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Thermal instabilities in nematic liquid crystals

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Abstract. This paper employs continuum theory to investigate the onset of a certain type of thermal instability when a sample of nematic liquid crystal confined between two horizontal flat plates is in the presence of a vertical temperature gradient. Two particularly simple experimental situations are examined, in one a parallel orientation is obtained at the plates and in the other the boundary orientation is perpendicular to the plates. Using a Fourier series method, we derive an expression for determining the critical temperature gradient at which instability sets in. In both cases, the analysis presented here allows for the presence of an applied magnetic field.

1. Introduction

In recent papers Dubois-Violette (1974) and Currie (1973) examine the occurrence of cellular thermal instabilities in a sample of nematic liquid crystal confined between two horizontal, infinite flat plates when subjected to a vertical temperature gradient. Two simple experimental situations of particular interest are considered, the initial orientation of the molecules being everywhere parallel to the bounding plates in one and everywhere perpendicular in the other. Assuming the principle of exchange of instabilities, both authors demonstrate that the initial equilibrium configurations become unstable when the temperature gradient reaches some critical value. Furthermore, they show that the value and sign of this gradient threshold depend upon the initial orientation.

After linearizing the field equations about the equilibrium state, Dubois-Violette (1974) uses 'an iterative procedure' on a computer to obtain the appropriate gradient thresholds for MBBA. The numerical results presented are found to be in good agreement with the experimental observations of Guyon and Pieranski (1972), Dubois-Violette *et al* (1973) and Pieranski *et al* (1973). However since no attempt is made to find an analytic solution to the problem, it must be noted that the results given are only pertinent to the one material MBBA. On the other hand, Currie (1973) makes various rough approximations concerning the magnitude of certain material parameters, and then employs the variational methods described by Chandrasekhar (1961) to find estimates for the gradient thresholds of P-azoxyanisole. Obviously such a calculation can only be expected to yield qualitative results at best.

For reasons already mentioned, it is apparent that the results obtained by Dubois-Violette (1974) and Currie (1973) are not particularly helpful in determining the exact value of the threshold gradient for every nematic material. The purpose of this paper is to present a method of solution which overcomes certain limitations encountered in those adopted by the aforementioned authors. Employing a Fourier series method used by Jeffreys (1928) to investigate the corresponding problem for a Newtonian fluid, the present paper obtains an exact expression for determining the threshold gradient of any nematic liquid crystal sample in either of the two particular experimental situations described above. It is then demonstrated that this expression provides an 'almost analytic' solution to the problem. In addition, the analysis presented here allows for the presence of an applied magnetic field whereas the analyses of Dubois-Violette (1974) and Currie (1973) do not.

2. Basic equations

In this paper we assume that the equations governing the behaviour of an incompressible nematic liquid crystal are those proposed by Leslie (1968a, b, 1969). In Cartesian tensor notation, they have the form

$$v_{i,i}=0 \tag{2.1}$$

$$d_i d_i = 1 \tag{2.2}$$

$$\rho\dot{v}_i = -p_{,i} - \left(\frac{\partial W}{\partial d_{k,j}} d_{k,i}\right)_{,j} + \hat{\sigma}_{ij,j} + F_i \tag{2.3}$$

$$\rho_1 \ddot{d}_i = \gamma d_i + \left(\frac{\partial W}{\partial d_{i,j}}\right)_{,j} - \frac{\partial W}{\partial d_i} + \hat{g}_i + G_i \tag{2.4}$$

$$\rho T\dot{S} = \rho r - q_{i,i} + \hat{\sigma}_{ij}A_{ij} - \hat{g}_i N_i, \qquad \rho S = -\frac{\partial W}{\partial T} \tag{2.5}$$

$$2W = 2W_0 + \alpha_2 d_{i,j}d_{i,j} + (\alpha_1 - \alpha_2 - \alpha_4) d_{i,i}d_{j,j} + \alpha_4 d_{i,j}d_{j,i} + (\alpha_3 - \alpha_2) d_i d_j d_{k,i} d_{k,j} \tag{2.6}$$

$$\hat{\sigma}_{ij} = \mu_1 d_k d_p A_{kp} d_i d_j + \mu_2 d_j N_i + \mu_3 d_i N_j + \mu_4 A_{ij} + \mu_5 d_j d_k A_{ki} + \mu_6 d_i d_k A_{kj} \tag{2.7}$$

$$\hat{g}_i = \lambda_1 N_i + \lambda_2 d_j A_{ji} \tag{2.8}$$

$$q_i = -\kappa_1 T_{,i} - \kappa_2 d_i d_k T_{,k} \tag{2.9}$$

$$2N_i = 2\dot{d}_i + (v_{k,i} - v_{i,k}) d_k \tag{2.10}$$

$$2A_{ij} = v_{i,j} + v_{j,i}. \tag{2.11}$$

Here $\boldsymbol{v}$ is the velocity vector, $\boldsymbol{d}$ is a unit vector specifying the preferred direction of the molecular axis, and superposed dots denote material derivatives. Associated with the constraints of incompressibility and (2.2) are two arbitrary functions, p the pressure and γ the director tension. $\boldsymbol{F}$ and $\boldsymbol{G}$ represent the effect of external forces, $\boldsymbol{F}$ being a body force per unit volume and $\boldsymbol{d} \wedge \boldsymbol{G}$ being a body couple per unit volume. r is the heat supply function per unit mass per unit time and will be taken to be zero throughout this paper. Further, ρ is the density, ρ_1 is a positive inertial coefficient, T is the temperature, and W is the form of the stored free energy per unit volume proposed by Frank (1958). The material functions ρ, ρ_1, W_0, κ_1, κ_2, α_1, α_2, α_3, α_4, μ_1, μ_2, μ_3, μ_4, μ_5, μ_6, λ_1, λ_2 are dependent upon temperature alone and are related by

$$\lambda_1 = \mu_2 - \mu_3, \qquad \lambda_2 = \mu_5 - \mu_6. \tag{2.12}$$

3. Formulation of the problem

We examine the stability of a sample of nematic liquid crystal confined between two horizontal, infinite flat plates in the presence of a vertical temperature gradient. The upper plate situated at $z = h$ is held at a temperature T_2 and the lower plate situated at $z = 0$ at a temperature T_1. Two particular boundary value problems are considered. In one a parallel orientation is obtained at the plates while in the other the boundary orientation is perpendicular.

Assuming that the external body forces arise from an applied uniform magnetic field $\boldsymbol{H}$ and gravity and accepting Ericksen's assumptions (1962):

$$\boldsymbol{F} = -\rho g \boldsymbol{k}, \qquad \boldsymbol{G} = \chi_a (\boldsymbol{H} \cdot \boldsymbol{d})\boldsymbol{H}, \qquad \operatorname{grad} T = \phi \boldsymbol{k}, \tag{3.1}$$

where g is the acceleration due to gravity, $\phi = \phi(z)$ is the vertical temperature gradient, χ_a is a constant coefficient denoting the anisotropic part of the magnetic susceptibility and $\boldsymbol{k}$ is the unit vector in the z direction. An obvious equilibrium solution is that in which $\boldsymbol{d}$ takes its boundary value throughout the material, provided either $\boldsymbol{H}$ is parallel to $\boldsymbol{d}$ or $\boldsymbol{H}$ is perpendicular to $\boldsymbol{d}$ and below the threshold value for a Frederiks transition (Leslie 1970). In the event that $\boldsymbol{H}$ is parallel to $\boldsymbol{d}$, the equilibrium state consisting of a zero velocity field, a constant director field $\boldsymbol{d}$, a temperature field T, a pressure field p and a constant director tension field $-\chi_a H^2$, where $H = \boldsymbol{H} \cdot \boldsymbol{d}$, is a possible configuration of the material. In the latter case the equilibrium state differs from that in the former in that there is now a zero director tension field.

To avoid undue repetition, it is assumed throughout the remainder of this paper that $\boldsymbol{H}$ is parallel to $\boldsymbol{d}$ unless stated otherwise. We now consider this equilibrium state to be disturbed by a small amplitude velocity field $\boldsymbol{v}$, associated with which is a director field $\boldsymbol{d}+\boldsymbol{n}$, a temperature field $T+s$, a pressure field $p+\bar{p}$ and a director tension field $-\chi_a H^2 + \bar{\gamma}$. In linearizing equations (2.1)–(2.5) about the equilibrium state, one adopts the usual Boussinesq approximation (1903) and ignores all variations of the material parameters with temperature except where associated with gravity. The linearized equations take the form

$$v_{i,i} = 0, \qquad d_i n_i = 0 \tag{3.2}$$

$$\rho \frac{\partial v_i}{\partial t} = -\rho' g k_i - \bar{p}_{,i} + A_{ijkm} v_{j,km} + B_{ijk} \frac{\partial n_{j,k}}{\partial t}, \qquad \rho' = \frac{\partial \rho}{\partial T} \tag{3.3}$$

$$\rho_1 \frac{\partial^2 n_i}{\partial t^2} = \bar{\gamma} d_i - \chi_a H^2 n_i + C_{ijkm} n_{j,km} + D_{ijk} v_{j,k} + \lambda_1 \frac{\partial n_i}{\partial t} \tag{3.4}$$

$$C \frac{\partial s}{\partial t} = \kappa_1 s_{,ii} + \kappa_2 d_j d_i s_{,ij} + \phi \kappa_2 (k_j d_i n_{j,i} + k_j d_j n_{i,i}), \qquad C = -T \frac{\partial^2 W_0}{\partial T^2} \tag{3.5}$$

where the coefficients A_{ijkm}, B_{ijk}, C_{ijkm} and D_{ijk} are given by Currie (1973, equation (3.7)). In equation (3.5) ϕ is a constant average temperature gradient defined by

$$\phi = (T_2 - T_1)/h. \tag{3.6}$$

Choosing Cartesian coordinate axes so that $\boldsymbol{d}$ is a unit vector in the positive x direction, we first examine the stability of a uniform parallel orientation with respect to disturbances of the form

$$\boldsymbol{n} = (0, 0, n) \exp(imx + wt), \qquad \boldsymbol{v} = (u, 0, v) \exp(imx + wt), \qquad \boldsymbol{s} = s \exp(imx + wt), \tag{3.7}$$

where n, u, v, s are functions of z alone. It follows that the appropriate boundary conditions to be applied at both $z=0$ and $z=h$ are

$$n=u=v=s=0. \tag{3.8}$$

For each value of the wavenumber m, one expects to find a critical value of ϕ, say $\phi_c(m)$, which is the value of ϕ with smallest modulus at which disturbances with this wavenumber become unstable. The value of $\phi_c(m)$ which has minimum modulus for all possible values of m is referred to as the critical temperature gradient or the gradient threshold of the sample. Since our aim is to obtain the critical values of ϕ for which (3.2)–(3.5) have non-trivial solutions for values of w with a positive real part in the neighbourhood of $w=0$, we follow Dubois-Violette (1974) and Currie (1973) in adopting the principle of exchange of instabilities. This principle asserts that the critical values are given when w is identically zero. Setting w equal to zero and making the change of variable

$$\tau=\pi z/h, \tag{3.9}$$

the elimination of $n, u, s, \bar{\gamma}$ and $\bar{p}$ from (3.2)–(3.5) yields an eighth-order linear differential equation for v as

$$(\mathrm{D}^4-\eta a^2\mathrm{D}^2+\eta_1 a^4)(\mathrm{D}^2-\alpha a^2)(\mathrm{D}^2-\kappa a^2)v=-R(\mathrm{D}^2+\lambda a^2)a^2 v, \tag{3.10}$$

where $\mathrm{D}\equiv \mathrm{d}/\mathrm{d}\tau$, $a=mh/\pi$ is a scaled non-dimensional wavenumber and

$$\eta=(2\mu_1+\eta_a+\eta_b)/\eta_a, \qquad \eta_1=\eta_b/\eta_a, \qquad \eta_a=\mu_4+\mu_3+\mu_6,$$
$$\eta_b=\mu_4+\mu_5-\mu_2, \qquad \alpha=\frac{\alpha_3}{\alpha_1}+\frac{\chi_a H^2h^2}{\alpha_1\pi^2a^2},$$
$$\kappa=\frac{(\kappa_1+\kappa_2)}{\kappa_1}, \qquad \lambda=\frac{\lambda_2-\lambda_1}{\lambda_2+\lambda_1}, \qquad R=-\frac{\rho' g\phi\kappa_2(\lambda_2+\lambda_1)h^4}{\alpha_1\kappa_1\pi^4\eta_a}. \tag{3.11}$$

The relevant boundary conditions to be applied at both $\tau=0$ and $\tau=\pi$ are readily derived from (3.8) together with (3.2)–(3.5) and take the form

$$v=\mathrm{D}v=(\mathrm{D}^4-\eta a^2\mathrm{D}^2)v=[\mathrm{D}^6-(\kappa+\eta)a^2\mathrm{D}^4+(\eta_1+\eta\kappa)a^4\mathrm{D}^2]v=0. \tag{3.12}$$

The stability of a uniform perpendicular orientation with respect to disturbances of the form

$$\boldsymbol{n}=(n,0,0)\exp(\mathrm{i}mx+wt), \qquad \boldsymbol{v}=(u,0,v)\exp(\mathrm{i}mx+wt), \qquad \boldsymbol{s}=s\exp(\mathrm{i}mx+wt), \tag{3.13}$$

may be examined in a similar manner. Proceeding as above, one obtains the equation for v as

$$(\mathrm{D}^4-\eta' a^2\mathrm{D}^2+\eta_1' a^4)(\mathrm{D}^2-\alpha' a^2)(\mathrm{D}^2-\kappa' a^2)v=-R'(\mathrm{D}^2+\lambda' a^2)a^2 v \tag{3.14}$$

with boundary conditions at $\tau=0$ and $\tau=\pi$ given by

$$v=\mathrm{D}v=(\mathrm{D}^4-\eta' a^2\mathrm{D}^2)v=[\mathrm{D}^6-(\eta'+\kappa')a^2\mathrm{D}^4+(\eta_1'+\eta'\kappa')a^4\mathrm{D}^2]v=0, \tag{3.15}$$

where

$$\eta'=\frac{\eta}{\eta_1}, \qquad \eta_1'=\frac{1}{\eta_1}, \qquad \alpha'=\frac{\alpha_1}{\alpha_3}+\frac{\chi_a H^2h^2}{\alpha_3\pi^2a^2},$$
$$\kappa'=\frac{1}{\kappa}, \qquad \lambda'=\frac{1}{\lambda}, \qquad R'=-\frac{\rho' g\phi\kappa_2(\lambda_2-\lambda_1)h^4}{\alpha_3(\kappa_1+\kappa_2)\pi^4\eta_b}. \tag{3.16}$$

Comparing (3.14) and (3.15) with (3.10) and (3.12), it is apparent that the solution of the former set of equations may be obtained from the solution of the latter by replacing η, η_1, α, κ, λ and R with their dashed counterparts. In addition, it is obvious from (3.10), (3.11) and (3.14), (3.16) that ϕh^4 is a universal function of a (Dubois-Violette 1974) only when there is no applied magnetic field. Finally, in the event that $\boldsymbol{H}$ is perpendicular to $\boldsymbol{d}$, lies in the xz plane and is below its appropriate critical value for a Frederiks transition (Leslie 1970), one obtains exactly the same equations as given above but with

$$\alpha=\frac{\alpha_3}{\alpha_1}-\frac{\chi_a H^2h^2}{\alpha_1\pi^2a^2} \quad \text{and} \quad \alpha'=\frac{\alpha_1}{\alpha_3}-\frac{\chi_a H^2h^2}{\alpha_3\pi^2a^2}. \tag{3.17}$$

4. Solution of the problem

We first examine the conditions under which there is a non-trivial solution of (3.10) subject to the homogeneous boundary conditions (3.12). Assuming that

$$D^8 v=\sum_{r=1}^{\infty} A_r \sin r\tau, \tag{4.1}$$

where the A_r are the constant coefficients of the sine series, repeated integration yields

$$v=\sum_{r=0}^{7}\frac{B_r t^r}{r!}+\sum_{r=1}^{\infty}\frac{A_r\sin r\tau}{r^8}\equiv P(t)+\sum_{r=1}^{\infty}\frac{A_r\sin r\tau}{r^8}, \tag{4.2}$$

where the B_r are constants of integration and we set

$$t=\pi/2-\tau \tag{4.3}$$

for convenience. Employing (4.2) in (3.10), one obtains

$$\sum_{r=1}^{\infty}\mu_r \sin r\tau=-(D_t^8-Q_1D_t^6+Q_2D_t^4-Q_3D_t^2+Q_4)P(t)\equiv L(t), \tag{4.4}$$

where $D_t \equiv d/dt$,

$$\mu_r=(1+Q_1r^{-2}+Q_2r^{-4}+Q_3r^{-6}+Q_4r^{-8})A_r \tag{4.5}$$

and

$$Q_1=(\alpha+\kappa+\eta)a^2, \qquad Q_2=(\alpha\kappa+\eta(\alpha+\kappa)+\eta_1)a^4,$$
$$Q_3=(\eta\eta_1\kappa+\eta_1(\alpha+\kappa))a^6-Ra^6, \qquad Q_4=\eta_1\alpha\kappa a^8+R\lambda a^4. \tag{4.6}$$

From (4.4), it is readily seen that

$$\mu_r=\frac{2}{\pi}\int_0^{\pi}L(t)\sin r\tau\,d\tau. \tag{4.7}$$

Using (4.4) to substitute for $L(t)$ in (4.7) and then employing the identity

$$\int_0^{\pi}t^n\sin r\tau\,d\tau=\begin{cases}\dfrac{2}{r}\left(\dfrac{\pi}{2}\right)^n\left[1-\dfrac{n(n-1)}{r^2}\left(\dfrac{2}{\pi}\right)^2+\dfrac{n(n-1)(n-2)(n-3)}{r^4}\left(\dfrac{2}{\pi}\right)^4-\dots\right], \\ \qquad n+r=2s+1, \\ 0, \qquad n+r=2s,\end{cases} \tag{4.8}$$

where s is an integer, we obtain

$$\frac{\pi r\mu_r}{4}=(Q_1B_6-Q_2B_4+Q_3B_2-Q_4B_0)+\frac{1}{2!}(-Q_2B_6+Q_3B_4-Q_4B_2)\left[\left(\frac{\pi}{2}\right)^2-\frac{2}{r^2}\right]$$
$$+\frac{1}{4!}(Q_3B_6-Q_4B_4)\left[\left(\frac{\pi}{2}\right)^4-\frac{12}{r^2}\left(\frac{\pi}{2}\right)^2+\frac{24}{r^4}\right]$$
$$-\frac{Q_4B_6}{6!}\left[\left(\frac{\pi}{2}\right)^6-\frac{30}{r^2}\left(\frac{\pi}{2}\right)^4+\frac{360}{r^4}\left(\frac{\pi}{2}\right)^2-\frac{6!}{r^6}\right] \tag{4.9}$$

when r is odd, and

$$\frac{\pi r\mu_r}{4}=(Q_1B_7-Q_2B_5+Q_3B_3-Q_4B_1)\frac{\pi}{2}+\frac{1}{3!}(-Q_2B_7+Q_3B_5-Q_4B_3)\left[\left(\frac{\pi}{2}\right)^3-\frac{6}{r^2}\frac{\pi}{2}\right]$$
$$+\frac{1}{5!}(Q_3B_7-Q_4B_5)\left[\left(\frac{\pi}{2}\right)^5-\frac{20}{r^2}\left(\frac{\pi}{2}\right)^3+\frac{5!}{r^4}\frac{\pi}{2}\right]$$
$$-\frac{Q_4B_7}{7!}\left[\left(\frac{\pi}{2}\right)^7-\frac{42}{r^2}\left(\frac{\pi}{2}\right)^5+\frac{840}{r^4}\left(\frac{\pi}{2}\right)^3-\frac{7!}{r^6}\frac{\pi}{2}\right] \tag{4.10}$$

when r is even. These expressions together with (4.2) and (4.5) give the formal solution of (3.10). From (4.9), (4.10) and (3.12), it is obvious that the even and odd B_r enter the solution entirely separately and hence the possible solutions split into two distinct sets, one symmetrical and the other antisymmetrical about the plane $t=0$. Utilizing the boundary conditions, one should now proceed to find the threshold gradients for each type of solution. However, in similar problems, it is common to find that the least stable mode is a symmetrical one. Hence, we only present the analysis for the fcrmer type of solution. In the appendix, it is demonstrated that this is in fact the correct choice to make in this case.

For a symmetrical solution, (4.10) implies that all the μ_{2n} and hence all the A_{2n} are identically zero. Employing (4.9) and (4.5) in (4.2) and then substituting the resulting expression for v into (3.12), one obtains four simultaneous equations for B_0, B_2, B_4 and B_6. After solving this set of linear equations for the B_{2i} and then using the resulting expressions in (4.9), it is found that

$$\frac{\pi(2r+1)\mu_{2r+1}}{4}=N(2r+1)\sum_{s=0}^{\infty}\frac{A_{2s+1}}{(2s+1)^7}, \tag{4.11}$$

where

$$N(2r+1)=(Q_1P_5-Q_2P_6+Q_3P_7-Q_4P_8)+\frac{1}{2!}(-Q_2P_5+Q_3P_6-Q_4P_7)$$
$$\times\left[\left(\frac{\pi}{2}\right)^2-\frac{2}{(2r+1)^2}\right]+\frac{1}{4!}(Q_3P_5-Q_4P_6)\left[\left(\frac{\pi}{2}\right)^4-\frac{12}{(2r+1)^2}\left(\frac{\pi}{2}\right)^2\right.$$
$$\left.+\frac{24}{(2r+1)^4}\right]-\frac{Q_4P_5}{6!}\left[\left(\frac{\pi}{2}\right)^6-\frac{30}{(2r+1)^2}\left(\frac{\pi}{2}\right)^4+\frac{360}{(2r+1)^4}\left(\frac{\pi}{2}\right)^2-\frac{6!}{(2r+1)^6}\right]$$

with

$$P_5=\frac{P_3\eta a^2-P_1a^4(\eta\kappa+\eta_1)}{P_2P_3-P_1P_4},\qquad P_6=\frac{\eta a^2-P_2P_5}{P_1},$$

$$P_7=\frac{2}{\pi}\left[1-\frac{P_6}{3!}\left(\frac{\pi}{2}\right)^3-\frac{P_5}{5!}\left(\frac{\pi}{2}\right)^5\right],\qquad P_8=-\left[\frac{P_7}{2!}\left(\frac{\pi}{2}\right)^2+\frac{P_6}{4!}\left(\frac{\pi}{2}\right)^4+\frac{P_5}{6!}\left(\frac{\pi}{2}\right)^6\right]$$

and

$$P_1=\frac{\pi}{2}-\frac{\eta a^2}{3}\left(\frac{\pi}{2}\right)^3,\qquad P_2=\frac{1}{2}\left(\frac{\pi}{2}\right)^3-\frac{\eta a^2}{30}\left(\frac{\pi}{2}\right)^5,$$

$$P_3=(\eta+\kappa)a^2\frac{\pi}{2}-\frac{(\eta_1+\eta\kappa)}{3}a^4\left(\frac{\pi}{2}\right)^3,$$

$$P_4=-\frac{\pi}{2}+\frac{(\eta+\kappa)}{2}a^2\left(\frac{\pi}{2}\right)^3-\frac{(\eta_1+\eta\kappa)}{30}a^4\left(\frac{\pi}{2}\right)^5.$$

After multiplying both sides of (4.11) by $[(2r+1)^8+Q_1(2r+1)^6+Q_2(2r+1)^4+Q_3(2r+1)^2+Q_4]^{-1}$ and then performing the summation over all integers $r\geqslant 0$, we finally use the relation (4.5) to obtain the consistency condition

$$\sum_{r=0}^{\infty}\frac{N(2r+1)}{[(2r+1)^8+Q_1(2r+1)^6+Q_2(2r+1)^4+Q_3(2r+1)^2+Q_4]}=\frac{\pi}{4}. \tag{4.12}$$

As noted in § 3, an examination of the solution of (3.14) subject to (3.15) leads to the same consistency condition (4.12) but with η, η_1, α, κ, λ and R replaced by their dashed counterparts.

5. Some numerical results

In the event that there are values of the parameters η, η_1, α, κ, λ, a and R for which the consistency condition (4.12) is satisfied, the problem described by equations (3.10) and (3.12) has a non-trivial solution. Physically this solution represents an undamped, or neutrally stable, disturbance with wavenumber specified by the dimensionless parameter a. Employing empirical data to prescribe η, η_1, α, κ and λ, we treat (4.12) as an equation in a and R and rewrite it symbolically as

$$f(a,R)=0. \tag{5.1}$$

For a fixed value of a, we compute $f(a,R)$ at $R=0,\pm R_1,\pm R_2,\ldots$, where $\{R_i\}$ is an increasing sequence of discrete values of R, and continue the process until $f(a,R)$ passes through a zero. After finding the approximate location of that root of (5.1) with the smallest value of $|R|$, an accurate value is obtained iteratively using the rule of false position. The position of this root is then used to initiate the search procedure for a neighbouring value of a, and the root-finding process is repeated for various values of a so as to obtain the solution locus in the (a,R) plane.

Employing available experimental data for MBBA, we adopt the Parodi relation (1970) and take the values for the viscosities as given by Gähwiller† (1971). Also we

† The values for the viscosities given by Gähwiller clearly do not satisfy the Parodi relation (1970). In a private communication Gähwiller has informed us that the value given for $(\mu_3+\mu_4+\mu_6)/2$ is in error and should be 24·8 centipoise. With this exception, we have employed the same set of material parameters as Dubois-Violette (1974).

consider the thermal conductivities and the elastic constants to have the values as stated by Dubois-Violette (1974), these being based on experimental observations of Vilanove *et al* (1974) and Haller (1972). In the event that there is no applied magnetic field present, the parameters η, η_1, α, κ and λ then take the values 5·435, 4·17, 1·167, 1·656 and 64·6 respectively, when the initial orientation is horizontal, and 1·302, 0·2396, 0·86, 0·604 and 0·0155, respectively, when the initial orientation is vertical. The solution locus, or neutral stability curve, for the former problem is represented by the full curve in figure 1. The broken curve in figure 1 represents an approximation to the neutral stability curve obtained by using only the first term of the series in the evaluation of $f(a, R)$. The minimum point on the approximate curve which is the point of physical interest, deviates from the true minimum by approximately 2% in both the parameters a and R. Since this error is well within the errors arising from inaccuracies in the empirical data, one may conclude that the infinite series (4.12) may safely be replaced by its first term. Figure 2 shows the neutral stability curve when the initial orientation is vertical, and in this case the approximate and true neutral stability curves are found to be indistinguishable.

On any line of constant a in the (a, R) plane, a value of R giving rise to a point outside the parabolic-type neutral stability curve ensures that any disturbance with wavenumber $a\pi/h$ is damped as time progresses. A value of R which yields a point in the inner region permits the existence of unstable disturbances with this wavenumber. The value of R at the minimum point on the curve gives a measure of the dimensionless temperature gradient which may be imposed before any unstable disturbances, of the form considered in this paper, exist and is therefore a quantity of physical interest.

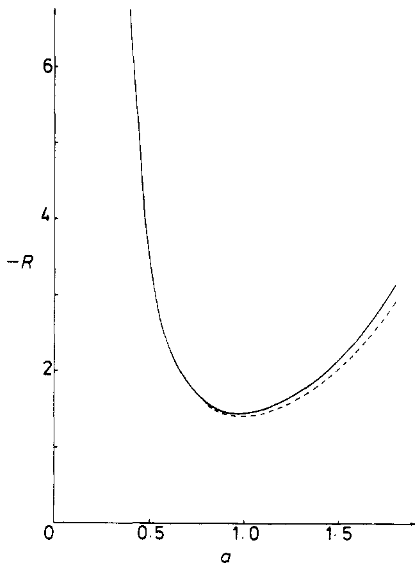

Figure 1. Instability curve for MBBA (having material parameters as specified in § 5), without magnetic field: parallel orientation. The temperature gradient stability parameter $-R$ defined in equation (3.11) is plotted against the scaled dimensionless wavenumber $a = mh/\pi$. The broken curve is the approximation obtained by using only the first term of the series in equation (4.12).

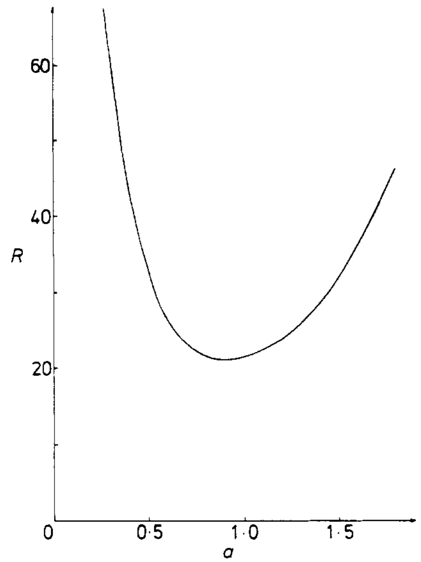

Figure 2. Instability curve for MBBA (having material parameters as specified in § 5), without magnetic field: perpendicular orientation. The temperature gradient stability parameter R' defined in equation (3.16) is plotted against the scaled dimensionless wavenumber $a = mh/\pi$. The approximation obtained by using only the first term of the series in equation (4.12) is indistinguishable from the exact result in this case.

Taking $\rho' g = -1 \text{ g cm}^{-2} \text{ s}^{-2} {}^\circ\text{C}^{-1}$, we find that the horizontal orientation becomes unstable when $-\phi h^4$ exceeds $2{\cdot}7 \times 10^{-3} \text{ cm}^3 {}^\circ\text{C}$, and that the vertical orientation becomes unstable when ϕh^4 exceeds $4{\cdot}9 \times 10^{-3} \text{ cm}^3 {}^\circ\text{C}$. For a sample 1 mm in thickness, the onset of instability is found to occur when

$$T_2 - T_1 = -2{\cdot}7 \,{}^\circ\text{C} \qquad \text{and} \qquad mh/2 = 1{\cdot}5$$

in the former case, and when

$$T_2 - T_1 = 4{\cdot}9 \,{}^\circ\text{C} \qquad \text{and} \qquad mh/2 = 1{\cdot}4$$

in the latter. These numerical results seem to confirm the theoretical predictions of Dubois-Violette (1974)† and appear to agree reasonably well with the experimental observations of Guyon and Pieranski (1972), Dubois-Violette *et al* (1973) and Pieranski *et al* (1973).

Recent experimental evidence (Cladis and Torza 1975) suggests that μ_3 becomes large and positive as the nematic–smectic transition temperature is approached. Keeping all other experimental measurements of Gähwiller (1971) fixed, we have examined the behaviour of the threshold as $-\mu_3/\mu_2$ increases up to 1. For a given sample thickness, it is found that the threshold gradient magnitude decreases when the initial orientation is horizontal but increases when it is vertical. However, we must admit that the Boussinesq approximation (1903) may become invalid near the transition temperature.

† The slight variation between our results and those of Dubois-Violette (1974) may be accounted for by the fact that we have used the corrected value of $\mu_3 + \mu_4 + \mu_6$.

6. Discussion

The above results are in agreement with the qualitative predictions of Dubois-Violette (1974) and Currie (1973). In addition the numerical results confirm the theoretical calculations of Dubois-Violette (1974) and are in good agreement with the experimental observations of Guyon and Pieranski (1972), Dubois-Violette *et al* (1973) and Pieranski *et al* (1973). However for the experimentalist wishing to compare theory and experiment, we believe that the present method of solution is an improvement upon those employed before. The method used by Currie (1973) suffers from the obvious disadvantages that it is inaccurate and not readily applicable to every nematic material. On the other hand the method adopted by Dubois-Violette (1974), although exact, requires one to solve (3.10) subject to (3.12) numerically for each new set of material parameters. An examination of such a numerical method of solution as outlined in the following appendix indicates the amount of computation involved. Employing (4.12), a comparatively trivial computation yields the threshold gradient for any nematic liquid crystal. In fact sufficiently accurate results may be obtained by using only the first term of the infinite series in (4.12), thus eliminating the necessity of a computer. In addition, we note that (4.12) allows for the presence of a magnetic field applied parallel or perpendicular to the initial director orientation.

In closing it must be admitted that only a certain class of infinitesimal disturbances has been considered. Hence one is unable to say anything concerning stability with respect to arbitrary infinitesimal disturbances below the threshold gradient predicted by (4.12). With this in mind, we suggest that further experimentation using different nematic materials over a variety of temperature ranges would serve as a useful check on the predictions of the continuum theory presented in this paper.

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Appendix

Scott (1973) has described the use of a matrix Ricatti transformation for the computation of eigenvalues of systems of linear ordinary differential equations of the form

$$\frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}\tau}=A\boldsymbol{U}+B\boldsymbol{V}, \qquad \frac{-\mathrm{d}\boldsymbol{V}}{\mathrm{d}\tau}=C\boldsymbol{U}+D\boldsymbol{V}, \tag{A.1}$$

where $\boldsymbol{U}$ and $\boldsymbol{V}$ are n-vectors and A, B, C and D are $n\times n$ matrices which depend on the independent variable τ and on some scalar parameter μ. Scott (1973) has used the method to find eigenvalues of (A.1) under the boundary conditions

$$\boldsymbol{U}(0)=\boldsymbol{0}, \qquad \boldsymbol{U}(x)=\boldsymbol{0}, \tag{A.2}$$

where $\boldsymbol{U}(\tau)$ denotes the value of $\boldsymbol{U}$ at the point τ. The Ricatti approach involves the related problem of calculating the characteristic lengths of (A.1) subject to (A.2), which, for a specified μ, are the positive values $\tau=x$ for which non-trivial solutions exist. The method is based on the introduction of the $n \times n$ matrix $T(\tau)$ via the Ricatti transformation

$$\boldsymbol{U}(\tau) = T(\tau)\boldsymbol{V}(\tau). \tag{A.3}$$

It may be shown that $T(\tau)$ satisfies the matrix Ricatti equation

$$T'(\tau) = B + AT(\tau) + T(\tau)D + T(\tau)CT(\tau), \tag{A.4}$$

where the prime denotes $\mathrm{d}/\mathrm{d}\tau$, and that (A.4) may be integrated using the simple initial condition

$$T(0) = \mathbf{0}. \tag{A.5}$$

Characteristic lengths are those positive values of x for which the condition

$$\det|T(x)| = 0 \tag{A.6}$$

is satisfied. If equation (A.4) is integrated numerically using condition (A.5), singularities of $\det|R(\tau)|$ may be encountered before the first characteristic length is reached and those are traversed by transferring to the system associated with $S(\tau) = T^{-1}(\tau)$, which is

$$-S'(\tau) = C + S(\tau)A + DS(\tau) + S(\tau)BS(\tau). \tag{A.7}$$

If equation (3.10) is written in terms of the independent variable $w = a\tau$ it becomes

$$(\mathrm{D}^4 - \eta\mathrm{D}^2 + \eta_1)(\mathrm{D}^2 - \alpha)(\mathrm{D}^2 - \kappa)v = -R(\mathrm{D}^2 + \lambda)v, \tag{A.8}$$

where D now denotes $\mathrm{d}/\mathrm{d}w$ and $\mu = R/a^4$. The boundary conditions

$$v = \mathrm{D}v = (\mathrm{D}^4 - \eta\mathrm{D}^2)v = [\mathrm{D}^6 - (\eta + \kappa)\mathrm{D}^4 + (\eta_1 + \eta\kappa)\mathrm{D}^2]v = 0 \tag{A.9}$$

hold at $w = 0$ and they also determine characteristic lengths. (A.8) and (A.9) may be written in the format of (A.1) and (A.2) if we let $\boldsymbol{U}$ be the column vector $[v, \mathrm{D}v, (\mathrm{D}^4 - \eta\mathrm{D}^2)v, (\mathrm{D}^6 - (\eta + \kappa)\mathrm{D}^4 + (\eta_1 + \eta\kappa)\mathrm{D}^2)v]$ and choose $\boldsymbol{V}$ conveniently. Using the empirical values for η, η_1, α, κ and λ as described in § 5, we obtained the first characteristic length x of the resulting system in $\boldsymbol{U}$ and $\boldsymbol{V}$ corresponding to various values of the parameter μ. If x_i is the first characteristic length associated with the parametric value $\lambda = \lambda_i$ then the first eigenvalue of (A.8) is λ_i with boundary conditions (A.9) imposed at $w = 0$ and $w = x_i$. The original equation (3.10) has a non-trivial solution with boundary conditions at $\tau = 0$ and $\tau = \pi$ for values $a_i = x_i/\pi$ and $R_i = \mu_i a_i^4$ of the parameters a and R. Sets of values (x_i, λ_i) enabled us to plot the neutral stability curve in the (a, R) plane.

Table 1. Parallel orientation problem: Ricatti results for neutral stability points.

μ	x	$a = x/\pi$	$R = \mu a^4$
−1·45	3·1501	1·003	−1·4657
−1·50	3·1226	0·994	−1·4637
−1·55	3·0965	0·986	−1·4626
−1·60	3·0716	0·978	−1·4620
−1·65	3·0479	0·970	−1·4619
−1·70	3·0253	0·963	−1·4620
−1·75	3·0036	0·956	−1·4623
−1·80	2·9829	0·949	−1·4630
−1·85	2·9630	0·943	−1·4642
−1·90	2·9439	0·937	−1·4652

For both problems considered the results obtained by the Ricatti approach coincided with those obtained by the Fourier method described in § 4. Characteristic lengths and associated points on the neutral stability curves are shown in tables 1 and 2 for the parallel and perpendicular orientation problems respectively. A point of interest is that the selection of the symmetric case in § 4 is now vindicated, since the Ricatti method obtains the least stable mode in evaluating the first characteristic length. The agreement between the different approaches shows that the symmetric mode is indeed the least stable.

Table 2. Perpendicular orientation problem: Ricatti results for neutral stability points.

μ	x	$a = x/\pi$	$R' = \mu a^4$
27·0	2·9608	0·942	21·301
28·0	2·9333	0·934	21·281
29·0	2·9072	0·925	21·267
29·5	2·8946	0·921	21·263
30·0	2·8823	0·917	21·259
30·5	2·8703	0·914	21·248
31·0	2·8586	0·910	21·249
31·5	2·8473	0·906	21·252
32·0	2·8361	0·903	21·258
33·0	2·8145	0·896	21·259

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