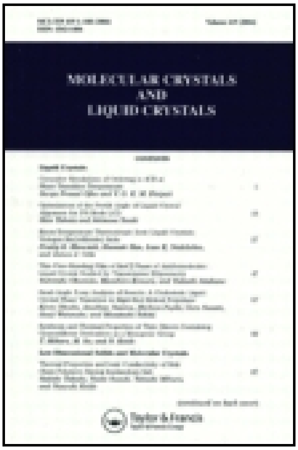

Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

Tensorial Form of Leslie-Ericksen Equations and Applications

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Version of record first published: 05 Oct 2009

Mol. Cryst. Liq. Cryst., Vol. 508, pp. 309/[671]–336/[698], 2009

ISSN: 1542-1406 print/1563-5287 online
DOI: 10.1080/15421400903065796

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Tensorial Form of Leslie-Ericksen Equations and Applications

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We propose a system of dynamical equations coupling a tensor Q_{ij} related to the molecular order with the flow velocity, whose structure is very similar to the Leslie-Ericksen equations. In particular, the Leslie viscosities and the Frank elastic constants appear explicitly, which contrasts with constitutive equations derived from the microscopic Doi theory and using the full order parameter tensor S_{ij}. The description in terms of the tensor Q_{ij} may be seen as intermediate between the director of Leslie-Ericksen theory and the order parameter tensor S_{ij} of microscopic theories. With our approach we take advantage of the fact that the Leslie viscosities and the Frank elastic constants are well-established for several real systems (as for example 5CB, 8CB, or MBBA). Our equations, that become manifestly equivalent to Leslie-Ericksen equations when a director may be defined, are used in order to regularise the director field at the position of the field singularities in a simple way. Our objective is to simulate the macroscopic behaviour of nematics containing a large assembly of defects under several experimental conditions (under shear and/or magnetic field). Since we are essentially concerned by the macroscopic response, the exact structure of the defects is secondary, it is why we believe this approach to be pertinent in studying the dynamics of the texture induced by defects. The model is applied to a spinning nematic (5CB) subjected to a magnetic field, and a relaxation mechanism involving topological defects is evidenced.

Keywords: Leslie-Ericksen theory; nematic; relaxation; spinning tube; topological defect

This work was partly supported by the Fundação para a Ciência e a Tecnologia (Portugal) under research grant SFRH/BPD/8894/2002 to A. Véron, and contract C2007-443-CENIMAT-1.

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I. INTRODUCTION

The understanding of the hydrodynamics of liquid crystals is of importance both for theoretical and practical reasons. At microscopic level liquid crystals are micro-structured fluids characterised by local order usually quantified by an order parameter. Within the scope of continuum theory the order parameter is considered as a field that couples with the velocity field. Accordingly, the full continuum theory also requires an equation of evolution for the order parameter field whose derivation constitutes a central part in the development of the theory. For liquid crystals composed of elongated molecules the microscopic order parameter is defined by

$$S_{ij} = \left\langle u_i u_j - \frac{1}{3}\delta_{ij} \right\rangle \tag{1}$$

where $\vec{u}$ is a unit vector parallel to the long molecular axis and $\langle\rangle$ denotes an average over a large ensemble of molecules. Without additional assumptions the continuum description should manipulate the symmetric and traceless tensor field S_{ij}. With the assumption of local uniaxiality the microscopic order parameter takes the particular form

$$S_{ij} = S\left(n_i n_j - \frac{1}{3}\delta_{ij}\right) \tag{2}$$

with $\vec{n}$ a unit vector called the director and indicating the local mean orientation of the molecules. If moreover the scalar S, that quantifies the degree of order, is assumed to be constant, then the director field completely describes the local order of the material. The Leslie-Ericksen (LE) theory has been built on these assumptions [1,2]. The evolution equation for the director is completely and unambiguously derived from the conservation of angular momentum. The main limitation of this theory lies in the description of special observed structures (defects) in terms of singularities in the director field. It is worth noting that singularity here actually means a region of space where the theory is no longer defined: no derivability at these points, divergence of the total free energy that consequently cannot be minimised, while it is necessary to define an equilibrium state. Moreover, with this approach mobile defects and creation/annihilation of defects cannot be described. To overcome these difficulties requires taking back into account at least some degrees of freedom of the full tensorial description that are 'frozen' in the director description.

The aim of this work is to propose a simple tensorial extension of LE theory that should be essentially equivalent to this theory everywhere except in the small regions of space occupied by the defect cores. In other words, the new theory should be able to regularise the LE theory. It is expected that the extended model will have the formal structure of LE theory in order to maintain its material parameters (Frank elastic constants and Leslie viscosities) while avoiding introducing too many additional parameters. The resulting model does not aim at describing correctly the core of the defects; it is based on the assumptions that (i) the spatial extension where LE fails is always limited to the core of the defects, i.e., a very small fraction of the total volume, and (ii) the director distribution far from the core is independent of the core structure. In other words, the domain of validity of the new model is essentially the one of LE theory. The final objective is to get theoretical and computational tools able to describe and simulate the texture of nematics containing many defects under several conditions with reasonable time consuming.

The model has been applied to the director dynamics in spinning nematic liquid crystals subjected to a static magnetic field and containing topological defects. More precisely we investigate the director response when (i) the tube containing the nematic rotates at a sufficiently high spinning rate leading to permanent director rotation and (ii) the director is strongly and homeotropically anchored.

II. THEORY

II-1. Fundamentals of the Theory

Local Order

One part of the methodology used in this work to regularise the LE theory is based on the remark that the product $n_i n_j$ appears almost everywhere in this theory so that a simple extension may consist in replacing the tensor $n_i n_j$ by a more general tensor Q_{ij} used to describe the local order. Thus, the order parameter S_{ij} is assumed to take the following form

$$S_{ij} = S\left(Q_{ij} - \frac{1}{3}\delta_{ij}\right) \tag{3}$$

with S constant. The property $S_{ii} = 0$ entrains $Q_{ii} = 1$; on the other hand, to maintain the meaning of scalar order parameter to the coefficient S we impose $\left(\frac{3}{2}S_{ij}S_{ij}\right)^{1/2} = S$, which entrains $Q_{ij}Q_{ij} = 1$. In summary, the order tensor Q_{ij} of this model satisfies the following set of conditions

$$\begin{cases} Q_{ij} = Q_{ji} \\ \mathrm{Tr}Q = 1 \\ \mathrm{Tr}Q^2 = 1 \end{cases} \tag{4}$$

We note that the description in terms of Q_{ij} is less general than the description in terms of S_{ij} since we have four independent components instead of five.

Total Free Energy

A basic quantity of micro-structured fluids is the total free energy associated with any configuration of the local order field, namely, the tensor Q_{ij} in our model. In general this free energy is a functional that takes the following form

$$\mathsf{F}[Q_{ij}] = \int_V F(Q_{ij}, Q_{ij,k})dV \tag{5}$$

where V denotes the space occupied by the material and F denotes the free energy density function of the order tensor and its first spatial derivatives.

Molecular Field

The minimisation of the total free energy leads to the definition of the molecular field. The variation $\delta\mathsf{F}[\delta Q_{ij}]$ associated with any variation δQ_{ij} reads

$$\delta\mathsf{F}[\delta Q_{ij}] = \int_V \left\{ \frac{\partial F}{\partial Q_{ij}}\delta Q_{ij} + \frac{\partial F}{\partial Q_{ij,k}}\frac{\partial \delta Q_{ij}}{\partial x_k} - \frac{1}{2}\mu\delta_{ij}\,\delta Q_{ij} - \frac{1}{2}\lambda Q_{ij}\,\delta Q_{ij} \right\} dV \tag{6}$$

The term $-(\mu\delta_{ij}\delta Q_{ij}+\lambda Q_{ij}\delta Q_{ij})/2$, where μ and λ are two Lagrange multipliers, has been added in the integrand of $\delta\mathsf{F}$ in order to release the two constraints $\mathrm{Tr}Q = 1$ and $\mathrm{Tr}Q^2 = 1$ (see Eq. (4)). Integration by parts of the second term of the integrand in Eq. (6) leads to

$$\begin{aligned} \delta\mathsf{F}[\delta Q_{ij}] = & \int_V \left\{ \frac{\partial F}{\partial Q_{ij}} - \frac{\partial}{\partial x_k}\left(\frac{\partial F}{\partial Q_{ij,k}}\right) - \frac{1}{2}\mu\delta_{ij} - \frac{1}{2}\lambda Q_{ij} \right\} \delta Q_{ij} dV \\ & + \int_{\partial V} \frac{\partial F}{\partial Q_{ij,k}} \delta Q_{ij} s_k dS \end{aligned} \tag{7}$$

where ∂V denotes the boundary of the domain V and $\vec{s}$ is an outward unit vector normal to ∂V. Taking into account the symmetry of δQ_{ij} (see Eq. (4)), $\delta\mathsf{F} = 0$ entrains

$$H_{ij} + \mu\delta_{ij} + \lambda Q_{ij} = 0 \tag{8}$$

with

$$H_{ij} = \frac{\partial}{\partial x_k}\left(\frac{\partial F}{\partial Q_{ij,k}}\right) + \frac{\partial}{\partial x_k}\left(\frac{\partial F}{\partial Q_{ji,k}}\right) - \frac{\partial F}{\partial Q_{ij}} - \frac{\partial F}{\partial Q_{ji}} \tag{9}$$

By analogy with the LE theory H_{ij} is called the molecular field. It should be noted that Eq. (8) entrains

$$\varepsilon_{pij} Q_{ik} H_{kj} = 0 \tag{10}$$

where ε_{ijk} denotes the Levi-Civitta tensor. The meaning of this latter equation will be given below.

Stress Tensor

A stress tensor may be deduced by evaluating the variation of the total free energy due to an infinitesimal displacement field $\vec{\xi}(\vec{r})$ while maintaining the tensor Q_{ij} parallel to itself; i.e., by considering the transformation defined by $r' = \vec{r} + \vec{\xi}(\vec{r})$ and $Q'_{ij}(\vec{r}') = Q_{ij}(\vec{r})$ where the prime denotes the final state. One gets

$$\delta \mathsf{F}\left[\vec{\xi}\right] = \int_V \sigma^d_{kl} \xi_{l,k} dV \tag{11}$$

with

$$\begin{cases} \sigma^d_{kl} = F\delta_{kl} + \sigma^e_{kl} \\ \sigma^e_{kl} = -\frac{\partial F}{\partial Q_{ij,k}} Q_{ij,l} \end{cases} \tag{12}$$

σ^d_{ij} is the distortion stress tensor and by analogy with LE theory σ^e_{ij} may be called the Ericksen stress tensor.

Rotational Identity

An identity may be derived from the invariance of the total free energy under the effect of a global rotation (i.e., applied simultaneously to the vector position $\vec{r}$ and the tensor field $Q_{ij}(\vec{r})$). For an infinitesimal rotation characterised by the rotation vector $\vec{\omega}$, the transformation is defined by

$$\begin{cases} x'_i = x_i + \varepsilon_{ijk}\, \omega_j\, x_k \\ Q'_{ij} = Q_{ij} + \left(\varepsilon_{ipq}\, Q_{qj} + \varepsilon_{jpq}\, Q_{iq}\right)\omega_p \end{cases} \tag{13}$$

After some algebraic manipulations and use of Eqs. (9) and (12) the variation of the free energy in any domain $\Omega \subset V$ reads

$$\delta \mathsf{F}[\vec{\omega}, \Omega] = \int_\Omega \left\{\varepsilon_{pqi}\sigma^e_{qi} - \varepsilon_{pqi} Q_{qj} H_{ji}\right\}\omega_p dV + \int_{\partial\Omega} \varepsilon_{pqi} Q_{qj} s_k \Pi_{kji}\omega_p dS \tag{14}$$

where we have defined the tensor Π_{kij} by

$$\Pi_{kij} = \frac{\partial F}{\partial Q_{ij,k}} + \frac{\partial F}{\partial Q_{ji,k}} \tag{15}$$

Finally the invariance by rotation, i.e., $\delta \mathsf{F} = 0$ for any $\vec{\omega}$, entrains the following rotational identity

$$\int_{\Omega} \varepsilon_{pij}\sigma_{ij}^{e} dV + \int_{\partial\Omega} \varepsilon_{pij} Q_{ik} s_l \Pi_{lkj} dS = \int_{\Omega} \varepsilon_{pij} Q_{ik} H_{kj} dV \quad (\forall p;\ \forall\Omega \subset V;\ \forall Q) \tag{16}$$

Because of Eq. (10), at equilibrium Eq. (16) simplifies to

$$\int_{\Omega} \varepsilon_{pij}\sigma_{ij}^{e} dV + \int_{\partial\Omega} \varepsilon_{pij} Q_{ik} s_l \Pi_{kjl} dS = 0 \quad (\forall p;\ \forall\Omega \subset V) \tag{17}$$

This latter equation may be interpreted as the balance of torque on any domain Ω at equilibrium.[1] In presence of a flow a viscous contribution σ_{ij}^{v} is added to σ_{ij}^{e} and, neglecting inertia, the balance of torque is rewritten as

$$\int_{\Omega} \varepsilon_{pij}\left(\sigma_{ij}^{e} + \sigma_{ij}^{v}\right) dV + \int_{\partial\Omega} \varepsilon_{pij} Q_{ik} s_l \Pi_{lkj} dS = 0 \quad (\forall p;\ \forall\Omega \subset V) \tag{18}$$

Use of the rotational identity (Eq. (16)), still valid out-of-equilibrium unlike Eq. (10), entrains

$$\int_{\Omega} \varepsilon_{pij}\left(\sigma_{ij}^{v} + Q_{ik} H_{kj}\right) dV = 0 \quad (\forall p;\ \forall\Omega \subset V) \tag{19}$$

Since this integral equation is valid for any domain $\Omega \subset V$, we arrive to the following equivalent local form of the torque balance equation

$$\varepsilon_{pij}\left(\sigma_{ij}^{v} + Q_{ik} H_{kj}\right) = 0 \quad (\forall p) \tag{20}$$

It is worth noting that (Eq. (20)) imposes a constraint to the local field at any time, accordingly it partially determines the time evolution of Q_{ij} once the free energy density F and the viscous stress σ^{v} have been defined. We note that the vectorial quantity $\varepsilon_{pij} Q_{ik} H_{kj}$ may be interpreted as a density of elastic torque and consequently Eq. (10) states that the density of elastic torque vanishes at equilibrium.

II-2. Constitutive Relations and Equations of Evolution

In this work we assume that the scalar order parameter $S = \left(\frac{3}{2} S_{ij} S_{ij}\right)^{1/2}$ is constant, even within the core of the defect. Considering that the scalar order parameter S is a pertinent variable that essentially determines the magnitude of the material parameters of the

[1] σ^{e} may be replaced by σ^{d} in Eq. (17) since $\sigma^{e} - \sigma^{d}$ is symmetric according to Eq. (12).

phenomenological theory, we conclude that the constancy of S justifies maintaining the visco-elastic coefficients of LE theory.

The equilibrium state is assumed to be described by an arbitrary homogeneous director $\vec{n}$ or equivalently by an order tensor of the form $Q_{ij} = n_i n_j$; accordingly any tensor of this form must be solution of the equilibrium equation (Eq. (8)), which requires a non-null contribution in the free energy density (noted F^b) even in the absence of inhomogeneities or external field; in other words F^b is uniquely function of the components Q_{ij}. It should be a function of the three independent invariants of the tensor Q_{ij}, namely, TrQ , TrQ^2, and TrQ^3.[2] According to the constraints given by Eq. (4) the simplest expression for F^b reads

$$F^b = -\frac{1}{6}\kappa_b Q_{kl} Q_{lp} Q_{pk} \tag{21}$$

The minus sign has been chosen to ensure that the desired equilibrium is obtained for $\kappa_b > 0$. Actually Eq. (21) is nothing but the Landau-de Gennes free energy density in terms of S_{ij} [2] written here using Eqs. (3) and (4).

When the local order is fully described by the director field $\vec{n}$ the free energy density is assumed to be given by the Frank free energy that is usually expressed in terms of the director components and its first spatial derivatives [2,4]. Gruhn *et al*. remarked that an equivalent expression might be obtained by maintaining explicit the product $n_i n_j$ even in the spatial derivatives [5]; this tensorial-like expression actually expresses the physical equivalence between $\vec{n}$ and $-\vec{n}$ more deeply than the original expression. Here we exploit this tensorial-like expression by replacing the product $n_i n_j$ by Q_{ij}, which yields

$$F^{el} = \frac{1}{4}K_2 Q_{ij,k} Q_{ij,k} + \frac{1}{2}(K_1 - K_2) Q_{ij,i} Q_{kj,k} + \frac{1}{4}(K_3 - K_1) Q_{ij} Q_{kl,i} Q_{kl,j} \tag{22}$$

The tensorial susceptibilities describing the response to an external magnetic field $\vec{B}$ or electric field $\vec{E}$ are assumed to be proportional to the molecular order parameter S_{ij} [2], which according to Eq. (3) readily entrains

$$F^{ext} = -\frac{1}{2}\frac{\chi_a}{\mu_0} Q_{ij} B_i B_j - \frac{1}{2}\varepsilon_0 \varepsilon_a Q_{ij} E_i E_j \tag{23}$$

[2]It is a consequence of the Cayley-Hamilton theorem that states that every square matrix satisfies its own characteristic equation. For 3×3 matrices the theorem reads $A^3 - \mathrm{Tr}(A)A^2 + \frac{1}{2}\Big((\mathrm{Tr}(A))^2 - \mathrm{Tr}(A^2)\Big)A - \det(A)I = 0$.

where μ_0 and ε_0 denote the magnetic permeability and the dielectric permittivity of the vacuum, χ_a the material's diamagnetic anisotropy and ε_a the material's dielectric anisotropy.

To the three contributions F^b, F^{el}, and F^{ext} to the free energy density correspond, according to Eq. (9), three contributions to the molecular field as follows

$$\begin{cases} H_{ij}^b = \kappa_b Q_{ik} Q_{kj} \\ H_{ij}^{el} = K_2 Q_{ij,kk} + (K_1 - K_2)\big(Q_{li,lj} + Q_{lj,li}\big) \\ \qquad + (K_3 - K_1)\big(Q_{kl,k} Q_{ij,l} + Q_{kl} Q_{ij,lk} - Q_{kl,i} Q_{kl,j}/2\big) \\ H_{ij}^{ext} = (\chi_a/\mu_0) B_i B_j + \varepsilon_0 \varepsilon_a E_i E_j \end{cases} \tag{24}$$

The frictional forces are induced by relative motion between adjacent elements of fluid. For fluids with local order described by a tensor, the rate of change of this tensor in a frame rotating with the fluid (i.e., the corotational or Jauman derivative) also contributes to friction. Mathematically this relative rate of change reads

$$\frac{DQ_{ij}}{Dt} = \frac{dQ_{ij}}{dt} - W_{ik} Q_{kj} + Q_{ik} W_{kj} \tag{25}$$

where d/dt denotes the material time derivative and W_{ij} the anti-symmetric part of the velocity gradient tensor. A natural and simple generalisation of the Leslie viscous stress tensor [1,2] using the tensor Q_{ij} and keeping the same structure with the same viscosity coefficients α_l $(l = 1, \ldots, 6)$ reads

$$\begin{aligned} \sigma_{ij}^v = {} & \alpha_1 Q_{kl} A_{kl} Q_{ij} + \alpha_2 Q_{ik} \frac{DQ_{jk}}{Dt} + \alpha_3 Q_{jk} \frac{DQ_{ik}}{Dt} + \alpha_4 A_{ij} + \alpha_5 Q_{ik} A_{kj} \\ & + \alpha_6 Q_{jk} A_{ki} \end{aligned} \tag{26}$$

where A_{ij} denotes the symmetric part of the velocity gradient tensor. From Eq. (26) we readily get

$$\varepsilon_{ikl} \sigma_{kl}^v = \varepsilon_{ikl} Q_{kp} \left(-\gamma_1 \frac{DQ_{pl}}{Dt} - \gamma_2 A_{pl} \right) \tag{27}$$

where $\gamma_1 = \alpha_3 - \alpha_2$ and $\gamma_2 = \alpha_6 - \alpha_5$.

Inserting Eq. (27) in Eq. (20) (i.e., the balance of torques) yields

$$\varepsilon_{pij} Q_{ik} \left(\gamma_1 \frac{DQ_{kj}}{Dt} + \gamma_2 A_{kj} - H_{kj} \right) = 0 \quad (\forall p) \tag{28}$$

Since any power of Q yields a symmetric tensor the Eq. (28) is satisfied when the term in brackets is assumed to be equal to an arbitrary polynomial of the tensor Q. Using moreover the Cayley-Hamilton theorem for 3×3 matrices (see footnote 2) we can limit the expansion in powers of Q to the second order. Accordingly, we replace Eq. (28) by

$$\gamma_1 \frac{DQ_{ij}}{Dt} + \gamma_2 A_{ij} - H_{ij} = \mu\delta_{ij} + \lambda Q_{ij} + \lambda' Q_{ik} Q_{kj} \quad (\forall p) \tag{29}$$

The Eq. (29) is a generalisation of Eq. (8), therefore the two arbitrary coefficients μ and λ must be still considered as 'Lagrange multipliers' in order to maintain $\mathrm{Tr}Q = 1$ and $\mathrm{Tr}Q^2 = 1$, even out-of-equilibrium. The additional coefficient λ' may be interpreted as a material parameter; however remarking that λ' can be included in the coefficient κ_b of the molecular field (see Eq. (24)) it is actually not an additional material parameter. Consequently we retain as the evolution equation for the tensor Q_{ij} the following equation

$$\gamma_1 \frac{DQ_{ij}}{Dt} = -\gamma_2 A_{ij} + H_{ij} + \mu\delta_{ij} + \lambda Q_{ij} \tag{30}$$

Before closing this section we give the equation describing the balance of force when inertia is neglected:

$$\frac{\partial}{\partial x_i}\left(\sigma^e_{ij} + \sigma^v_{ij} - P\delta_{ij}\right) = 0 \tag{31}$$

where P denotes the pressure. Eqs. (30) and (31) form the set of coupled equations used in the sequel in order to determine the velocity and the Q fields.

III. APPLICATION TO A SPINNING TUBE

III-1. Preliminaries

We consider the set-up illustrated in Figure 1. A cylindrical tube filled with a nematic fluid is rotated around its axis with the spinning rate Ω and subjected to a homogeneous and constant magnetic field normal to the tube axis. In the sequel the x_1 and x_2 axes are chosen normal to the tube axis and the x_3 axis parallel to it; the magnetic field is parallel to the x_2 axis. Three unit vectors $\vec{e}_i$ ($i = 1, 2, 3$) are taken parallel to the corresponding x_i axes. The simulations are performed within one section of the tube; for convenience this section lies at $x_3 = 0$. Finally, the origin of the system of axes is chosen at the centre of this section.

Boundary and initial conditions are required to solve Eqs. (30) and (31). Concerning the velocity we assume non-slipping conditions on the boundaries. For the relaxation process (i.e., $\Omega = 0$) the initial

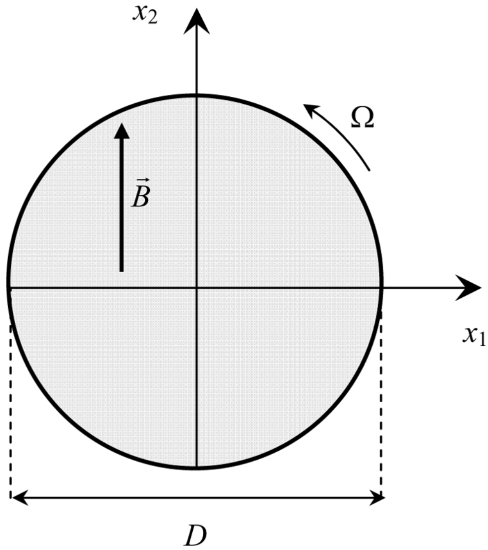


FIGURE 1 Normal section of the tube spinning with angular velocity Ω; the velocity of a point of the tube with coordinates (x_1, x_2) is $v_1 = -\Omega x_2$, $v_2 = \Omega x_1$ and $v_3 = 0$. A magnetic field $\vec{B}$ normal to the tube axis is applied.

velocity field is set to zero; for the spinning process (i.e., $\Omega \neq 0$) the initial velocity field is assumed to be given by $\vec{v} = \vec{\Omega} \times \vec{r}$ in the plane $x_3 = 0$. The director is assumed to be rigidly and homeotropically anchored on the wall of the tube; that entrains a total topological charge equal to $+1$ and consequently topological defects must be present in the initial state. For simplicity we have assumed that initially one defect with charge $+1$ lies in the centre of the disk. In order to build this initial state we first define a singular tensor field $\boldsymbol{Q}^S$ equivalent to a radial director field singular at the centre of the disk, namely,

$$\begin{cases} Q_{ij}^S = n_i^S n_j^S \\ n_1^S = \cos \theta^S \\ n_2^S = \sin \theta^S \\ n_3^S = 0 \\ \theta^S(x_1, x_2) = \tan^{-1}(x_1/x_2) \end{cases} \tag{32}$$

In a second stage, in order to regularise $\boldsymbol{Q}^S$ we define a new tensor field $\boldsymbol{Q}_{ij}^R$ by

$$Q_{ij}^R = \alpha Q_{ij}^S + \beta u_i u_j + \gamma v_i v_j \tag{33}$$

where $\vec{u}$ and $\vec{v}$ are two unit vectors defined by

$$\begin{cases} \vec{u} = n_2^S \vec{e}_1 - n_1^S \vec{e}_2 \\ \vec{v} = \vec{e}_3 \end{cases} \tag{34}$$

so that the triplet $(\vec{n}, \vec{u}, \vec{v})$ forms an orthonormal basis. The conditions $\mathrm{Tr}\boldsymbol{Q}^R = 1$ and $\mathrm{Tr}(\boldsymbol{Q}^R \boldsymbol{Q}^R) = 1$ are satisfied if β and γ are related to α as follows (more details are given in [6]):

$$\begin{cases} \beta(\alpha) = \frac{1}{2}\left((1-\alpha) + \sqrt{(1+3\alpha)(1-\alpha)}\right) \\ \gamma(\alpha) = 1 - \alpha - \beta(\alpha) \end{cases} \tag{35}$$

The free variable α is defined as a regular function of space satisfying $\alpha = 1$ far from the singular point (which entrains $\beta = \gamma = 0$ and $\boldsymbol{Q}^R = \boldsymbol{Q}^S$ so that Q_{ij}^R satisfies the same boundary conditions as Q_{ij}^S) and $\alpha = \beta$ at the singular point. In order to show the regularity of $Q_{ij}^R(x_1, x_2)$ at the origin we must prove that the limits of $Q_{ij}^R(x_1, x_2)$ and its space derivatives when $(x_1, x_2) \to (0, 0)$ are path independent and finite. We can write $Q_{ij}^R = \alpha\left(n_i^S n_j^S + u_i u_j + v_i v_j\right) + (\beta - \alpha) u_i u_j + (\gamma - \alpha) v_i v_j$; noting that $\delta_{ij} = n_i^S n_j^S + u_i u_j + v_i v_j$ since $(\vec{n}, \vec{u}, \vec{v})$ forms an orthonormal basis, we get $Q_{ij}^R = \alpha\delta_{ij} + (\beta - \alpha) u_i u_j + (\gamma - \alpha) v_i v_j$. Since $\alpha\delta_{ij} + (\gamma - \alpha) v_i v_j$ is obviously regular, we must examine the regularity of $\Delta Q_{ij}^R = (\beta - \alpha) u_i u_j$. The assumption that $\beta - \alpha \to 0$ when approaching the singular point whatever the path entrains the continuity of ΔQ_{ij}^R; if moreover $\beta - \alpha$ and its derivatives vanish sufficiently rapidly when approaching the singular point as well, then $Q_{ij}^R(x_1, x_2)$ is regular. For more general initial conditions with several defects at arbitrary positions the more complex procedure to generate $\boldsymbol{Q}^S$ and $\boldsymbol{Q}^R$ fields is described elsewhere [6].

In the sequel we assume that the flow is essentially bidimensional and within the normal section of the tube, i.e., we impose $v_3 = 0$ when solving the Eqs. (30) and (31). This sensibly reduces the computational time consuming. On the contrary no particular assumptions are made for the tensor Q_{ij} since in the vicinity of the core defects it might be quite general. The evolution equation for the tensor Q_{ij} (Eq. (30)) is solved by using the fourth order Runge-Kutta explicit scheme and the velocity equation (Eq. (31)) is solved by using the Successive Over-Relaxation iterative scheme, while evaluating the pressure by solving a Poisson equation [7]. The results presented in this work have been obtained with the material parameters of 5CB at $T_{NI} - T = 10°C$ [8,9] given in Table 1. For κ_b (see Eq. (21)) we used the highest value compatible with our choice of the increment parameters Δt and Δx, namely, $\kappa_b = 1.0 \times 10^2\ \mathrm{J/m^3}$. This value is rather small in comparison

TABLE 1 Material Parameters of 5CB for $T_{NI} - T = 10°C$

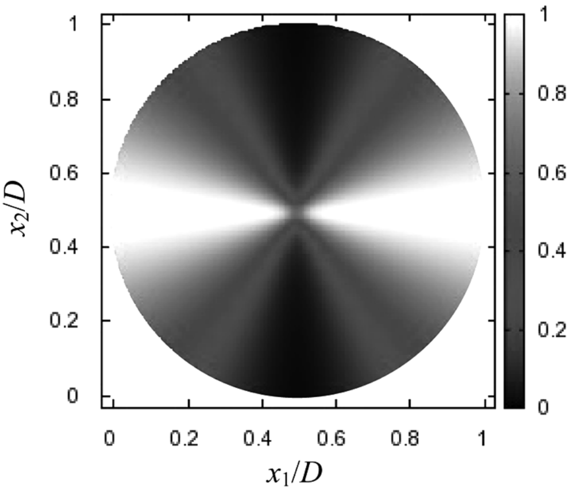
Leslie viscosities [8]	Frank elastic constants [9]
$\alpha_1 = -0.006 \mathrm{Pa\,s}^{-1}$	
$\alpha_2 = -0.081 \mathrm{Pa\,s}^{-1}$	$K_1 = 1.15 \times 10^{-11}\mathrm{N}$
$\alpha_3 = -0.005 \mathrm{Pa\,s}^{-1}$	$K_2 = 0.60 \times 10^{-11}\mathrm{N}$
$\alpha_4 = 0.065 \mathrm{Pa\,s}^{-1}$	$K_3 = 1.53 \times 10^{-11}\mathrm{N}$
$\alpha_5 = 0.064 \mathrm{Pa\,s}^{-1}$	
$\alpha_6 = -0.022 \mathrm{Pa\,s}^{-1}$	

with data given in literature; the consequence is to increase the size of the defect core (i.e., the region where Q_{ij} notably differs from $n_i n_j$). We expect that it has no great importance inasmuch as we are essentially concerned with the macroscopic texture in the whole sample while the volume of the defects core is negligible. For the external constraints we used $\Omega = 60\,\mathrm{Hz}$ (for the spinning process), $B = 2\,\mathrm{T}$ and $\chi_a/\mu_0 = 1.14$; for the geometrical parameters we used $D = 80\ \mu\mathrm{m}$. The small diameter D used in this work is not realistic, it has been used essentially to avoid huge computer time consuming. Concerning the numerical parameters we used $\Delta x_1 = \Delta x_2 = 0.31\mu\mathrm{m}$ for the space increments and $\Delta t = 60\mu\mathrm{s}$ or $\Delta t = 30\mu\mathrm{s}$ for the time increments in the relaxation process or the spinning process, respectively.

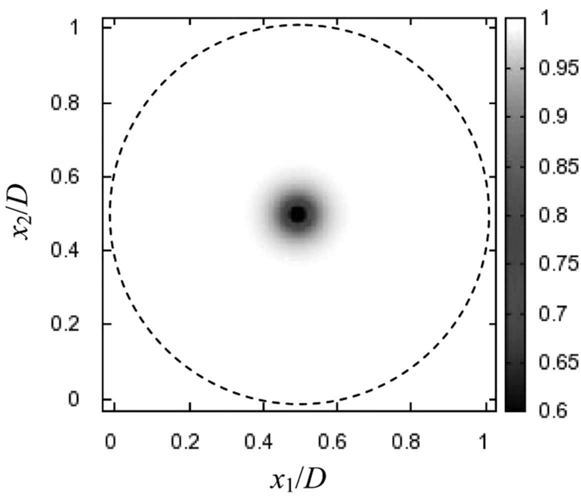
III-2. Results and Discussion

When the tensor Q_{ij} is equivalent to a director (i.e., $Q_{ij} = n_i n_j$) $\mathrm{Tr}\boldsymbol{Q}^3 = 1$; it turns out that within the core of the defects $\mathrm{Tr}\boldsymbol{Q}^3$ becomes smaller than 1 (in terms of energy this means that the bulk energy density F^b within the core is higher than outside the core (see Eq. (21)). Accordingly a 2D plot of the spatial dependence of $\mathrm{Tr}\boldsymbol{Q}^3$ will exhibit a circular depression with small diameter (presumably related to κ_b). On the other hand one can visualise the defects position and dynamics by plotting $\mathrm{Tr}\boldsymbol{Q}^3$ using a colour scale; the defect will appear as a small spot in a uniformly coloured background.

In a first stage we relax the analytical configuration defined by the tensor field $\boldsymbol{Q}^R$ in section III-1 under the effect of the magnetic field alone ($\Omega = 0$). Figs. 2 to 7 show the time evolution of the component Q_{11} (Figs. 2a to 7a) and $\mathrm{Tr}\boldsymbol{Q}^3$ (Figs. 2b to 7b); Figure 2 shows the initial configuration defined by the analytical tensor field $\boldsymbol{Q}^R$, and corresponding to a radial distribution of the director and regularised in the centre. A grey scale is used for both quantities: for Q_{11} the



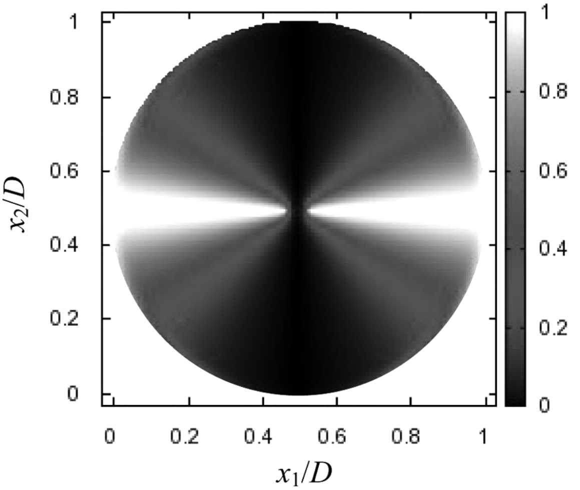
(a)



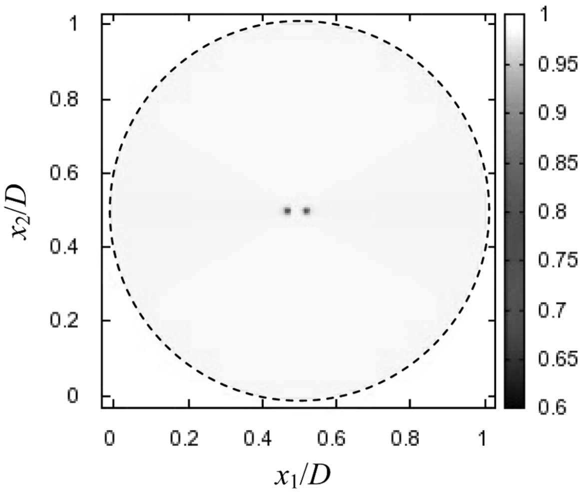
(b)

FIGURE 2 2D plots of (a) Q_{11} and (b) $\mathrm{Tr}\boldsymbol{Q}^3$ at time $t = 0$ ms; the circle in (b) materialises the wall of the tube. The configuration corresponds to the tensor field $\boldsymbol{Q}^R$ defined in section III-1.

correspondence between colours and values is white for $Q_{11} = 1$ and black for $Q_{11} = 0$ (thus black regions correspond to directors parallel to the magnetic field and white regions to directors normal to the magnetic field); for $\mathrm{Tr}\boldsymbol{Q}^3$ the correspondence is white for $\mathrm{Tr}\boldsymbol{Q}^3 = 1$



(a)



(b)

FIGURE 3 2D plots of (a) Q_{11} and (b) Tr$\boldsymbol{Q}^3$ at time $t = 12$ ms when a magnetic field with magnitude $B = 2\,\mathrm{T}$ has been applied at time $t = 0$ ms on the state described by the Figure 2. The tube is at rest, i.e., $\Omega = 0$. The circle in (b) materialises the wall of the tube.

and black for Tr$\boldsymbol{Q}^3 = 0.6$, this latter value corresponds approximately to the bottom of the depression in Tr$\boldsymbol{Q}^3$. The relaxation process may be divided in two stages. During the first one ($t < 50$ ms, see Figs. 3 and 4)

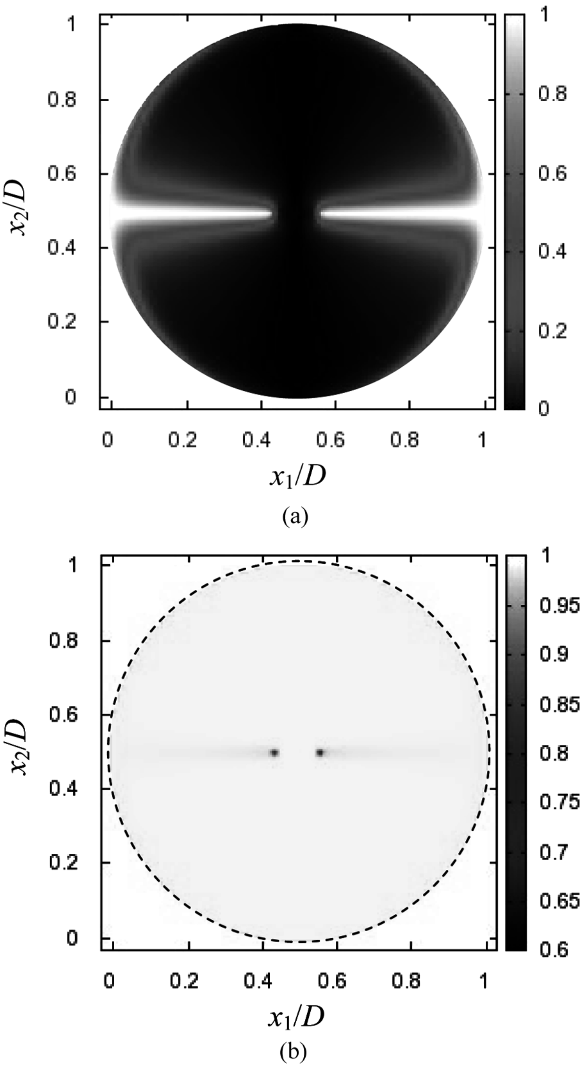
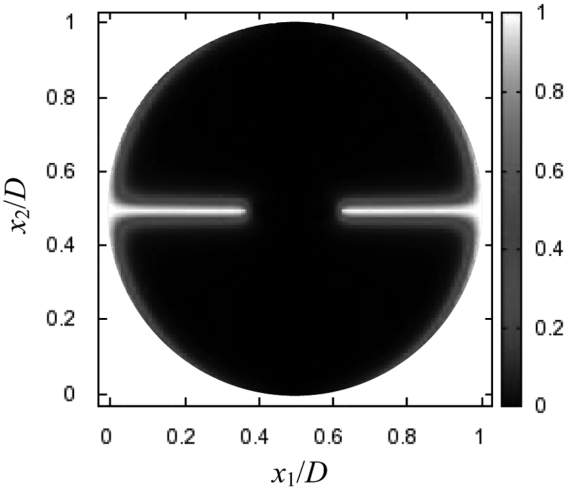
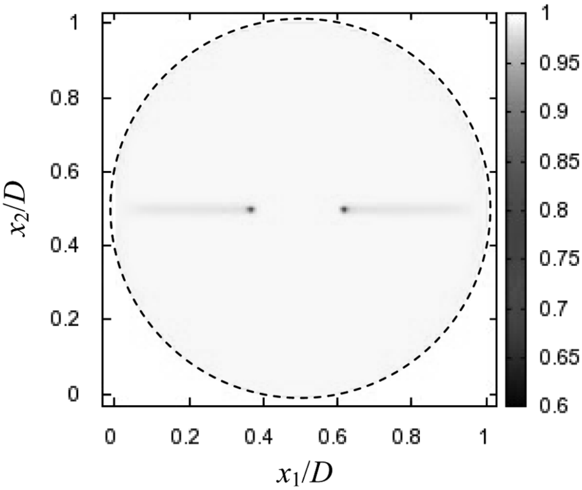


FIGURE 4 2D plots of (a) Q_{11} and (b) TrQ^3 at time $t = 36$ ms when a magnetic field with magnitude $B = 2\,\mathrm{T}$ has been applied at time $t = 0$ ms on the state described by the Figure 2. The tube is at rest, i.e., $\Omega = 0$. The circle in (b) materialises the wall of the tube.

the black colour in the figures showing Q_{11} invades the most part of the disk, except within two thin horizontal bands enveloping the x_1 axis, starting from a region close to the centre and joining the



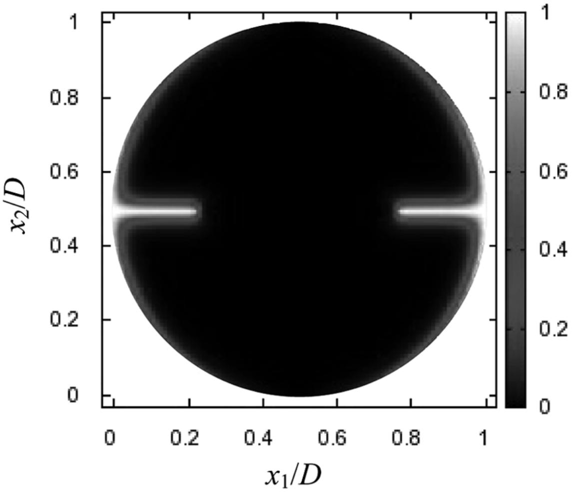
(a)



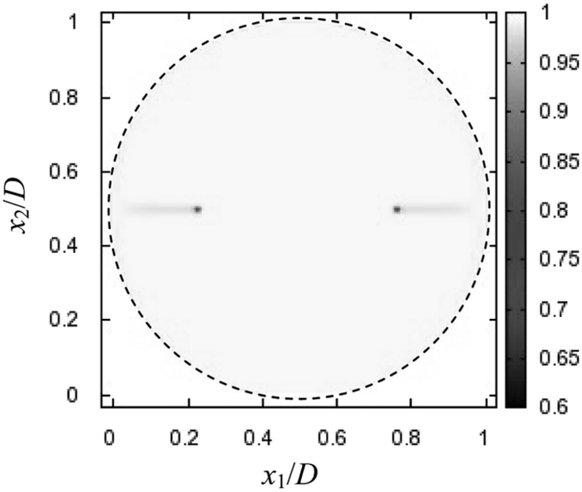
(b)

FIGURE 5 2D plots of (a) Q_{11} and (b) Tr$\boldsymbol{Q}^3$ at time $t = 72$ ms when a magnetic field with magnitude $B = 2$ T has been applied at time $t = 0$ ms on the state described by the Figure 2. The tube is at rest, i.e., $\Omega = 0$. The circle in (b) materialises the wall of the tube.

boundary. That reflects the alignment of the director with the magnetic field almost everywhere; the presence of defects avoids the full alignment of the director within the white bands. Simultaneously,



(a)



(b)

FIGURE 6 2D plots of (a) Q_{11} and (b) TrQ^3 at time $t = 144$ ms when a magnetic field with magnitude $B = 2\,\mathrm{T}$ has been applied at time $t = 0$ ms on the state described by the Figure 2. The tube is at rest, i.e., $\Omega = 0$. The circle in (b) materialises the wall of the tube.

during this first stage the single $+1$ defect splits into two $+1/2$ defects, which manifests by the appearance of two dark spots in the Figures 3a and 4a. The two defects start to repel from each other while moving

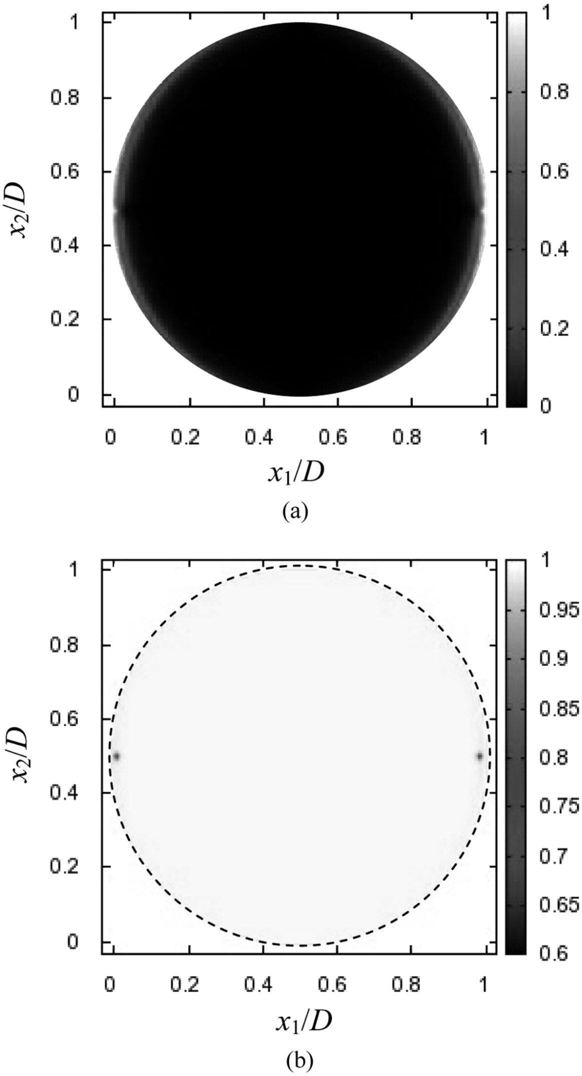


FIGURE 7 2D plots of (a) Q_{11} and (b) TrQ^3 at time $t = 300$ ms when a magnetic field with magnitude $B = 2\,\mathrm{T}$ has been applied at time $t = 0$ ms on the state described by the Figure 2. The tube is at rest, i.e., $\Omega = 0$. The configuration described by this figure is stationary. The circle in (b) materialises the wall of the tube.

along the x_1 axis and towards the boundary. This motion being slower than the alignment of the director just described above, it actually characterises the second stage of the relaxation where the width of the white bands is constant in time (Figs. 5 to 7). After a sufficiently long delay ($t \approx 300$ ms) the two defects stabilise at two diametrically opposite positions on the x_1 axis and close to the tube surface (Fig. 7b).

The motion of the two defects may be interpreted as follows. Within the white band connecting one defect to the boundary, the director is normal to the magnetic field; accordingly the bands mainly contribute to the energy of the system. Obviously, by reducing the length of the bands the system reduces its energy; which manifests by the motion of the defects ending the bands. However, the two white regions cannot vanish completely in the vicinity of the two positions ($x_1 = -D/2$, $x_2 = 0$) and ($x_1 = D/2$, $x_2 = 0$) because of rigid anchoring. It should be noted that in practice the anchoring is not perfectly rigid, it is described by a finite anchoring energy according to Rapini-Papoular model [10], therefore a competition will appear between the anchoring strength and the magnetic strength. The results presented here require that the anchoring strength dominates the magnetic strength.

One may wonder whether the mobility of the defects is correctly described by our model inasmuch as the core is not correctly described. In other words, does the core structure of the defect influence the defect mobility or not? When backflows are neglected the mobility is dictated by the total free energy that tends to reach a minimum corresponding to a steady configuration. The minimisation of the total free energy takes into account not only the energy of the core but also the energy in a large volume around the core where the director is defined and strongly inhomogeneous. Accordingly, it seems not unreasonable to attribute a notable role in the defect mobility to the director pattern around a defect. It should be noted that it is implicitly the assumption of models using the director description outside of a tubular region surrounding the disclination line, assuming moreover a definite energy per unit of length within the tubular region [2].

The steady configuration of the tensor field Q reached during the relaxation process described above is used as the initial condition for Q when the tube is spun. It is worth recalling the fundamental results concerning the director time evolution of a spinning homogeneous nematic at spinning rate Ω and subjected to the magnetic field $\vec{B}$ normal to the axis of rotation. Within the scope of Leslie-Ericksen theory, the angle θ between the director, assumed to stay normal to the tube axis, and the magnetic field obeys to the following equation

$$\frac{d\theta}{dt} + \Omega_c \sin 2\theta = \Omega \tag{36}$$

with

$$\Omega_c = \frac{\chi_a B^2}{2\mu_0 \gamma_1} \tag{37}$$

Two kinds of solution exist according to the value of Ω with respect to Ω_c [11]; for $\Omega < \Omega_c$ a steady orientation is reached; on the contrary for $\Omega > \Omega_c$ the director permanently rotates according to

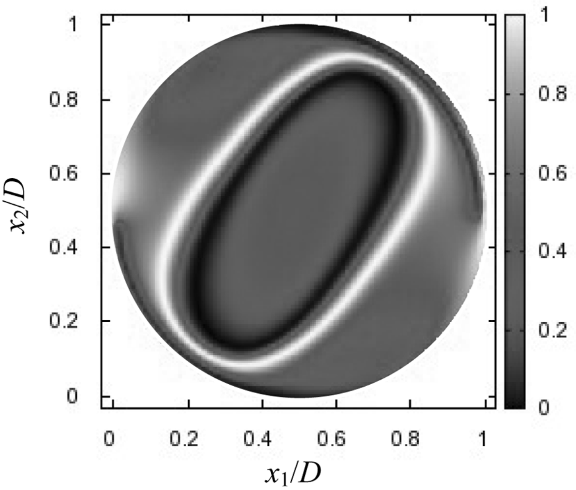
$$\tan\theta = \frac{\Omega_c}{\Omega} + \sqrt{1 - \left(\frac{\Omega_c}{\Omega}\right)^2}\tan(\omega t + \varphi) \tag{38}$$

with

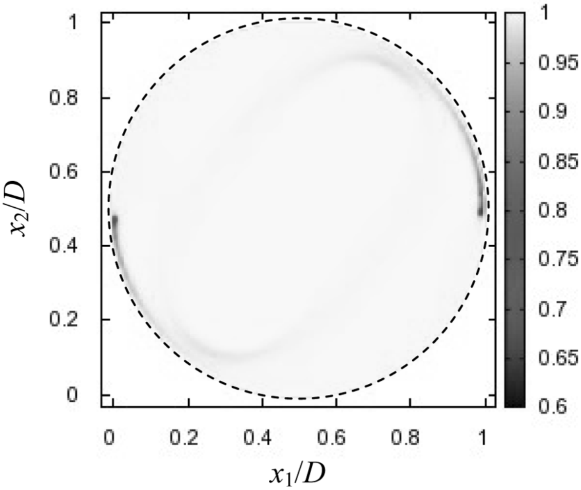
$$\omega = \sqrt{\Omega^2 - \Omega_c^2} \tag{39}$$

The question arises of what should happen for $\Omega > \Omega_c$ when the director is rigidly anchored on the surface of the tube. The rotation of the director in the vicinity of the boundary would be locked by the anchoring. Accordingly, a circular stationary layer close to the tube wall should appear as a ring in a 2D plot with a colour scale and with increase of time an accumulation of such rings reflecting the winding up of the director is expected. Actually the dynamics evidenced by the simulations performed for $\Omega/\Omega_c = 2$ is notably different as shown by the 2D plots of Q_{11} and $\mathrm{Tr}\boldsymbol{Q}^3$ in Figures 8 to 13. During each period of director rotation an elliptic white ring appears, develops, breaks in two parts, and finally vanishes. When the ring becomes clearly defined it looks like an ellipse whose long axis coincides with one diameter of the tube while the short axis is significantly smaller than the diameter. The long axis makes approximately an angle of 35° with the magnetic field. Subsequently, the ring ‘breaks’ at two diametrically opposite positions where it was thinner, namely, at the extremities of the long axis and near the boundary (Figs. 10a and 11a). Subsequently each semi-ring behave like the two white bands of the relaxation process, they shorten but without completely disappearing because of strong anchoring.

When we compare the figures showing Q_{11} and $\mathrm{Tr}\boldsymbol{Q}^3$ we observe that the thinnest part of the white ring and the position of its breaking points coincide with the occurrence of a depression in $\mathrm{Tr}\boldsymbol{Q}^3$ (compare the position of the dark streak in Figure 9b with the position of the white ring in Fig. 9a) and the appearance of two spots in Figure 10b. The frontier between a white and a black ring is a wall corresponding to a rotation by $\pi/2$ of the director; the breaking of such a wall generates a pair of defects $\pm 1/2$. The creation of a pair of defects arises as



(a)



(b)

FIGURE 8 2D plots of (a) Q_{11} and (b) Tr$\boldsymbol{Q}^3$ at time $t = 192$ ms for $B = 2$ T and $\Omega/\Omega_c = 2$ (Ω_c is defined by Eq. (37)) when the state at time $t = 0$ ms corresponds to the steady state shown in Figure 7. The circle in (b) materialises the wall of the tube.

follows: where the ring is thinner, i.e., where the gradients are stronger, Tr$\boldsymbol{Q}^3$ starts to become slightly smaller than 1, the depression in Tr$\boldsymbol{Q}^3$ becomes deeper with increase of time and its spatial extension

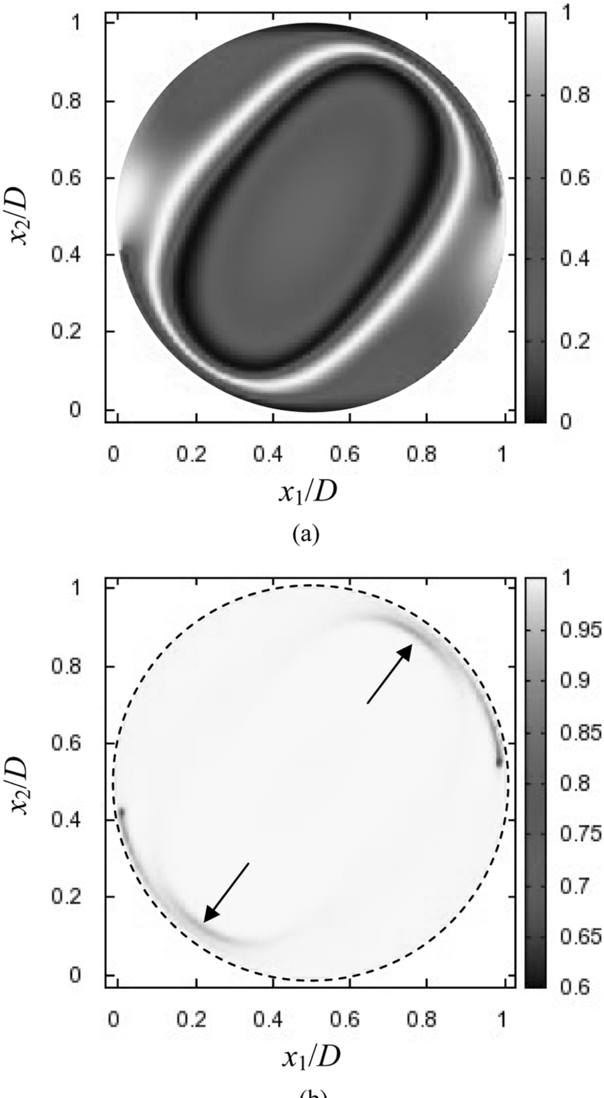
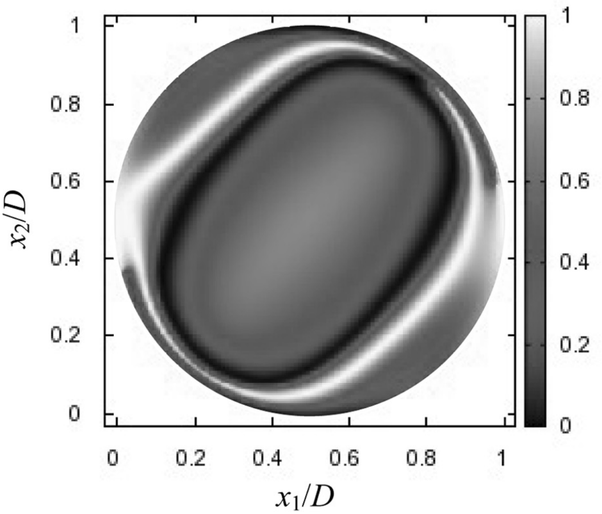
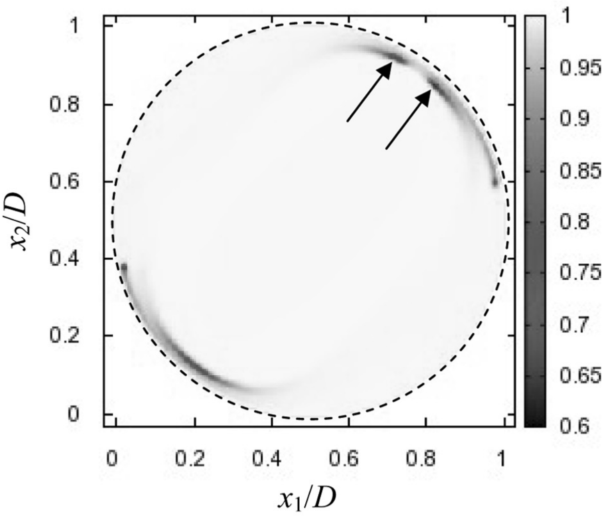


FIGURE 9 2D plots of (a) Q_{11} and (b) TrQ^3 at time $t = 204$ ms for $B = 2$ T and $\Omega/\Omega_c = 2$ (Ω_c is defined by Eq. (37)) when the state at time $t = 0$ ms corresponds to the steady state shown in Figure 7. The circle in (b) materialises the wall of the tube. The two dark streaks indicated by the arrows in (b) coincide with the thinnest part of the white ring for Q_{11} in (a).

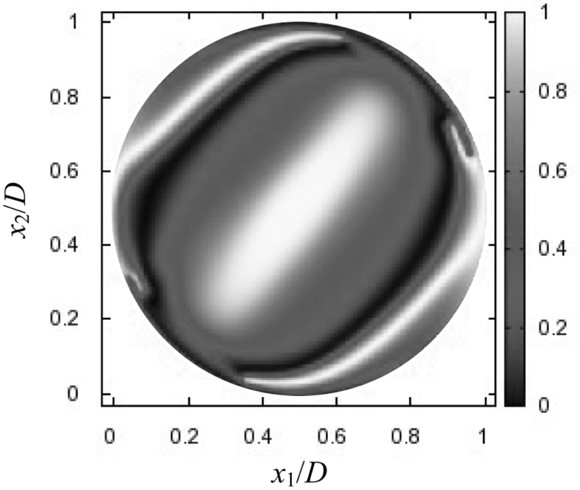


(a)

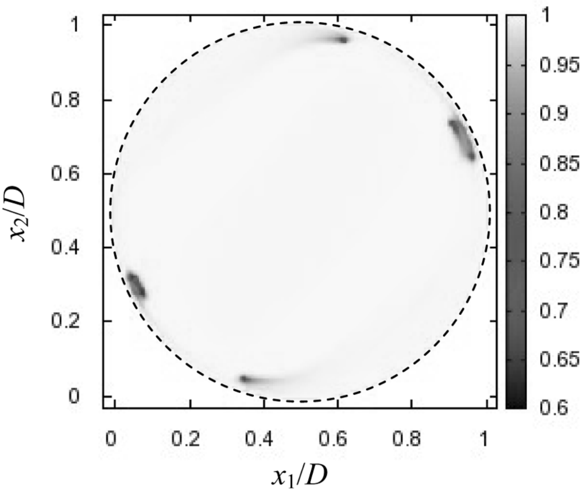


(b)

FIGURE 10 2D plots of (a) Q_{11} and (b) Tr$\boldsymbol{Q}^3$ at time $t = 216$ ms for $B = 2$ T and $\Omega/\Omega_c = 2$ (Ω_c is defined by Eq. (37)) when the state at time $t = 0$ ms corresponds to the steady state shown in Figure 7. The circle in (b) materialises the wall of the tube. The appearance of two dark spots in (b) coincides with the breaking of the white ring for Q_{11} in (a).



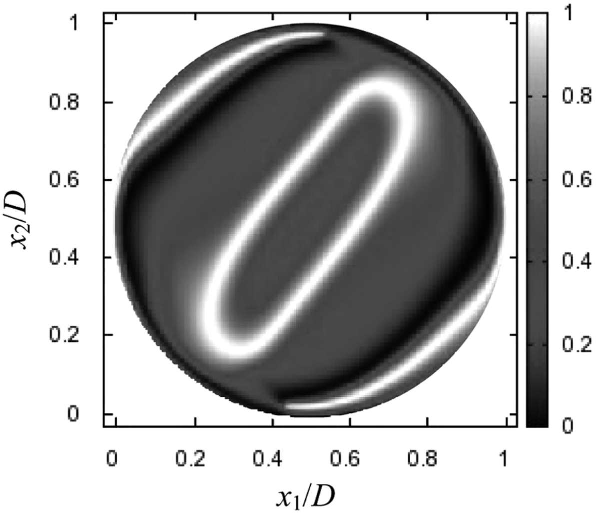
(a)



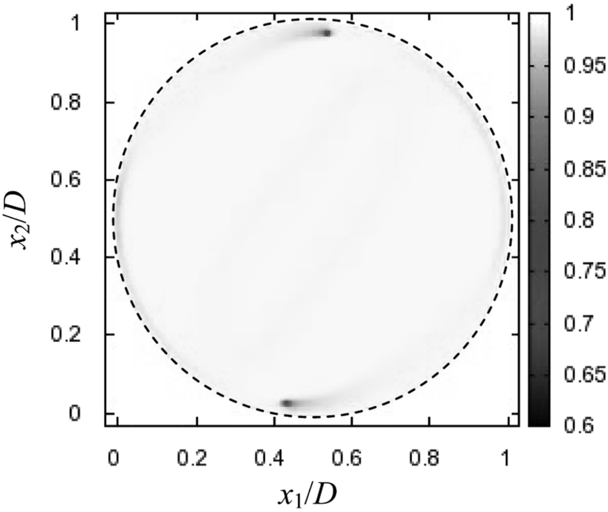
(b)

FIGURE 11 2D plots of (a) Q_{11} and (b) TrQ^3 at time $t = 228$ ms for $B = 2$ T and $\Omega/\Omega_c = 2$ (Ω_c is defined by Eq. (37)) when the state at time $t = 0$ ms corresponds to the steady state shown in Figure 7. The circle in (b) materialises the wall of the tube.

follows a portion of the ring in the plot of Q_{11}, subsequently the central part of the extended curvilinear depression raises up towards one, thus forming two separate depressions (two spots in Fig. 10b). Finally,



(a)



(b)

FIGURE 12 2D plots of (a) Q_{11} and (b) Tr$\boldsymbol{Q}^3$ at time $t = 240$ ms for $B = 2$ T and $\Omega/\Omega_c = 2$ (Ω_c is defined by Eq. (37)) when the state at time $t = 0$ ms corresponds to the steady state shown in Figure 7. The circle in (b) materialises the wall of the tube. The comparison with Figure 11 indicates that two pairs of defects have annihilated while a new elliptic white ring has appeared.

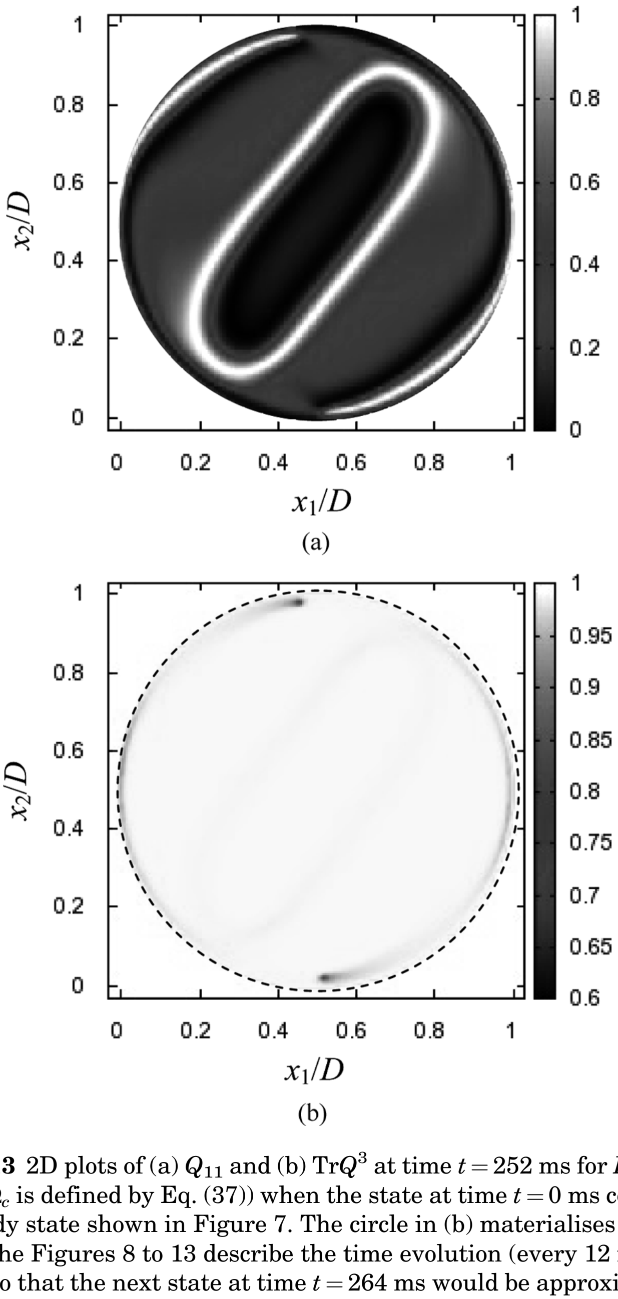


FIGURE 13 2D plots of (a) Q_{11} and (b) Tr$\boldsymbol{Q}^3$ at time $t = 252$ ms for $B = 2$ T and $\Omega/\Omega_c = 2$ (Ω_c is defined by Eq. (37)) when the state at time $t = 0$ ms corresponds to the steady state shown in Figure 7. The circle in (b) materialises the wall of the tube. The Figures 8 to 13 describe the time evolution (every 12 ms) during one cycle, so that the next state at time $t = 264$ ms would be approximately the one shown in Figure 8.

two thin circular depressions are formed indicating the presence of two defects. Immediately after the double breaking of the ring, six defects exist (two defects were already present before the breaking, they result from the previous cycle), four with the charge $+1/2$ and two with the charge $-1/2$. They move while staying close to the tube wall and finally two of the new defects annihilate with the two previously existing defects as shown in Figures 10b to 12b. The breaking and the vanishing of the rings clearly avoid the continuous increasing of the elastic energy; thus, the process of creation/annihilation of defects appears as a mechanism to relax the elastic energy.

IV. CONCLUSION

We proposed a tensorial extension of the Leslie-Ericksen theory that regularises the original theory within the core of the defects. We first defined a tensor field with four degrees of freedom to describe the local order. Fundamental quantities and relations have been deduced from an arbitrary free energy density and invariance by rotation. The balance of torque provided a system of three equations that must satisfy the order tensor at any time. The evolution equation for the order tensor is derived from constitutive equations for the free energy density and the viscous stress, they have been chosen the closest possible to the corresponding relations in the LE theory. Thus, the model uses the visco-elastic coefficients of LE theory plus one additional parameter to stabilise the uniaxial state. Finally, an evolution equation for the order tensor compatible with the balance of torque is proposed.

The model has been applied to (a section of) a spinning tube filled with a nematic fluid (5CB) subjected to a magnetic field and initially containing one defect with topological charge $+1$ at the centre of the tube section. We first observed that the $+1$ defect splits into two $+1/2$ defects during the relaxation stage under the magnetic field alone. When the tube is spun, a (quasi) periodic regime occurs where pairs of defects are created and annihilated, avoiding the winding up of the director and the permanent increase of the elastic energy. This process of creation/annihilation of defects appears thus as a way to relax the distortion generated by permanent rotation of the director combined with strong anchoring.

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