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Two-dimensional hydrodynamical description of a rotating nematic sample in a magnetic field

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Nematodynamic equations are applied to the description of a cylindrical nematic sample, rotating around its axis with constant angular velocity, in the presence of a perpendicular magnetic field. The system is described by the director orientation \mathbf{n} and by the velocity vector \mathbf{v} fields in the cylinder volume. Equations are simplified by considering the director orientation \mathbf{n} constrained in a planar section of the cylinder and by neglecting coupling with the velocity field, which is completely determined by the angular speed rate. Boundary conditions for perfect alignment of the director \mathbf{n} perpendicularly to the walls are assumed. It is shown that a dynamical equation can be obtained which is amenable to numerical analysis for the spatial and time dependence of the director orientation. Transient distributions and stationary solutions are found and discussed.

1. Introduction

According to the hydrodynamical description of nematic liquid crystals [1, 2], an incompressible nematic sample is described by two vector fields in space: the director unit vector $\mathbf{n}(\mathbf{r}, t)$, which gives the orientation of the director at space point \mathbf{r} and time t , and the velocity vector $\mathbf{v}(\mathbf{r}, t)$. Constitutive equations [1, 2] provide a closed set of partial differential relations which are in principle able to describe the fluid both in space and time, if explicit boundary and initial conditions are given and either analytical or (more likely) numerical solution techniques are available. In most cases one has to resort to drastic approximations.

We shall consider in the following a well known case, namely a rotating sample in the presence of a constant perpendicular magnetic field. A tube containing a nematic liquid crystal is spinning at a constant angular velocity about its symmetry axis, while a uniform magnetic field is turned on in a horizontal plane. Equivalent or related rheological measurements with analogous geometrical set-ups have been made in the past, initially by Tsevtkov [3], who actually used a stationary sample in a rotating magnetic field. Gasparoux and Prost measured the torque exerted by the fluid on the cylinder as a function of the rotational speed [4], and Leslie *et al.* performed studies on the electron spin resonance spectrum of a paramagnetic probe dissolved in the nematic

[5]. Emsley *et al.* also measured the deuterium NMR spectrum for the nematic phase of a partly deuteriated liquid crystal as a function of sample spinning speed [6], and Knepe and Schneider measured the rotational viscosity coefficient of the liquid crystal [7]. Experiments related to fixed geometries of the initial orientation of the director in the bulk with respect to the magnetic field have also been conducted, more recently, by Martins and coworkers [8].

In this communication, we describe the full dependence upon space and time of the director orientation, taking into account boundary conditions at the internal walls of the tube and assuming a defect-controlled experimental set-up. Under the two basic approximations of neglecting the dynamical coupling between the velocity and director vector fields, and of constraining the director motion in the horizontal plane containing the magnetic field, we recover a closed, albeit non-linear, partial differential equation for the director orientation and we present our preliminary findings. A time-dependent solution is calculated which takes into account the spatial gradients, and it is shown that its dynamical evolution goes first through a long-lived transient behaviour, with rather complex spatial patterns, and then always reaches a stationary distribution. The spatial patterns depend on the value of the spinning rate, and their complexity appears to be higher for values close to Leslie's critical velocity.

In §2 the model is discussed and the full time evolution equation for the director orientation is introduced. Neglecting any spatial dependence, simple and well-known

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solutions are obtained whose validity is limited by the fact that boundary conditions must necessarily be discarded and that a forced uniformity of the director orientation is imposed upon the whole sample. These are revised in §3. New insight is gained when the spatial dependence is fully taken into account, although the solutions are much more difficult to obtain and one has to resort to numerical algorithms, as discussed in §4. Preliminary results are presented in §5, and concluding remarks are given in §6.

2. The model

The geometrical set-up is sketched in figure 1, which shows a representative planar section of the sample. The plane is defined by the axes \mathbf{e}_1 and \mathbf{e}_2 ; a point in space is identified by the vector \mathbf{r} , which is defined by the Cartesian coordinates (r_1, r_2, r_3) : in the plane $r_3 = 0$. The radius of the cylinder is R . The magnetic field is defined as $\mathbf{H} = (H, 0, 0)$. Finally the constant angular velocity vector for the cylinder is $\boldsymbol{\Omega} = (0, 0, \Omega)$. For each position \mathbf{r} , the vector fields \mathbf{v} and \mathbf{n} are defined as having components in the plane only, i.e. $\mathbf{v} = (v_1, v_2, 0)$, $\mathbf{n} = (n_1, n_2, 0)$, choice (1).

Next we neglect any complexity in the velocity profile, i.e. we assume that the vector field is obtained as the linear velocity of a rigid cylinder of angular velocity Ω , choice (2). This approximation allows us to uncouple the director \mathbf{n} from the velocity \mathbf{v} in the nematodynamic equations. Since $\mathbf{n}^2 = 1$, we may summarize these choices

by writing:

$$\mathbf{v} = \boldsymbol{\Omega} \times \mathbf{r} = (-\Omega r_2, \Omega r_1, 0) \quad (1)$$

$$\mathbf{n} = (\cos \phi, \sin \phi, 0). \quad (2)$$

Notice that equation (1) satisfies the incompressibility condition, $\nabla \cdot \mathbf{v} = 0$, where ∇ is the gradient with respect to \mathbf{r} . Both choices (1) and (2) may be considered as reasonable assumptions. The imposed planarity should be lifted if boundary conditions requiring adjustments along the third coordinates are imposed. The real velocity profile is distorted in the intermediate regions of the sample, especially at high rotation speeds [7].

From the constitutive equation of nematodynamics we have:

$$\xi \frac{d^2 n_i}{dt^2} = G_i + g_i + \pi_{kik} \quad (3)$$

$$g_i = \lambda n_i - \frac{\partial W}{\partial n_i} + g'_i \quad (4)$$

where ξ is the inertial constant, G_i is the i -component of the external director body force due to the magnetic field, and g_i is that of the internal director body force, which contains a dissipative contribution g'_i ($i = 1, 2$); W is the Helmholtz free energy and $\pi_{ji} = \partial W / \partial n_{ij}$; λ is an arbitrary function. The material time derivative is d/dt . The external director body force is given simply by

$$G_i = \chi_a H_j n_j H_i \quad (5)$$

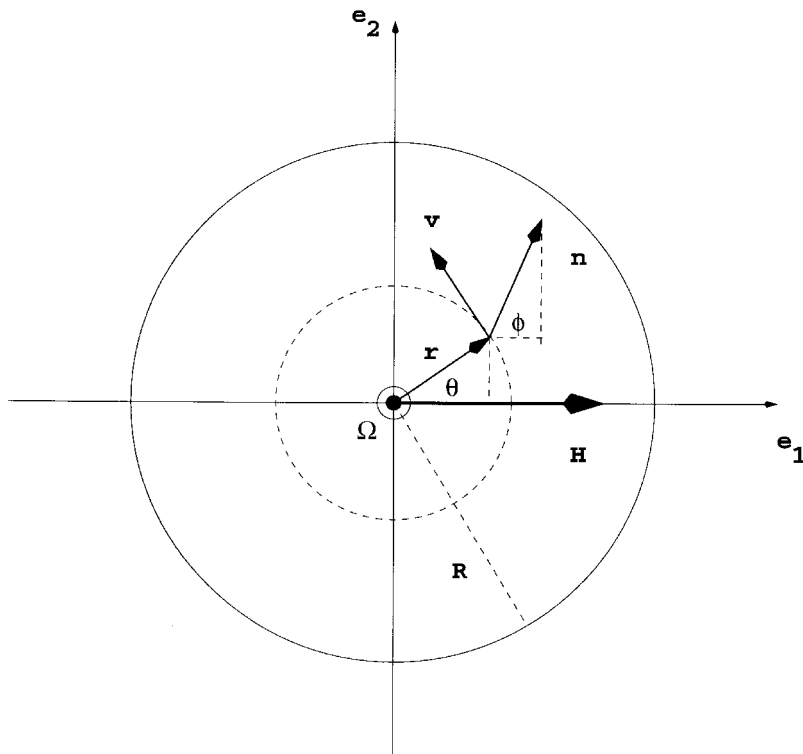


Figure 1. Geometrical set-up.

where $\chi_a = \chi_{\parallel} - \chi_{\perp}$, χ_{\parallel} and χ_{\perp} being the principal diamagnetic susceptibilities per unit volume. Einstein's summation convention is employed, if not stated otherwise explicitly. By simple algebraic manipulations, taking into account that $\mathbf{n}^2 = 1$, one gets the following equation for the unknown angle ϕ :

$$\xi \left(n_2 \frac{d^2 n_1}{dt^2} - n_1 \frac{d^2 n_2}{dt^2} \right) + \frac{1}{2} \chi_a H^2 \sin 2\phi + n_2 g'_1 - n_1 g'_2 + \mathcal{K} = 0 \quad (6)$$

where \mathcal{K} is obtained as:

$$\mathcal{K} = n_2 \left(-\frac{\partial W}{\partial n_1} + \pi_{k1,k} \right) + n_1 \left(-\frac{\partial W}{\partial n_2} + \pi_{k2,k} \right). \quad (7)$$

The intrinsic director body force components g'_i are obtained in terms of the components of the director field, and of the angular speed Ω :

$$g'_1 = -\gamma_1 \left(\frac{dn_1}{dt} + \Omega n_2 \right) \quad (8)$$

$$g'_2 = -\gamma_1 \left(\frac{dn_2}{dt} - \Omega n_1 \right) \quad (9)$$

Here γ_1 is a rotational viscosity parameter. We may now substitute these expressions in equation (6). We neglect the inertial contribution, by assuming ξ small (3); also we may write explicitly the material time derivative as

$$\frac{d}{dt} = \frac{\partial}{\partial t} + (\Omega \times \mathbf{r}) \cdot \nabla. \quad (10)$$

The following equation is then obtained:

$$\gamma_1 \left[\frac{\partial \phi}{\partial t} - \Omega \left(1 + r_2 \frac{\partial \phi}{\partial r_1} - r_1 \frac{\partial \phi}{\partial r_2} \right) \right] + \frac{1}{2} \chi_a H^2 \sin 2\phi + \mathcal{K} = 0. \quad (11)$$

The function \mathcal{K} can be evaluated from equation (7); for the sake of simplicity we shall adopt the spherical approximation (4) for the elastic energy W [9]

$$W = \frac{1}{2} K n_{ij} n_{ij} \quad (12)$$

where K is an averaged elastic constant. In this case \mathcal{K} is simply given by (see Appendix):

$$\mathcal{K} = K(n_2 \nabla^2 n_1 - n_1 \nabla^2 n_2). \quad (13)$$

In order to simplify as much as possible our final equation, it is convenient to change our representation from Cartesian to cylindrical, or polar as far as the plane is concerned, i.e. from r_1, r_2 to r, θ (*cf.* figure 1), and to introduce a rescaled radius $x = r/d$, where x is now an adimensional quantity and d is a constant length. Finally,

the time evolution of the director is governed by the following equation:

$$\frac{\partial \phi}{\partial t} + \Omega \left(\frac{\partial \phi}{\partial \theta} - 1 \right) + \Omega_c \sin 2\phi - \Omega_K \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{1}{x} \frac{\partial \phi}{\partial x} + \frac{1}{x^2} \frac{\partial^2 \phi}{\partial \theta^2} \right) = 0. \quad (14)$$

Parameters Ω_c and Ω_K have dimensions of frequencies and are defined as:

$$\Omega_c = \frac{\chi_a H^2}{2\gamma_1} \quad (15)$$

$$\Omega_K = \frac{K}{\gamma_1 d^2}. \quad (16)$$

The fundamental time scales which enter the description of the system are then related to the speed of rotation (Ω), to the ratio between the field intensity H and the viscosity parameter γ_1 (Ω_c), and to the ratio between the averaged elastic constant K and γ_1 (Ω_K). Depending on their relative values, different stationary and dynamical regimes can be analysed. The case $\Omega = 0$ corresponds to a fixed geometry, i.e. no rotation: in this case, the stationary solution, $\partial \phi / \partial t = 0$ does not depend upon the viscosity γ_1 , but only on the field intensity and the elastic constant.

3. Space-independent approximation

Let us now review the traditional treatment of equation (14), when spatial dependence is totally neglected. All derivatives with respect to x and θ are discarded and the following simplified ordinary differential equation for $\phi(t)$ is found:

$$\frac{d\phi}{dt} - \Omega + \Omega_c \sin 2\phi = 0 \quad (17)$$

where in this section d/dt is the ordinary derivative with respect to time. A stationary solution, $d\phi/dt = 0$, is possible only for $\Omega/\Omega_c \leq 1$, in which case

$$\phi = \frac{1}{2} \arcsin \frac{\Omega}{\Omega_c} \quad (18)$$

otherwise the angle ϕ basically rotates in time, with an effective frequency given by $(\Omega^2 - \Omega_c^2)^{1/2}$ [10]. Two considerations are in order. First, the assumption of spatial independence is a very drastic approximation, especially in so far as boundary conditions are concerned. Second, the prediction of a rotating director even in the bulk of the fluid, especially at high rotating speeds of the sample, could be strongly modified when spatial dependence comes into consideration. In fact additional stationary solutions can manifest themselves once the condition of independence of ϕ upon x and

especially θ is released. This will be the subject of the analysis continued in §4.

It is interesting to note that even under the condition of negligible spatial gradient of the director, additional stationary solutions can be predicted if one assumes modified constitutive equations, as was done by Martins [11] in his continuum theory of liquid crystal polymers, where he allowed for some non-affinity of the response of polymer strands to an imposed rate of deformation. The only changes are in equations (8) and (9), which become

$$g'_1 + \tau \left(\frac{dg'_1}{dt} + \Omega g'_2 \right) = -\gamma_1 \left(\frac{dn_1}{dt} + \Omega n_2 \right) \quad (19)$$

$$g'_2 + \tau \left(\frac{dg'_2}{dt} - \Omega g'_1 \right) = -\gamma_1 \left(\frac{dn_2}{dt} - \Omega n_1 \right) \quad (20)$$

where τ is a time constant. Neglecting time derivatives and combining these expression with equation (6) we obtain the following condition for stationary solutions:

$$\sin 2\phi = \frac{\Omega}{\Omega_c(1 + \tau^2 \Omega^2)}. \quad (21)$$

For $\tau=0$ we re-obtain the simple description based on Leslie's equations. For $\tau>0$ two cases are possible: if $\tau^2 \Omega_c^2 > 1/4$, a stationary solution is always found, since the right hand member of equation (21) is always less than 1. Otherwise two critical velocities $\Omega_{1,2}$ are predicted:

$$\Omega_{1,2} = \frac{1}{\tau^2 \Omega_c} \left[\frac{1}{2} \pm \left(\frac{1}{4} - \tau^2 \Omega_c^2 \right)^{1/2} \right] \quad (22)$$

such that stationary solutions are possible for $\Omega \leq \Omega_1$ and for $\Omega \geq \Omega_2$. Thus for finite values of τ , a richer collection of situations (no critical velocity at all, or two critical velocities) can in principle be obtained even without considering the director spatial dependence.

However, a more careful analysis of the problem gives a different perspective. First, in most plausible experimental conditions Ω_c ranges from 10^{-2} to 10^{-4} s^{-1} . Estimates of τ range from 10^{-3} to 10^0 s at most. Thus the condition of no critical velocities is practically rarely attained, except maybe for short molecules, for which γ_1 is significantly small. Two critical velocities are usually predicted for liquid crystal polymers, with $\Omega_1 \approx \Omega_c$ and $\Omega_2 \approx 1/\tau^2 \Omega_c \gg \Omega_c$. Second, although modified equation (21) predicts a necessary condition for the existence of stationary solutions, it is by no means a sufficient condition. A complete numerical analysis of the problem in time, based on the solution of the time equation in $\phi(t)$ shows that in all cases for $\Omega \geq \Omega_2$ the possible stationary solution is unstable, i.e. it does not constitute a true limit for infinite time, whereas for $\Omega \leq \Omega_1 \approx \Omega_c$, the stationary solution is stable.

4. Space-dependent treatment

We shall first define boundary and initial conditions for the system under study. Up to now surface effects have not been considered fully, since the approximate elastic free energy we have chosen is defined minus surface terms, which have been neglected. For simplicity we shall consider only the case of equal boundary conditions on the whole internal surface of the cylinder, i.e. having the same dependence upon θ . Let us assume then normal or radial boundary conditions at the surface:

$$\phi(X, \theta, t) = \theta \quad (23)$$

for all times. In the following we shall also consider ϕ as a periodic function of θ of period 2π . The spatial variables θ and x are thus defined as ranging within the limits $0 \leq \theta \leq 2\pi$, $0 \leq x \leq X = R/d$. Next we shall assume that at $x=0$ the generic solution $\phi(0, \theta, t)$ is a finite well-behaved function.

Naturally, different boundary conditions could be assumed: for instance, the director could be assumed to be tangential to the wall of the cylinder, instead of being perpendicular to it, or one could assume the existence of a defect (divergent ϕ) at $x=0$. Initial conditions should also be specified. For the sake of simplicity, we shall assume that at $t=0$ the system is prepared in the simplest stationary state compatible with the absence of rotational speed and magnetic field ($\Omega = \Omega_c = 0$), i.e. a perfect radial alignment of the director:

$$\phi(x, \theta, 0) = \theta. \quad (24)$$

Solutions of the full time and space dependent equation cannot be recovered analytically. However, a numerical solution can be found, by considering an expansion in a suitable set of functions. Let us first define a related function

$$\varphi = \phi - \theta. \quad (25)$$

The time evolution equation in φ is now:

$$\begin{aligned} \frac{\partial \varphi}{\partial t} + \Omega \frac{\partial \varphi}{\partial \theta} + \Omega_c \sin 2(\theta + \varphi) \\ - \Omega_K \left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{1}{x} \frac{\partial \varphi}{\partial x} + \frac{1}{x^2} \frac{\partial^2 \varphi}{\partial \theta^2} \right) = 0. \end{aligned} \quad (26)$$

Initial and boundary conditions are now simply stated as:

$$\varphi(X, \theta, t) = 0 \quad (27)$$

$$\varphi(x, \theta, 0) = 0 \quad (28)$$

and the conditions of φ being periodic in θ and finite in $x=0$ are maintained. By neglecting the terms in Ω and Ω_c , one is left essentially with a Laplace equation in the

plane

$$\frac{\partial \varphi_0}{\partial t} = \Omega_K \left(\frac{\partial^2 \varphi_0}{\partial x^2} + \frac{1}{x} \frac{\partial \varphi_0}{\partial x} + \frac{1}{x^2} \frac{\partial^2 \varphi_0}{\partial \theta^2} \right). \quad (29)$$

Generic finite solutions are then completely defined in the form [12]:

$$\varphi_0(x, \theta, t) = \sum_m \sum_n a_{mn}(t) |mn\rangle \quad (30)$$

where the basis functions in θ and x are

$$|mn\rangle = \frac{1}{\pi^{1/2} X J_{m+1}(\alpha_{mn} X)} \exp(im\theta) J_m(\alpha_{mn} X). \quad (31)$$

Index m assumes all integer values, index n assumes all integer values minus 0; functions $|mn\rangle$ are orthonormal with respect to integration in θ and x ,

$$\langle mn | mn' \rangle = \delta_{m,m'} \delta_{n,n'} \quad (32)$$

and they are eigenfunctions of the Laplacian operator, with eigenvalues α_{mn}^2 . Boundary conditions are taken into account by the condition imposed on the Bessel functions [13]

$$J_m(\alpha_{mn} X) = 0 \quad (33)$$

which defines real coefficients α_{mn} , while coefficients a_{mn} are defined from the initial conditions and have a simple exponential dependence on time:

$$a_{mn}(t) = a_{mn}(0) \exp(-\Omega_K \alpha_{mn}^2 t). \quad (34)$$

Initial conditions are used to specify all $a_{mn}(0)$. One can now use an expression similar to equation (30) to write the general solution of equation (26):

$$\varphi(x, \theta, t) = \sum_m \sum_n A_{mn}(t) |mn\rangle \quad (35)$$

but with corrected time dependent coefficients $A_{mn}(t)$. The time dependence is defined according to the non linear system of the differential equation in t only:

$$\dot{A}_{mn} + (im\Omega + \Omega_K \alpha_{mn}^2) A_{mn} + \Omega_c B_{mn} = 0 \quad (36)$$

where $B_{mn}(t)$ is defined as the average:

$$B_{mn} = \langle mn | \sin 2(\theta + \varphi) \rangle \quad (37)$$

and they depend on all A_{mn} . Initial conditions can be assumed to be $A_{mn}(0) = 0$ for all m, n . Equation (36) is obtained by substituting (35) in the time evolution expression for φ , equation (26). The expression obtained is then premultiplied for a generic $\langle m, n |$ function and integrated with respect to θ and x ; taking into account the orthonormality condition (32), and the fact that functions $|m, n\rangle$ are eigenfunctions of the Laplacian operator, equation (36) is recovered.

The system of equation (36) lends itself to a recursive solution, since it is solved analytically for the A_{mn} once the B_{mn} are known; first some simple dependence for the A_{mn} is assumed, the B_{mn} are calculated and the procedure

is iterated till convergence is reached. In other words, the functions A_{mn} are obtained from the recursive expressions:

$$A_{mn}^{(k+1)}(t) = -\Omega_c \exp[(im\Omega + \Omega_K \alpha_{mn}^2)t] \\ \times \int_0^t d\tau \exp[-(im\Omega + \Omega_K \alpha_{mn}^2)\tau] B_{mn}^{(k)}(\tau) \quad (38)$$

$$B_{mn}^{(k)} = \langle mn | \sin 2(\theta + \varphi^{(k)}) \rangle \quad (39)$$

and $\varphi^{(k)}$ is obtained from $A_{mn}^{(k)}$ through equation (35). A reasonable starting choice is simply $A_{mn}^{(1)} = 0$. Notice that in practice one considers only values of $m > 0$ and $n > 1$, due to the symmetries imposed by the fact that the solution is real. This procedure turns out to be very effective: transient behaviour and stationary solutions are well reproduced by a small number of complex exponential and Bessel functions, around 5–7, depending on the relative magnitude of the parameters. Convergence in the iteration procedure is usually reached after no more than 10 steps.

5. Preliminary numerical results

The non linear nature of equation (35) and its dependence on three independent parameters makes the complete analysis of the system rather complex. Also, it would be interesting to explore effects due to changes in the boundary and initial conditions, and possibly to introduce three-dimensional features, e.g. the distribution of the director orientation in the z direction of the sample. Our aim in this work is to present the reader with a few examples for a ‘realistic’ choice of parameters. It is interesting to consider which values are to be expected for Ω_c , and Ω_K . For a relatively low intensity field, 14 000 G, and assuming $\chi_a = 10^{-7}$ for a short molecule nematic, and $\gamma_1 = 100$ P we get a value for Leslie’s critical velocity of $\Omega_c = 9.8 \times 10^{-2} \text{ s}^{-1}$. If we take $K = 5 \times 10^{-6}$ dyne and we choose $d = (K/\chi_a)^{1/2} / H = 5.5 \times 10^{-4}$ cm (magnetic coherence length) we get $\Omega_K = 1.7 \times 10^{-1} \text{ s}^{-1}$. Let us assume a radius $R = 0.1$ mm, corresponding to a rescaled radius $X = 18.2$. We have now defined all the parameters which describe the rotating sample, except the spinning rate Ω . Let us consider five possible cases: $\Omega = 0 \text{ s}^{-1}$, $\Omega = 4.9 \times 10^{-2} \text{ s}^{-1}$, $\Omega = 9.8 \times 10^{-2} \text{ s}^{-1}$, $\Omega = 19.6 \times 10^{-2} \text{ s}^{-1}$, $\Omega = 9.8 \times 10^{-1} \text{ s}^{-1}$, i.e. 0, $\Omega_c/2$, Ω_c , $2\Omega_c$ and $10\Omega_c$.

The distribution of the director orientation is shown for each case in figures 2–6. Four snapshots have been collected, at increasing times different for each case, labelled respectively (a), (b), (c) and (d) in a clockwise direction. Each snapshot shows a colour plot of function $|\sin \phi|$: a yellow hue characterizes areas where $|\sin \phi|$ is close to 1, i.e. the director is aligned with the y -axis (perpendicular to the magnetic field, cf. figure 1); a

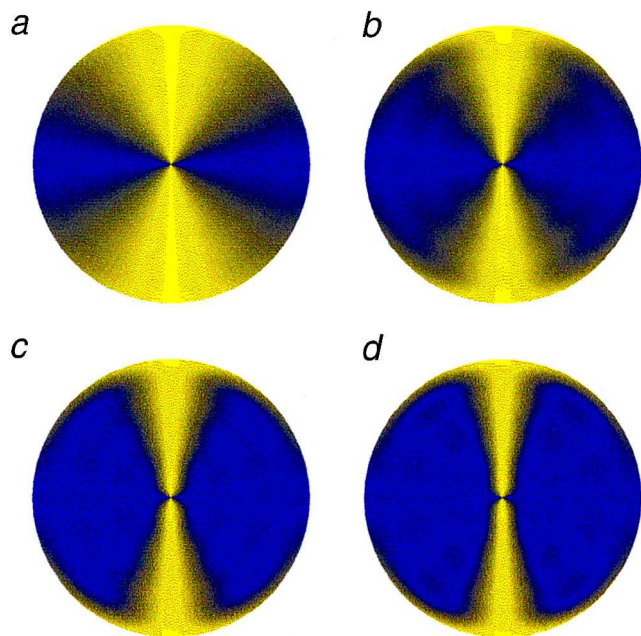


Figure 2. Colour plots of the director orientation in the sample for $\Omega=0$, $\Omega_c=9.8 \times 10^{-2} \text{ s}^{-1}$ and $\Omega_K=1.7 \times 10^{-1} \text{ s}^{-1}$, obtained from the numerical solution of equation (35): (a) $t=1 \text{ s}$, (b) $t=5 \text{ s}$, (c) $t=10 \text{ s}$, (d) $t=25 \text{ s}$.

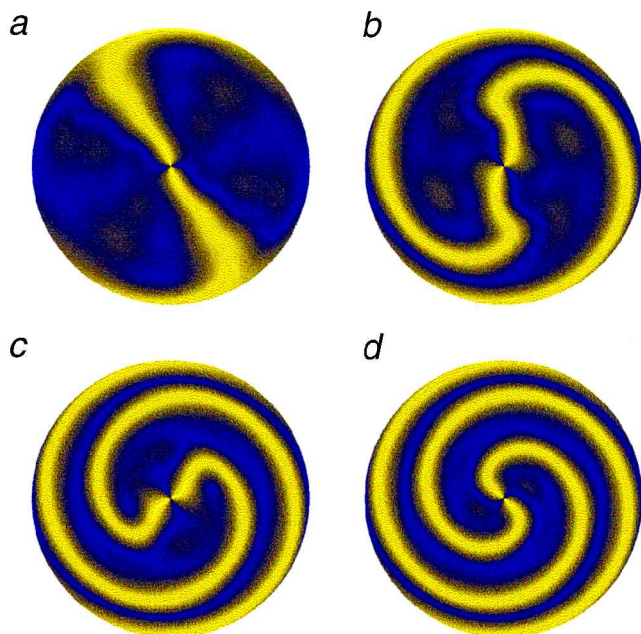


Figure 3. Colour plots of the director orientation in the sample for $\Omega=\Omega_c/2$, and Ω_c , Ω_K as in figure 2: (a) $t=20 \text{ s}$, (b) $t=100 \text{ s}$, (c) $t=200 \text{ s}$, (d) $t=400 \text{ s}$.

violet hue characterizes areas where $|\sin \phi|$ is close to 0, i.e. the director is aligned with the x -axis (parallel to the magnetic field). In all cases, the last snapshot is practically the stationary solution. A few conclusions can be immediately derived: (i) a stationary solution is always attained, independent of the ratio between the

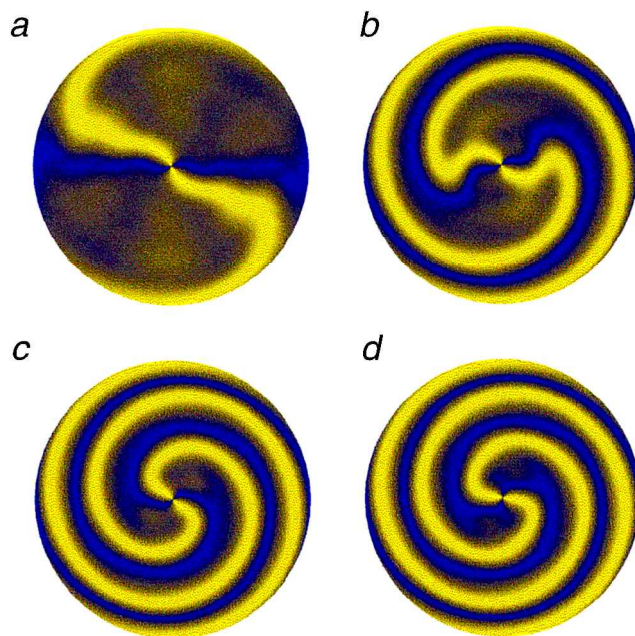


Figure 4. Colour plots of the director orientation in the sample for $\Omega=\Omega_c$, and Ω_c , Ω_K as in figure 2: (a) $t=20 \text{ s}$, (b) $t=100 \text{ s}$, (c) $t=200 \text{ s}$, (d) $t=400 \text{ s}$.

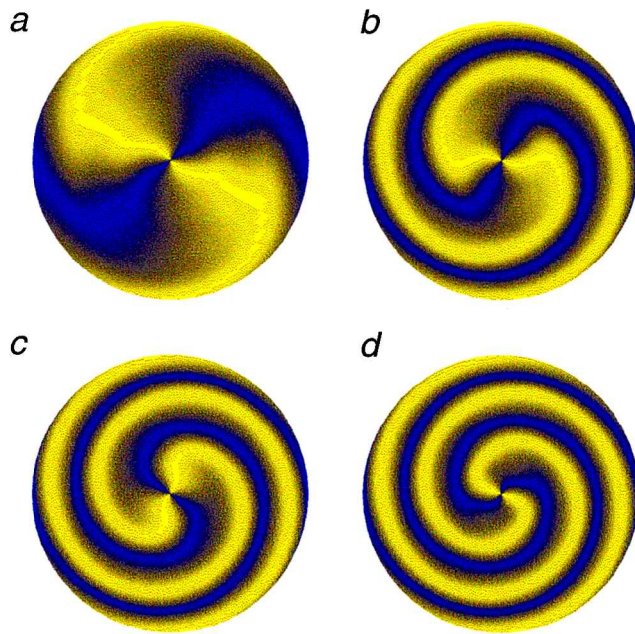


Figure 5. Colour plots of the director orientation in the sample for $\Omega=2\Omega_c$, and Ω_c , Ω_K as in figure 2: (a) $t=40 \text{ s}$, (b) $t=200 \text{ s}$, (c) $t=300 \text{ s}$, (d) $t=500 \text{ s}$.

spinning velocity and Leslie's critical velocity; (ii) a complex pattern of director orientations occurs for low and intermediate spinning velocities, roughly between half and twice Leslie's critical velocity Ω_c , with areas of parallel and perpendicular alignment to the magnetic field which alternate along both the angular and the

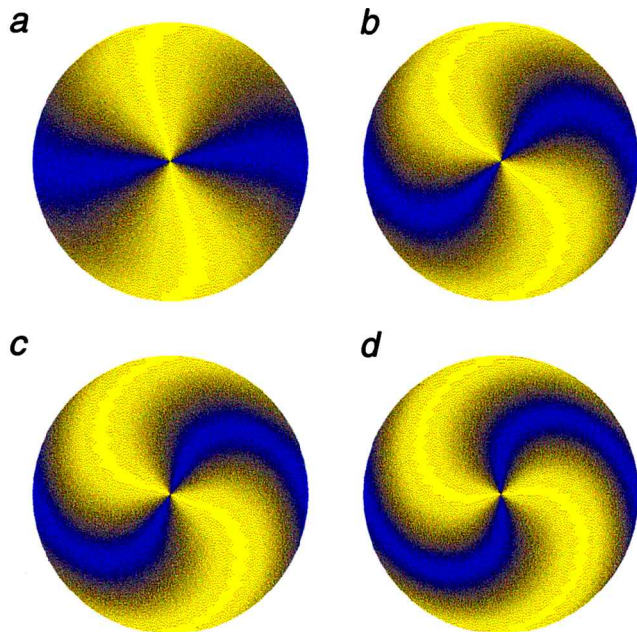


Figure 6. Colour plots of the director orientation in the sample for $\Omega = 10\Omega_c$, and Ω_c , Ω_K as in figure 2: (a) $t = 40$ s, (b) $t = 200$ s, (c) $t = 300$ s, (d) $t = 500$ s.

radial coordinate; (iii) the stationary solution is closer to θ for increasing Ω , in accordance with the obvious observation that for high rotation speed both elastic and magnetic contributions become perturbational terms and the dominant stationary solution is given by the spinning term only; (iv) transient phenomena can be relatively long lived and they can persist for times comparable to the inverse of Leslie's critical velocity.

6. Concluding remarks

The objective of this work has been to show that the constitutive equations of a nematic liquid crystal sample, subjected to a constant spinning motion and a magnetic field, can be numerically solved when the full spatial dependence is taken into account. A reasonably complex partial differential equation for the director orientation is recovered by imposing four conditions.

- (1) Confinement of the spatial dependence to a plane.
- (2) Choice of the simplest possible velocity profile.
- (3) Neglect of inertial terms.
- (4) Assumption of the spherical approximation.

The complete time evolution equation is easily written in spatial polar coordinates θ , x and boundary and initial conditions can be written clearly for simple cases. The numerical treatment of the resulting problem can be based on a combination of a Fourier expansion in θ and in an expansion in terms of Bessel functions in x , combined with a recursive procedure for determining the exact time dependence. Preliminary calculations

reported here show that complex patterns arise, depending on the chosen values of the spinning velocity, intensity of magnetic field and elastic constant, and that transient behaviours always give rise to a stationary solution.

A comment is certainly due concerning the physical reliability of some of our assumptions and choices. Basically, in this preliminary work our main concern was to start by considering the spatial dependence of director orientation in a spinning nematic sample, in an attempt to go beyond the standard treatment, and to present the reader with a clear methodology to do this. To this purpose, a drastic simplification has been intentionally sought by limiting our treatment to planar geometries, neglecting time dependent velocity profiles and using very simple boundary and initial conditions (radial alignment at the walls at all times, and throughout the whole sample at $t=0$). With these choices, the resulting final equations are simple enough to be solved quickly by a straightforward computational procedure. The price to be paid is of course a certain departure from the description of a realistic physical system. For instance, initial conditions in a real sample, at least in the presence of a magnetic field, should be taken rather as an alignment of the director with the field in the bulk of the sample. This would require more complicated, although still straightforward to calculate, initial conditions for the coefficients A_{mn} . Only for the sake of clarity has the simplest assumption of perfect radial alignment been made.

A number of extensions of the treatment presented in this work are possible, corresponding to lifting some or all of the approximations used to recover equation (35), and making the description closer to the full equations of nematodynamics. Conditions (3) and (4), related to inertial terms and elastic constants, can be eliminated easily, at the limited cost of a more complicated algebraic description. More significant are conditions (1) and (2). Extension of our treatment to three dimensions, inclusion of backflow effects in terms of time dependent velocity profiles, and choice of realistic initial conditions are probably the most relevant ingredients in describing actual experimental situations, since it should be possible to consider explicitly the formation of convection fluxes along the third dimension and to accommodate more realistic boundary conditions (e.g. with a parallel alignment to the cylinder internal walls) and initial conditions (e.g. with an initial alignment of the sample almost parallel to the magnetic field). Work is currently near completion which attempts to answer at least partially some of these issues [14]. We expect that the existence of long lived transient patterns and of a stationary solution should be confirmed by a 3-D analysis, although the detailed description of patterns in the distribution of the director orientation should be different.

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Appendix

Explicit form of function \mathcal{K}

In the case under consideration, W and \mathcal{K} can be written explicitly as:

$$W = \frac{1}{2}K(n_{1,1}^2 + n_{1,2}^2 + n_{2,1}^2 + n_{2,2}^2) \quad (\text{A1})$$

$$\mathcal{K} = n_2\pi_{k1,k} - n_1\pi_{k2,k}. \quad (\text{A2})$$

It is straightforward to show that:

$$\pi_{ki,k} = K\hat{\nabla}^2 n_i. \quad (\text{A3})$$

In Cartesian space coordinates it is simple to evaluate the effect of the Laplacian over n_i :

$$\frac{\partial^2 n_1}{\partial r_1^2} = -n_1 \left(\frac{\partial \phi}{\partial r_1} \right)^2 - n_2 \frac{\partial^2 \phi}{\partial r_1^2} \quad (\text{A4})$$

$$\frac{\partial^2 n_1}{\partial r_2^2} = -n_1 \left(\frac{\partial \phi}{\partial r_2} \right)^2 - n_2 \frac{\partial^2 \phi}{\partial r_2^2} \quad (\text{A5})$$

$$\frac{\partial^2 n_2}{\partial r_1^2} = -n_2 \left(\frac{\partial \phi}{\partial r_1} \right)^2 + n_1 \frac{\partial^2 \phi}{\partial r_1^2} \quad (\text{A6})$$

$$\frac{\partial^2 n_2}{\partial r_2^2} = -n_2 \left(\frac{\partial \phi}{\partial r_2} \right)^2 - n_1 \frac{\partial^2 \phi}{\partial r_2^2}. \quad (\text{A7})$$

Substituting in equation (A2) one gets:

$$\mathcal{K} = -K \left(\frac{\partial^2 \phi}{\partial r_1^2} + \frac{\partial^2 \phi}{\partial r_2^2} \right) \quad (\text{A8})$$

and in polar coordinates:

$$\mathcal{K} = -K \left(\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \phi}{\partial \theta^2} \right). \quad (\text{A9})$$

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