$[\nabla_{\boldsymbol{x}}^4 F(\boldsymbol{x}_0, \beta_0) \cdot (\boldsymbol{t}_0 \otimes \boldsymbol{t}_0 \otimes \boldsymbol{t}_0)]_{\mathcal{K}} + 3[\nabla_{\boldsymbol{x}}^3 F(\boldsymbol{x}_0, \beta_0) \cdot (\ddot{\boldsymbol{x}}_0 \otimes \boldsymbol{t}_0)]_{\mathcal{K}} + 3\ddot{\beta}_0 (\mathbf{B}_0 \boldsymbol{t}_0)_{\mathcal{K}} + \dddot{\beta}_0 \boldsymbol{b}_{0\mathcal{K}} = 0; \tag{35c}$$

in Eq. (35c) for brevity we have defined

$$\mathbf{B}_0 := \frac{\partial}{\partial \beta} \nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}_0, \beta_0). \tag{36}$$

Now, in $\mathcal{K}^\perp$ the hessian $\nabla_{\boldsymbol{x}}^2 F(\boldsymbol{x}_0, \beta_0)$ is non-singular; therefore, Eq. (35b) can be solved for $\ddot{\boldsymbol{x}}_0$, according to Eq. (32):

$$\ddot{\boldsymbol{x}}_{0\mathcal{K}^\perp} = -\overline{(\nabla_{\boldsymbol{x}}^2 F)^{-1}}(\boldsymbol{x}_0, \beta_0)\left[\left[\nabla_{\boldsymbol{x}}^3 F(\boldsymbol{x}_0, \beta_0) \cdot (\boldsymbol{t}_0 \otimes \boldsymbol{t}_0)\right]_{\mathcal{K}^\perp} + \ddot{\beta}_0 \boldsymbol{b}_{0\mathcal{K}^\perp}\right] \tag{37}$$

By recalling Theorem (4.1), we know that a necessary condition for the existence of a solution branch in a transverse direction is $\boldsymbol{b}_{0\mathcal{K}} = \mathbf{0}$.

6. Final Remarks

Equations (35) should now be analyzed by discriminating cases according to the norm of the projection of such vector in $\mathcal{K}$. This yields the explicit bifurcation equations that can be implemented in the numerical code. In adition to that, an explicit analytical condition to identify tricriticality can be written. Details of the procedure, and on the code itself are reported elsewhere [19]. Although the equations presented are in a very general and raw form, which could not be applied directly to the case of biaxial nematic liquid crystals, they are the starting point from which the bifurcation scenario is revealed; they can be used independently to reconstruct qualitatively the phase sequence to be expected and compared to the experimental evidence.

A version of the code will be made available for download from the website http:\\smmm.unipv.it

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