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A numerical investigation into thermal instabilities in homeotropic nematics heated from below

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This paper employs continuum theory to examine the onset of a particular type of cellular thermal instability in a sample of nematic liquid crystal confined between two infinite, horizontal flat plates when subjected to a vertical temperature gradient. We consider the case in which the anisotropic axis is initially uniformly aligned perpendicular to the plates. Using Chebyshev polynomials, accurate numerical solutions for the critical temperature gradient are obtained and the variation of this quantity with a uniform magnetic field applied vertically across the plates is investigated. In particular we obtain the value of the magnetic field at which the nature of the instability changes from an oscillatory type to a stationary one.

1. Introduction

The occurrence of thermal instabilities in a sample of nematic liquid crystal confined between two horizontal, infinite flat plates when subjected to a vertical temperature gradient has been the subject of several investigations in recent years. Dubois-Violette (1974), Currie (1973) and Barratt & Sloan (1976) analyse the onset of a stationary convective instability in two particular simple experimental situations. In one the anisotropic axis is initially uniformly aligned everywhere parallel to the plates (planar orientation) while in the other it is everywhere perpendicular to the plates (homeotropic orientation). Employing the continuum theory proposed by Ericksen (1961) and Leslie (1968*a*, *b*, 1969), the theoretical predictions of the above authors, for samples of thickness 1 or $\frac{1}{2}$ mm, are in good agreement with the experimental observations of Guyon & Pieranski (1972), Dubois-Violette, Guyon & Pieranski (1973) and Pieranski, Dubois-Violette & Guyon (1973*a*). In particular they found that a stationary-roll-type instability was possible at much lower thresholds than that required for isotropic liquids of similar properties, and in the case of a homeotropic configuration one must heat the upper plate.

An obvious question which poses itself is whether convection is possible when the lower plate is heated. In an attempt to answer this question, Lekkerkerker (1977, 1979) presents analyses which predict that an oscillatory convective instability is possible in this event. Guyon, Pieranski & Salan (1979) describe observations of just such an instability in samples of 5 mm thickness and they employ a simple one-dimensional model to analyse their results. For such comparatively thick samples, it appears necessary to apply a uniform magnetic field vertically across the plates so as to maintain the initial homeotropic alignment at the boundaries. Guyon *et al.* (1979) and Lekkerkerker (1979) examine the variation of the critical temperature gradient with magnetic

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field and predict the strength of magnetic field at which there is a transition from the oscillatory instability to a stationary one. Velarde & Zuniga (1979) have employed a rather crude Galerkin method to obtain approximate numerical solutions to this problem.

Since a very nice physical description and explanation of the mechanism which induces the oscillatory type of instability may be found in the papers by Lekkerkerker (1977, 1979) and Guyon *et al.* (1979), we do not dwell upon it here. The purpose of this paper is to present a detailed numerical investigation into the occurrence of both stationary and oscillatory convective instabilities in homeotropic configurations when a uniform magnetic field is applied parallel to the initial molecular orientation. We seek to obtain accurate numerical values for the critical temperature gradient at which instability occurs. To achieve this the governing equations are linearized about a known equilibrium solution and a system of linear, ordinary differential equations is obtained which determines the behaviour of the individual Fourier modes of the disturbance. Employing expansions in Chebyshev polynomials to approximate the solution of this system of differential equations, one then uses the QR matrix eigenvalue algorithm to solve the resulting linear, algebraic eigenvalue problem. The method employed here is analogous to that used by Orszag (1971) in his treatment of the Orr–Sommerfeld stability equation. The results obtained are then compared with those of other authors.

2. The continuum equations

Detailed accounts of the physical properties of nematic liquid crystals and the continuum theory describing their macroscopic behaviour are readily available in the books by de Gennes (1974) and Chandrasekhar (1977) and the reviews by Stephen & Straley (1974), Ericksen (1976) and Leslie (1980). Hence only a summary of the phenomenological equations proposed by Ericksen (1961) and Leslie (1968*a*, *b*, 1969) to describe their behaviour is given here.

The theory provides equations which determine the velocity vector field $\mathbf{v}$, the director $\mathbf{d}$ and temperature T, where $\mathbf{d}$ is a unit vector which describes the orientation of the anisotropic axis of these transversely isotropic liquids. With the assumption of incompressibility, the pertinent equations are the constraints

$$\operatorname{div} \mathbf{v} = 0, \quad \mathbf{d}.\mathbf{d} = 1 \tag{2.1}$$

and the balance laws

$$\rho \dot{v}_i = -p_{,i} - \left(\frac{\partial W}{\partial d_{k,j}} d_{k,i}\right)_{,j} + \tilde{t}_{ij,j} + F_i, \tag{2.2}$$

$$\sigma \ddot{d}_i = \gamma d_i + \left(\frac{\partial W}{\partial d_{i,j}}\right)_{,j} - \frac{\partial W}{\partial d_i} + \tilde{g}_i + G_i, \tag{2.3}$$

$$T\dot{S} = r - q_{i,i} + \tilde{t}_{ij} A_{ij} - \tilde{g}_i N_i, \quad S = -\partial W/\partial T, \tag{2.4}$$

where

$$\left.\begin{aligned} \tilde{t}_{ij} &= \alpha_1 d_k d_p A_{kp} d_i d_j + \alpha_2 d_j N_i + \alpha_3 d_i N_j + \alpha_4 A_{ij} + \alpha_5 d_j d_k A_{ki} + \alpha_6 d_i d_k A_{kj}, \\ \tilde{g}_i &= -\gamma_1 N_i - \gamma_2 A_{ik} d_k, \quad q_i = -\kappa_1 T_{,i} - \kappa_2 d_i d_k T_{,k} \\ 2A_{ij} &= v_{i,j} + v_{j,i}, \quad 2N_i = 2\dot{d}_i + (v_{k,i} - v_{i,k})\, d_k. \end{aligned}\right\} \tag{2.5}$$

Cartesian tensor notation is employed, so that repeated tensor indices are subject to the usual summation convention and a comma preceding a subscript denotes differentiation with respect to the appropriate spatial co-ordinate. In addition a superposed dot indicates a material time derivative. In these equations ρ is the density, σ a positive inertial coefficient and r the heat supply function per unit volume per unit time, taken to be zero throughout this paper. The arbitrary scalar functions p and γ arise from the constraints of incompressibility (2.1a) and fixed director magnitude (2.1b), respectively, while $\mathbf{F}$ represents any external body force present and $\mathbf{G}$ any generalized external body force acting. W is the stored-energy function per unit volume and we adopt the form proposed by (Oseen 1929) and Frank (1958)

$$2W = 2W_0 + K_2 d_{i,j}\, d_{i,j} + (K_1 - K_2 - K_4)\, d_{i,i}\, d_{j,j} + K_4 d_{i,j}\, d_{j,i} + (K_3 - K_2)\, d_i\, d_j\, d_{k,i}\, d_{k,j}. \tag{2.6}$$

The material parameters in the theory are dependent upon temperature alone and must satisfy the relations

$$\gamma_1 = \alpha_3 - \alpha_2, \quad \gamma_2 = \alpha_6 - \alpha_5. \tag{2.7}$$

In calculations, we assume the additional constraint proposed by Parodi (1970)

$$\alpha_2 + \alpha_3 = \alpha_6 - \alpha_5. \tag{2.8}$$

3. Formulation of the problem

The problem under investigation here concerns the stability of a sample of nematic liquid crystal contained between two horizontal plates of infinite extent when subjected to a vertical temperature gradient. The upper plate situated at $z = h$ is held at a constant temperature T_2 while the lower plate situated at $z = 0$ is kept at a constant temperature T_1. This paper examines the particular problem in which a homeotropic orientation obtains at the plates and a uniform magnetic field is applied vertically across the plates.

We assume that external body forces only arise from an applied uniform magnetic field $\mathbf{H} = (0, 0, H)$ and gravity. Thus, accepting the forms proposed by Ericksen (1962), it readily follows that

$$\mathbf{F} = (0, 0, -\rho g), \quad \mathbf{G} = \chi_a(\mathbf{H} \,.\, \mathbf{d})\mathbf{H}, \tag{3.1}$$

where g is the acceleration due to gravity and χ_a is a constant coefficient denoting the anisotropic part of the magnetic susceptibility. One obvious solution of equations (2.1)–(2.4) is the equilibrium configuration in which

$$\mathbf{v} = 0, \quad \mathbf{d} = (0, 0, 1), \quad T = T^0(z), \tag{3.2}$$

and hence

$$\gamma = -\chi_a H^2, \quad T^0 = \phi z + T_1, \quad p = \hat{p} - \rho g z, \tag{3.3}$$

where ϕ is the constant temperature gradient $(T_2 - T_1)/h$ and $\hat{p}$ is a constant. We now examine the situation in which this equilibrium configuration is disturbed by a small-amplitude velocity field $\mathbf{v}$ with which one associates a director field $\mathbf{d} + \mathbf{n}$, a temperature field $T^0(z) + s$, a pressure field $p + \bar{p}$ and a director tension field $-\chi_a H^2 + \bar{\gamma}$. Assuming that the magnitudes of the perturbation fields $\mathbf{v}$, $\mathbf{n}$, $\bar{p}$, s, $\bar{\gamma}$ and their derivatives are small compared to unity, one now linearizes equations (2.1)–(2.4) about the above equilibrium solution. Adopting the usual Boussinesq approximation (1903) the linearized equations take the form

$$v_{i,i} = 0, \quad d_i n_i = 0, \tag{3.4}$$

$$\frac{\rho\,\partial v_i}{\partial t} = -\rho' g e_i - \bar{p}_{,i} + A_{ijkm} v_{j,km} + B_{ijk}\frac{\partial}{\partial t} n_{j,k}, \quad \rho' = \frac{\partial \rho}{\partial T}, \tag{3.5}$$

$$\frac{\sigma\,\partial^2 n_i}{\partial t^2} = \bar{\gamma} d_i - \chi_a H^2 n_i + C_{ijkm} n_{j,km} + D_{ijk} v_{j,k} - \gamma_1 \frac{\partial n_i}{\partial t}, \tag{3.6}$$

$$\frac{\partial s}{\partial t} + \phi v_3 = \kappa_1 s_{,ii} + \kappa_2 d_j d_i s_{,ij} + \phi\kappa_2 (e_j d_i n_{j,i} + e_j d_j n_{i,i}), \tag{3.7}$$

where the coefficients A_{ijkm}, B_{ijk}, C_{ijkm} and D_{ijk} are defined by

$$\begin{aligned} 2A_{ijkm} &= 2\alpha_1 d_i d_j d_k d_m + (\alpha_2+\alpha_5)\,\delta_{ik} d_j d_m + (\alpha_3+\alpha_6)\,\delta_{km} d_i d_j + \alpha_4 \delta_{ij}\delta_{km} \\ &\quad + (\alpha_5-\alpha_2)\,\delta_{ij} d_k d_m, \\ B_{ijk} &= \alpha_2 \delta_{ij} d_k + \alpha_3 \delta_{jk} d_i, \quad 2D_{ijk} = (\gamma_1-\gamma_2)\,\delta_{ij} d_k - (\gamma_2+\gamma_1)\,\delta_{ik} d_j, \\ C_{ijkm} &= K_2 \delta_{ij}\delta_{km} + (K_1-K_2)\,\delta_{jk}\delta_{im} + (K_3-K_2)\,\delta_{ij} d_k d_m, \end{aligned}$$

δ_{ij} is the Kronecker delta and $\mathbf{e} \equiv (0,0,1)$. We note that (3.7) results when (2.4) is divided by the quantity $-T\partial^2 W_0/\partial T^2$. Hence in (3.7) the κ's represent thermal diffusivities whereas in (2.4) they represent thermal conductivities.

One now investigates the stability of the uniform homeotropic configuration with respect to disturbances of the form

$$\mathbf{v} = (v_1, 0, v_3)\exp[im(x-kt)], \quad \mathbf{n} = i(n,0,0)\exp[im(x-kt)], \tag{3.8a, b}$$

$$s = s\exp[im(x-kt)], \tag{3.8c}$$

where v_1, v_3, n and s are functions of z alone and k is in general complex. One observes that (3.4b), (3.5b) and (3.6b) are satisfied identically by (3.8) while (3.6c) determines $\bar{\gamma}$ and (3.4) gives v_1 in terms of v_3. Elimination of $\bar{p}$ between equations (3.5a, c) finally yields the system of equations

$$(D^4 + A_1 m^2 D^2 + A_2 m^4)\,v_3 + (A_3 m^2 D^2 + A_4 m^4)\,n + A_5 m^4 s = 0, \tag{3.9a}$$

$$(D^2 + B_1 m^2)\,v_3 + (B_2 D^2 + B_3 m^2)\,n = 0, \tag{3.9b}$$

$$(D^2 + E_1 m^2)\,s + E_2 m^2 n + E_3 m^2 v_3 = 0, \tag{3.9c}$$

where

$$\begin{aligned} &A_1 = \{-(2\alpha_1+\eta_a+\eta_b)+2\rho ikm\}/\eta_b, \quad A_2 = (\eta_a - 2i\rho k/m)/\eta_b, \\ &A_3 = -2\alpha_2 ki/\eta_b, \quad A_4 = -2\alpha_3 ki/\eta_b, \quad A_5 = 2\rho' g/m^2\eta_b, \\ &B_1 = \frac{\gamma_2+\gamma_1}{\gamma_2-\gamma_1}, \quad B_2 = \frac{2K_3 m}{\gamma_1-\gamma_2}, \quad B_3 = \frac{-2(K_1 m - \gamma_1 ik + \chi_a H^2/m - \sigma imk^2)}{\gamma_1-\gamma_2}, \\ &E_1 = (-m\kappa_1 + ik)/m\kappa, \quad E_2 = -\phi\kappa_2/m\kappa, \quad E_3 = -\phi/m^2\kappa, \\ &\eta_a = \alpha_4+\alpha_3+\alpha_6, \quad \eta_b = \alpha_4+\alpha_5-\alpha_2, \quad \kappa = \kappa_1+\kappa_2, \quad D \equiv d/dz. \end{aligned}$$

For reasons discussed by Pieranski *et al.* (1973b), it seems reasonable to neglect the director inertia term in (3.9b) and so we set $\sigma \equiv 0$ throughout the remainder of this paper. One now requires to solve the three equations (3.9) for v_3, n and s subject to the boundary conditions

$$v_3 = Dv_3 = s = n = 0, \tag{3.10}$$

on $z = 0$ and $z = h$.

Solutions are obtained using expansions in Chebyshev polynomials and, to invoke the orthogonality properties of this set of polynomials, it is convenient to impose boundary conditions at ± 1. To this end one introduces the new independent variable

$$\zeta = (2z-h)/h \tag{3.11}$$

and makes a transformation from z to ζ in (3.9) and (3.10). Transformation of (3.9) yields the set of equations

$$(D_1^4+\mu_1 D_1^2+\mu_2)\bar{v}+\mu_3\bar{s}+ik\{(\delta_1 D_1^2+\delta_2)\bar{v}+(\delta_3 D_1^2+\delta_4)\bar{n}\} = 0, \tag{3.12a}$$

$$(D_1^2+\mu_4)\bar{v}+(\mu_5 D_1^2+\mu_6)\bar{n}+ik\delta_5\bar{n} = 0, \tag{3.12b}$$

$$(D_1^2+\mu_7)\bar{s}+\mu_8\bar{n}+\mu_9\bar{v}+ik\delta_6\bar{s} = 0, \tag{3.12c}$$

where $D_1 \equiv d/d\zeta$ and $\bar{v}$, $\bar{s}$ and $\bar{n}$ are the transforms of v_3, s and n respectively. The coefficients in (3.12) are real quantities defined by

$$b^2A_1 = \mu_1+ik\delta_1,\quad b^4A_2 = \mu_2+ik\delta_2,\quad b^2A_3 = ik\delta_3,\quad b^4A_4 = ik\delta_4,\quad b^4A_5 = \mu_3,$$

$$b^2B_1 = \mu_4,\quad B_2 = \mu_5,\quad b^2B_3 = \mu_6+ik\delta_5,\quad b^2E_1 = \mu_7+ik\delta_6,\quad b^2E_2 = \mu_8,\quad b^2E_3 = \mu_9,$$

where b is a non-dimensional wavenumber defined by $b = \frac{1}{2}mh$. One now requires to find solutions of the equations (3.12) subject to the transformed boundary conditions

$$\bar{v} = D_1\bar{v} = \bar{s} = \bar{n} = 0, \tag{3.13}$$

on $\zeta = \pm 1$.

For a given value of the magnetic field, H, the mathematical problem is that of determining values of the parameters b, ϕ and k for which there are non-trivial solutions of (3.12) and (3.13). Apart from H, b, ϕ and k, all quantities appearing in the coefficients of (3.12) are material parameters which are determined from empirical data. For prescribed values of b and ϕ suppose that non-trivial solutions exist for a set of k values denoted by $k^{(j)} = k_R^{(j)}+ik_I^{(j)}$, $j = 1, 2, \ldots$, where $k_R^{(j)}$ and $k_I^{(j)}$ are real, and values are ordered so that $k_I^{(1)} \geqslant k_I^{(2)} \geqslant k_I^{(3)} \geqslant \ldots$. The value $k^{(1)}$ corresponds to the least stable mode associated with the prescribed temperature gradient, ϕ, and wavenumber, b, and this mode is unstable only if $k_I^{(1)} > 0$. If an unstable mode is found for a particular wavelength, the temperature gradient at which disturbances of this wavelength become unstable is determined by adjusting ϕ until $k_I^{(1)} = 0$. Values of b and ϕ for which this occurs yield a point on the neutral stability curve and the value of ϕ with minimum modulus on this curve is called the critical temperature gradient for the liquid crystal sample.

In the introduction reference is made to stationary and oscillatory convective instabilities in liquid crystal samples. The nature of an unstable mode is determined by the sign of the real part of k associated with this mode. Suppose a non-trivial solution exists for $k = k_R+ik_I$, where $k_I > 0$. If $k_R = 0$ the solution corresponds to a stationary instability whereas if $k_R \neq 0$ the solution corresponds to an oscillatory instability. In this latter case we shall see that a solution also exists for $k = -k_R + ik_I$. It follows that oscillations in the disturbance arise from the terms

$$\exp(\pm imk_R t) = \exp(\pm 2ibk_R t/h)$$

and that they have frequency $\omega = 2b|k_R|/h$. It is of interest to note at this point that the principle of exchange of stabilities, as used by Barratt & Sloan (1976), may only be employed to determine critical temperature gradients if the least stable mode is stationary, that is if $k_R^{(1)} = 0$.

4. Method of solution

We seek approximate solutions to (3.12) and (3.13) using expansions in series of Chebyshev polynomials. Orszag (1971), in his treatment of the Orr–Sommerfeld equation, discusses the advantages of Chebyshev polynomials relative to other sets of orthogonal polynomials. In particular, he shows that if the coefficients of a linear differential equation are infinitely differentiable the approximation obtained is of infinite order in the sense that errors decrease more rapidly than any power of $1/N$ as $N \to \infty$, where N is the number of Chebyshev polynomials retained in the approximation. The required properties of Chebyshev polynomials are outlined below and further details, if required, may be obtained in the paper by Orszag (1971).

Suppose $v(\zeta)$ is an infinitely differentiable function for $-1 \leqslant \zeta \leqslant 1$ and let the Chebyshev expansions of $v(\zeta)$ and its derivatives $d^q v/d\zeta^q$ be

$$d^q v(\zeta)/d\zeta^q = \sum_{n=0}^{\infty} a_n^{(q)} T_n(\zeta), \tag{4.1}$$

where $a_n^{(0)} \equiv a_n$ and $T_n(\zeta)$ is the nth-degree Chebyshev polynomial of the first kind, defined by

$$T_n(\cos\theta) = \cos n\theta \tag{4.2}$$

for $n = 0, 1, 2, \ldots$. The properties of $T_n(\zeta)$ may be used to express $a_n^{(q)}$ in terms of coefficients in the expansion of $d^{q-1}v(\zeta)/d\zeta^{q-1}$. Orszag (1971) has shown that

$$c_{p-1} a_{p-1}^{(q)} - a_{p+1}^{(q)} = 2p a_p^{(q-1)}, \quad p \geqslant 1, \tag{4.3}$$

where $c_0 = 2$ and $c_p = 1$ for $p > 0$. By adding equations (4.3) for $p = n+1, n+3, n+5, \ldots$ and assuming that $|a_p^{(q)}|$ and $|a_p^{(q-1)}|$ vanish appropriately as $p \to \infty$ one obtains

$$\left.\begin{aligned} c_n a_n^{(q)} = 2 \sum_{p=n+1}^{\infty} p a_p^{(q-1)}, \quad n \geqslant 0, \\ p+n \equiv 1 \pmod 2. \end{aligned}\right\} \tag{4.4}$$

The set of differential equations (3.12) contains derivatives of orders two and four and in order to relate Chebyshev expansions of derivatives such as $d^2v(\zeta)/d\zeta^2$ and $d^4v(\zeta)/d\zeta^4$ to the Chebyshev expansion of $v(\zeta)$ it is essential to express $a_n^{(2)}$ and $a_n^{(4)}$ in terms of the coefficients in (4.1) with $q = 0$. These results are readily obtained on setting $q = 1, 2, 3, 4$ in (4.4), and the required relationships are

$$\left.\begin{aligned} c_n a_n^{(2)} = \sum_{p=n+2}^{\infty} p(p^2-n^2) a_p, \quad n \geqslant 0, \\ p \equiv n \pmod 2. \end{aligned}\right\} \tag{4.5}$$

and

$$\left.\begin{aligned} 24c_n a_n^{(4)} = \sum_{p=n+4}^{\infty} p(p^2-n^2)[(p-n)^2-4][(p+n)^2-4]a_p, \quad n \geqslant 0,\\ p \equiv n \pmod 2). \end{aligned}\right\} \tag{4.6}$$

We now return to the system of differential equations (3.12) and approximate the dependent variables and their derivatives by means of the truncated Chebyshev expansions

$$\left.\begin{aligned} d^q\bar{v}(\zeta)/d\zeta^q &= \sum_{n=0}^{N} \phi_n^{(q)} T_n(\zeta),\\ d^q\bar{s}(\zeta)/d\zeta^q &= \sum_{n=0}^{N} \eta_n^{(q)} T_n(\zeta),\\ d^q\bar{n}(\zeta)/d\zeta^q &= \sum_{n=0}^{N} \theta_n^{(q)} T_n(\zeta). \end{aligned}\right\} \tag{4.7}$$

If the expansions (4.7) are substituted in (3.12) the orthogonality properties of Chebyshev polynomials may be used to derive a system of linear algebraic equations in $\phi_n^{(q)}$, $\eta_n^{(q)}$ and $\theta_n^{(q)}$ for $q = 0, 2, 4$ and $n = 0, 1, \ldots, N$. Coefficients with superscripts 2 and 4 may be eliminated from this algebraic system by means of the relationships (4.5) and (4.6). The appendix to this paper contains the derivation of a system of homogeneous, linear equations in $\phi_n \equiv \phi_n^{(0)}, \eta_n = \eta_n^{(0)}, \theta_n = \theta_n^{(0)}$ for $n = 0, 1, \ldots, N$. The solution of this linear system may be used with expansions (4.7) to provide an approximate solution to the differential equations (3.12) and boundary conditions (3.13). Here, of course, we are only interested in finding values of k for which the linear system of algebraic equations has a non-trivial solution.

In the appendix it is shown that the linear algebraic equations in ϕ_n, η_n, θ_n separate into two sets with no coupling between odd subscript coefficients and even subscript coefficients. Solutions of the even-subscript system yield approximations to $\bar{v}$, $\bar{s}$ and $\bar{n}$ which are even functions of ζ and solutions of the odd-subscript system yield approximations to $\bar{v}$, $\bar{s}$ and $\bar{n}$ which are odd functions of ζ. In the even system it is convenient to replace N by $2M$, n by $2m$, and to introduce the transformations

$$\phi_{2m} = \hat{\phi}_m, \quad \eta_{2m} = \hat{\eta}_m, \quad \theta_{2m} = \hat{\theta}_m.$$

In the appendix we show that the linear system associated with the even solution of (3.12) is

$$\begin{aligned} \frac{16}{3}\sum_{q=m+2}^{M} F_{qm}[(q-m)^2-1][(q+m)^2-1]\hat{\phi}_q + 8\mu_1 \sum_{q=m+1}^{M} F_{qm}\hat{\phi}_q + \mu_2 c_m \hat{\phi}_m + \mu_3 c_m \hat{\eta}_m \\ + ik\left[8\delta_1 \sum_{q=m+1}^{M} F_{qm}\hat{\phi}_q + \delta_2 c_m \hat{\phi}_m + 8\delta_3 \sum_{q=m+1}^{M} F_{qm}\hat{\theta}_q + \delta_4 c_m \hat{\theta}_m\right] = 0, \end{aligned} \tag{4.8a}$$

$$8\sum_{q=m+1}^{M} F_{qm}\hat{\phi}_q + \mu_4 c_m \hat{\phi}_m + 8\mu_5 \sum_{q=m+1}^{M} F_{qm}\hat{\theta}_q + \mu_6 c_m \hat{\theta}_m + ik\delta_5 c_m \hat{\theta}_m = 0, \tag{4.8b}$$

$$8\sum_{q=m+1}^{M} F_{qm}\hat{\eta}_q + \mu_7 c_m \hat{\eta}_m + \mu_8 c_m \hat{\theta}_m + \mu_9 c_m \hat{\phi}_m + ik\delta_6 c_m \hat{\eta}_m = 0, \tag{4.8c}$$

where $F_{qm} = q(q^2-m^2)$ and $m = 0, 1, \ldots, M$. The linear algebraic equations associated with the even-subscript solution of the boundary conditions are

$$\sum_{q=0}^{M} \hat{\phi}_q = 0, \quad \sum_{q=0}^{M} q^2\hat{\phi}_q = 0, \quad \sum_{q=0}^{M} \hat{\eta}_q = 0, \quad \sum_{q=0}^{M} \hat{\theta}_q = 0. \tag{4.9}$$

Linear equations analogous to (4.8) and (4.9) and associated with the odd-subscript solution are given in the appendix. We shall see later, however, that interest is centred on the even solution.

Equations (4.8) and (4.9) constitute a system of $3M+7$ equations in $3M+3$ unknowns and this system has only the trivial solution in which all Chebyshev coefficients are zero. We resolve this over-specification by means of Lanczos's τ method (Lanczos 1956). The integer m is restricted to the range $m = 0, 1, \ldots, M-2$ in the first equation of (4.8) and to the range $m = 0, 1, \ldots, M-1$ in the second and third equations. The restriction imposed upon m is equivalent to solving the original set of equations (3.12) and (3.13) for an approximate solution which is even in ζ, with the additional terms

$$\tau_{N-2}^{(1)} T_{N-2}(\zeta) + \tau_N^{(1)} T_N(\zeta), \quad \tau_N^{(2)} T_N(\zeta), \quad \tau_N^{(3)} T_N(\zeta),$$

on the right-hand sides of the first, second and third equations, respectively, in (3.12). The parameters $\tau_{N-2}^{(1)}$ and $\tau_N^{(j)}, j = 1, 2, 3$, may be obtained, if required, in terms of the coefficients

$$\phi_0, \phi_2, \ldots, \phi_N; \quad \eta_0, \eta_2, \ldots, \eta_N; \quad \theta_0, \theta_2, \ldots, \theta_N.$$

The τ parameters may be used to estimate the errors in the approximations. Similar arguments apply to the odd solution and the over-specification is resolved on restricting m in the manner described for the even solution.

With m restricted as described, system (4.8)–(4.9) may be written in matrix form as

$$(\mathbf{A} + ik\mathbf{B})\mathbf{X} = 0, \tag{4.10}$$

where $\mathbf{A}$ and $\mathbf{B}$ are real matrices of order $3M+3$ and $\mathbf{X}$ is a vector whose components are the Chebyshev coefficients $\hat{\phi}_j, \hat{\eta}_j, \hat{\theta}_j, j = 0, 1, \ldots, M$. In the computations to be described, rows $3M$ to $3M+3$ of (4.10) were formed using the boundary equations (4.9) so that the final four rows of $\mathbf{B}$ contain only zero entries. Equation (4.10) may be written as

$$\mathbf{AX} = \lambda\mathbf{BX}, \tag{4.11}$$

where $k = \lambda i$, and the problem of finding values of k for which there are non-trivial solutions of (3.12) and (3.13) becomes that of solving the generalized eigenvalue problem described by (4.11). Permissible values of λ occur in complex conjugate pairs and this verifies a point made in § 3 that permissible values of k with non-zero real part occur in pairs $\pm k_R + ik_I$.

The first stage in solving (4.11) for eigenvalues λ exploits the fact that $\mathbf{B}$ has zeros in all entries of the final four rows. Using column operations, with partial pivoting, all elements in the final four rows of $\mathbf{A}$ are set to zero, apart from those on or to the right of the main diagonal. The matrix $\mathbf{A}$ has thus been transformed to $\mathbf{A}^{(1)} = \mathbf{AQ}$, where $\mathbf{Q}$ is a non-singular matrix representing the column operations. The same transformation is applied to $\mathbf{B}$ and (4.11) is thereby transformed to

$$\mathbf{A}^{(1)}\mathbf{X}^{(1)} = \lambda\mathbf{B}^{(1)}\mathbf{X}^{(1)},$$

where $\mathbf{X}^{(1)} = \mathbf{Q}^{-1}\mathbf{X}$, $\mathbf{B}^{(1)} = \mathbf{B}\mathbf{Q}$ and $\mathbf{B}^{(1)}$ has zeros in the final four rows. If the product

$$\prod_{i=3M}^{3M+3} a_{i,i}^{(1)}$$

differs from zero the eigenvalues are solutions of $\det[\mathbf{A}^{(2)} - \lambda\mathbf{B}^{(2)}] = 0$, where $\mathbf{A}^{(2)}$ and $\mathbf{B}^{(2)}$ are the leading $3M-1$ by $3M-1$ submatrices of $\mathbf{A}^{(1)}$ and $\mathbf{B}^{(1)}$, respectively, and $[\mathbf{A}^{(1)}]_{i,j} = a_{i,j}^{(1)}$. If the aforementioned product is zero the reduction fails. This failure did not occur in any of the computations which were performed. When $\mathbf{B}^{(2)}$ has full rank the values of λ are given as the eigenvalues of $[\mathbf{B}^{(2)}]^{-1}\mathbf{A}^{(2)}$. Assuming no difficulties are encountered in the inversion of $\mathbf{B}^{(2)}$, the matrix $[\mathbf{B}^{(2)}]^{-1}\mathbf{A}^{(2)}$ is balanced using the algorithm described by Wilkinson and Reinsch (1971) and the eigenvalues are obtained by means of the QR algorithm.

The method described above was used with some of the data and no difficulties arose. However, to guard against the possibility of $\mathbf{B}^{(2)}$ having numerical rank less than $3M-1$ we include a modification based on the work of Gary & Helgason (1970). The method is clearly described by these authors and an outline should suffice here. Row and column operations are used with complete pivoting to find non-singular $\mathbf{P}^{(2)}$ and $\mathbf{Q}^{(2)}$ so that $\mathbf{B}^{(3)} = \mathbf{P}^{(2)}\mathbf{B}^{(2)}\mathbf{Q}^{(2)}$ is diagonal, with

$$|B_{i,i}^{(3)}| \geqslant |B_{i+1,i+1}^{(3)}| \quad \text{for} \quad i = 1, 2, \ldots, 3M-2.$$

If

$$|B_{i,i}^{(3)}| > \epsilon \quad \text{for} \quad i \leqslant R \quad \text{and} \quad |B_{i,i}^{(3)}| \leqslant \epsilon \quad \text{for} \quad i > R,$$

where ϵ is a small positive tolerance, then the rank of $\mathbf{B}^{(3)}$ is taken as R. In the computation ϵ was given the value 10^{-6}. $\mathbf{A}^{(2)}$ is now transformed to $\mathbf{A}^{(3)} = \mathbf{P}^{(2)}\mathbf{A}^{(2)}\mathbf{Q}^{(2)}$ and column operations are then used to nullify those elements of $\mathbf{A}^{(3)}$ which lie to the left of the main diagonal in rows $R+1$ to $3M-1$. If the transformed $\mathbf{A}^{(3)}$ is $\mathbf{A}^{(4)} = \mathbf{A}^{(3)}\mathbf{Q}^{(3)}$ then $\mathbf{B}^{(3)}$ is transformed to $\mathbf{B}^{(4)} = \mathbf{B}^{(3)}\mathbf{Q}^{(3)}$. Assuming the product

$$\prod_{i=R+1}^{3M-1} a_{i,i}^{(4)}$$

differs from zero the eigenvalues are solutions of $\det[\mathbf{A}^{(5)} - \lambda\mathbf{B}^{(5)}] = 0$, where $\mathbf{A}^{(5)}$ and $\mathbf{B}^{(5)}$ are the leading R by R submatrices of $\mathbf{A}^{(4)}$ and $\mathbf{B}^{(4)}$, respectively. Thereafter the method is as described in the previous paragraph. The reduction algorithm of Gary & Helgason (1970) was included in the calculations described in the next section and in all cases it was found that $R = 3M-1$.

5. Numerical results

Employing available experimental data for MBBA, we adopt the Parodi (1970) relation and take the values for viscosities as given by Gähwiller (1971). Also we 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 c.g.s. units we therefore set the parameters $(\alpha_1, \alpha_2, \ldots, \alpha_6)$, (K_1, K_3), (γ_1, γ_2), (κ_1, κ_2) equal to the values $(6{\cdot}5 \times 10^{-2}$, $-77{\cdot}5 \times 10^{-2}$, $-1{\cdot}2 \times 10^{-2}$, $83{\cdot}2 \times 10^{-2}$, $46{\cdot}3 \times 10^{-2}$, $-32{\cdot}4 \times 10^{-2})$, $(6 \times 10^{-7}, 7 \times 10^{-7})$, $(76{\cdot}3 \times 10^{-2}$, $-78{\cdot}7 \times 10^{-2})$, $(9{\cdot}3 \times 10^{-4}, 6{\cdot}1 \times 10^{-4})$. The constant χ_a which denotes the anisotropic part of the magnetic susceptibility is given the value $1{\cdot}23 \times 10^{-7}$ and the applied

M	$10^3 \times k^{(1)}$
9	$-9{\cdot}28420+6{\cdot}46919i$
10	$-9{\cdot}28522+6{\cdot}46808i$
11	$-9{\cdot}28520+6{\cdot}46785i$
12	$-9{\cdot}28514+6{\cdot}46781i$
13	$-9{\cdot}28504+6{\cdot}46778i$

TABLE 1. Approximations to $k^{(1)}$ using $M+1$ even-degree, Chebyshev polynomials with $H = 0$, $\phi = -24$, $b = 1{\cdot}5$.

Mode number	Even or odd	$10^3 \times k^{(j)}, j = 1, 2, \ldots, 8$
1	E	$-9{\cdot}285+6{\cdot}468i$
2	E	$+9{\cdot}285+6{\cdot}468i$
3	E	$-0{\cdot}205i$
4	O	$-0{\cdot}206i$
5	O	$-0{\cdot}888i$
6	E	$-0{\cdot}900i$
7	E	$-1{\cdot}243i$
8	O	$-1{\cdot}423i$

TABLE 2. The eight least stable modes for $H = 0$, $\phi = -24$, $b = 1{\cdot}5$. Even (E) and odd (O) eigenmodes are listed.

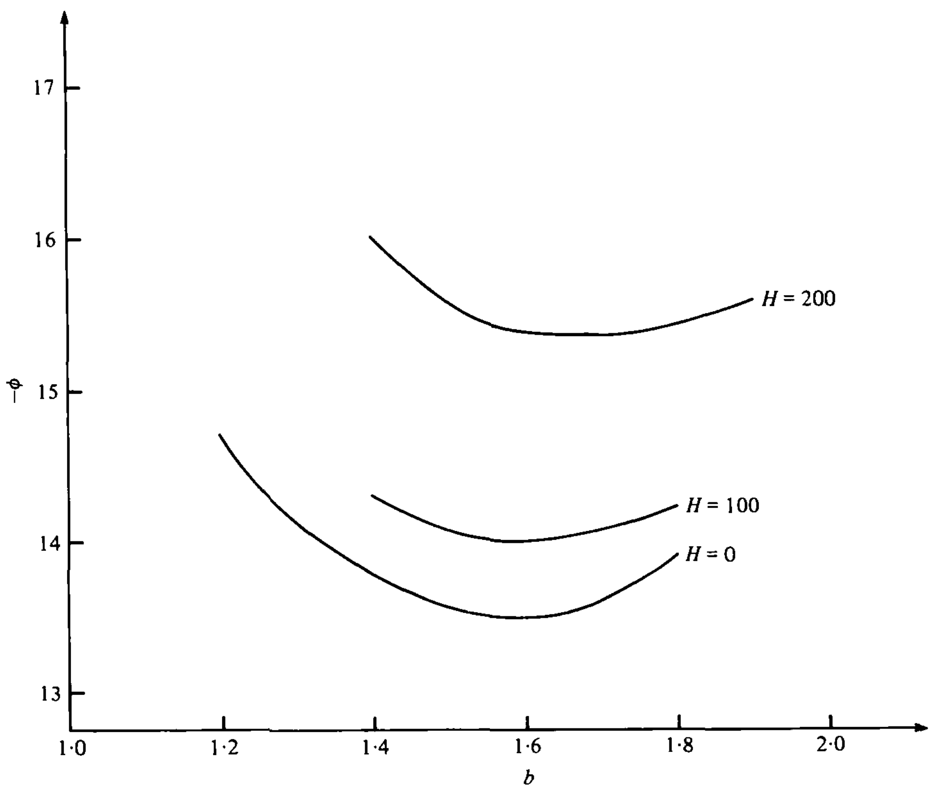

FIGURE 1. Neutral stability curve for MBBA at three values of magnetic field.

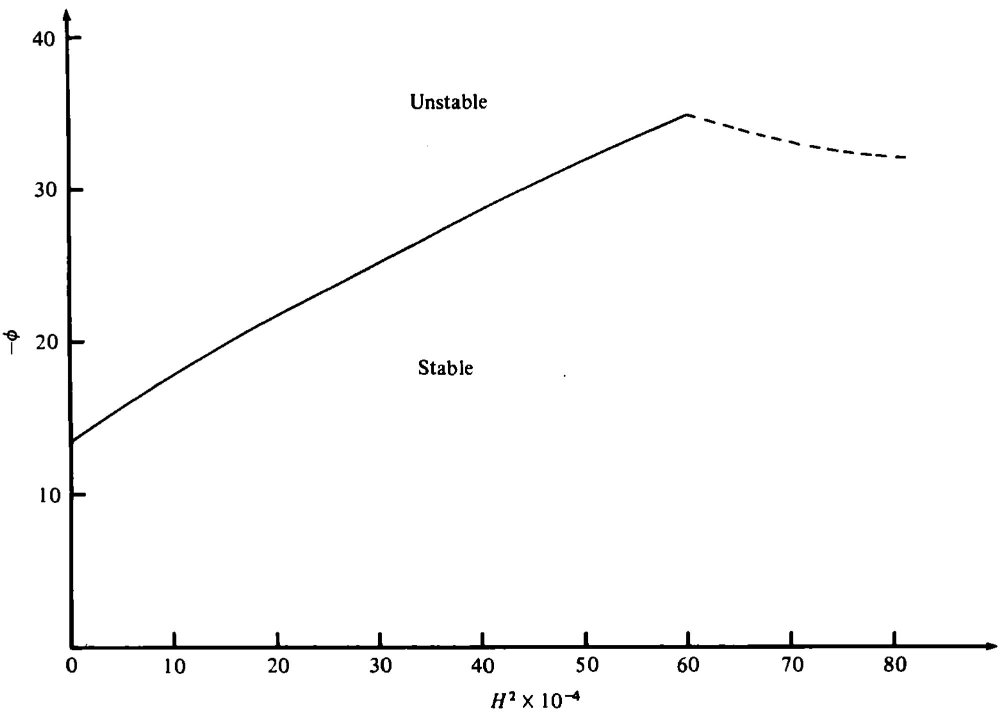

FIGURE 2. Effect of magnetic field on stability. Critical temperature gradient $-\phi$ is plotted against $H^2 \times 10^{-4}$. Heavy line and broken line correspond, respectively, to oscillatory and stationary modes of convection.

magnetic field, H, is expressed in gauss. The density ρ is given the value 1, the term $\rho' g$ is taken as -1 and the sample thickness is assumed to be 5 mm throughout the calculations.

Preliminary numerical experiments were conducted to determine a suitable value for the integer M, where $M+1$ is the number of even or odd Chebyshev polynomials used in the expansions of dependent variables. Noting the relation $k = \lambda i$, we see that as M increases the eigenvalue of (4.17) should converge to those values of $-ik$ for which there are non-trivial solutions of the equations (3.12)–(3.13). In all computations a large positive real eigenvalue of (4.17) is obtained. This eigenvalue varies greatly with M and it is considered to be a spurious eigenvalue of equations (3.12)–(3.13). Interest is directed on the least stable mode of this differential system and trial computations indicate that the associated value $k^{(1)}$ may be obtained sufficiently accurately with $M = 11$. Table 1 gives several approximations to $k^{(1)}$ for the even solution with $H = 0$, $\phi = -24$, $b = 1{\cdot}5$. For this data set, $k^{(1)}$ may be obtained correct to 4 significant figures with $M = 11$. This value of M was used throughout the computations on the assumption that computational errors might then be less than errors in experimental data. Trial computations also indicate that the least stable mode is associated with the even solution. In table 2, for example, the eight least stable modes are listed for $H = 0$, $\phi = -24$ and $b = 1{\cdot}5$. We note that the pairs of modes 3 and 4, 5 and 6 are almost coincident. Since the least stable mode is associated with symmetric eigenmodes we restrict our attention henceforth to the even solutions.

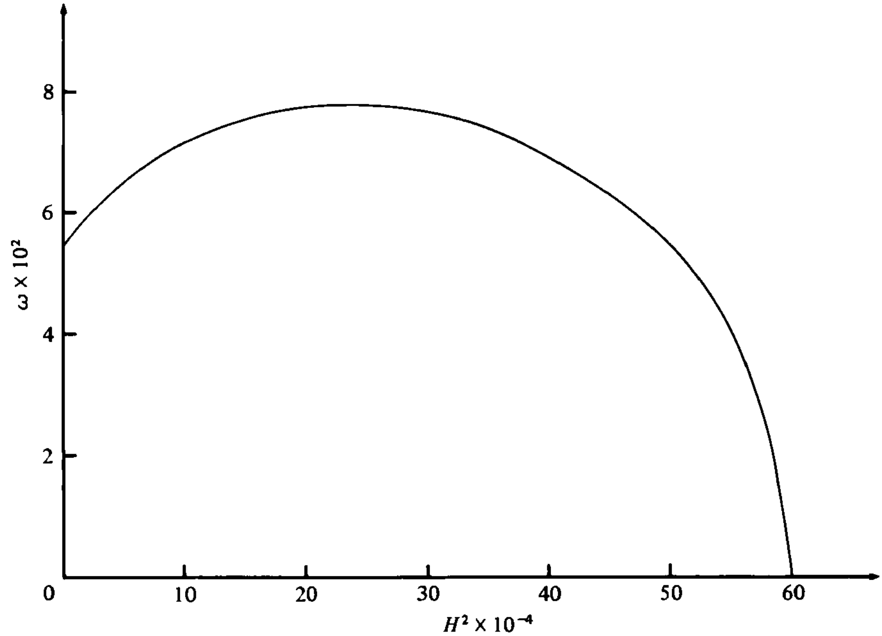

FIGURE 3. Frequency of oscillation of oscillatory modes. Frequency of the least stable mode is plotted against $H^2 \times 10^{-4}$.

Figure 1 shows the neutral stability curve for MBBA at three values of the applied, transverse magnetic field. For a particular value of the dimensionless wavenumber, b, the point on the neutral stability curve is obtained by computing $k^{(1)}$ at a set of increasing values of $-\phi$. The value of $-\phi$ is found for which $k_1^{(1)} = 0$ and this yields a point on the curve. If the magnitude of the temperature gradient, $-\phi$, is less than this value any disturbance with wavenumber $m = 2b/h$ is damped as time progresses. A value of ϕ which yields a point in the inner region of the curve permits the existence of unstable disturbances with this wavenumber. The value of ϕ at the minimum point on the curve gives a measure of the dimensionless temperature gradient which may be imposed before disturbances of the type considered here become unstable. This is the critical temperature gradient and it is therefore a quantity of physical interest. The critical temperature gradients are $\phi = -13{\cdot}5$, $\phi = -14{\cdot}0$ and $\phi = -15{\cdot}4$, respectively, for $H = 0$, $H = 100$ and $H = 200$. At $H = 0$ the minimum occurs at $b = 1{\cdot}6$ and the value of b at the minimum increases slowly with H, taking the value $1{\cdot}7$ at $H = 200$. We observe that the liquid crystal sample becomes more stable as the magnetic field increases from zero.

To examine the effect of magnetic field on stability, we obtained the minimum points on the neutral stability curves at increasing values of H. Figure 2 shows the critical temperature gradient, $-\phi$, plotted as a function of $H^2 \times 10^{-4}$ over a wide range of magnetic field. For H between 0 and approximately 775 the critical temperature gradient increases almost linearly with H^2. The deviation from linearity arises from a slight concavity of the curve in this region. The value of b at the critical points increases from $1{\cdot}6$ at $H = 0$ to $2{\cdot}3$ at $H = 775$. The real part of $k^{(1)}$ is non-zero over

	Guyon *et al.*	Barratt & Sloan	Velarde & Zuniga	Lekkerkerker
Critical temperature difference ΔT_c $(H = 0)$	5·5° C	6·75 °C	12 °C	
Period $2\pi/\omega$ $(H = 0)$		117 s	120 s	200 s
Period $(2\pi/\omega)$ $(\omega = \max)$	110 s	80 s	170 s	170 s
Magnetic field H $(\omega = \max)$	400 gauss	490 gauss	300 gauss	180 gauss
Magnetic field H_T at transition between instabilities	650 gauss	775 gauss	660 gauss	
Critical temperature difference ΔT_c $(H = H_T)$	15 °C	17·3 °C		

TABLE 3

this portion and the least stable mode is of oscillatory type with frequency given by $\omega = 2b|k_R|/h$. Figure 3 shows the behaviour of ω with $H^2 \times 10^{-4}$ and we observe that ω initially increases to a maximum around $H = 490$ and then it diminishes with further increase in H, reaching the value zero at $H = 775$. For $H > 775$ the value of $k^{(1)}$ is purely imaginary for ϕ close to the critical value and the least stable mode is stationary in this region. At approximately 775 gauss there is a transition from an oscillatory instability to a stationary instability. The broken line in figure 2 shows the temperature gradient at which the least stable stationary mode becomes unstable. We observe that as the magnetic field is increased beyond the transition point there is an initial destabilizing effect. When H is greater than the transition value the least stable mode is a stable oscillatory mode for values of $-\phi$ well below the value shown by the broken curve in figure 2. As $-\phi$ is increased $k_I^{(1)}$ increases and $|k_R^{(1)}|$ decreases and the latter becomes zero at a value of $-\phi$ below the broken curve. For $-\phi$ between this point and the critical value $k^{(1)}$ and $k^{(2)}$ are purely imaginary with $k_I^{(1)}$ and $k_I^{(2)}$ both negative. There is therefore a region immediately below the broken curve in figure 2 within which the least stable mode is a stable stationary mode. The interface of physical interest is that which separates the stable and unstable regions, however, and this is given by the curve in figure 2.

6. Discussion of results

Employing expansions in Chebyshev polynomials, we have obtained accurate numerical solutions for threshold gradients at which thermal convection appears when a homeotropically aligned nematic is heated from below. Our results together with the experimental results of Guyon *et al.* (1979) and the theoretical results of Velarde & Zuniga (1979) and Lekkerkerker (1979) are listed in table 3 above. It should be noted that some results are not given explicitly by other authors but have been estimated from graphs presented by them. Also, although all results reported are for MBBA, the values of material parameters used in calculations are not usually stated. The period referred to in table 3 is the period of oscillation of the least stable mode at the onset of instability.

The most comprehensive comparison of our results possible is with the experimental results of Guyon *et al.* (1979). The agreement between them both qualitatively and quantitatively seems rather good. Apart from experimental error, some differences in results could arise if the empirical values for material parameters employed in calculations are not precisely those pertaining to the material used in the experiments. The greatest discrepancies between theory and experiment seem to occur when large magnetic fields are present and hence higher threshold gradients are required for the onset of the thermal instability. In such cases with temperature differences as high as 15–20 °C other physical effects, neglected in the preceding analysis, may well become important and so render the above results unreliable. In particular the Boussinesq (1903) approximation is probably invalid for such large temperature differences where changes in the material parameters with temperature might well be significant. This could be related to the fact that observed thresholds are lower than those predicted by the theory employed. From a qualitative viewpoint, our results confirm that the main physical features of the instability are well described by the rather simpler analyses of Guyon *et al.* (1979) and Lekkerkerker (1979). In comparing our results with those found by Velarde & Zuniga (1979) using a first-order Galerkin method, it is not surprising that there are some noticeable quantitative differences between them. The most significant being that in the absence of any magnetic field they predict a critical temperature gradient which is approximately double that found here. Finally it is of interest to note that the least stable mode is an even mode as was found to be the case by Barratt & Sloan (1976) in two rather similar experimental situations.

In closing, it must be admitted that only a limited class of infinitesimal disturbances has been considered and consequently one is unable to say anything concerning stability with respect to arbitrary infinitesimal disturbances below the threshold gradients predicted here. However, they are more general than those allowed for by Guyon *et al.* (1979) and Lekkerkerker (1977, 1979) and also seem to be consistent with experimental observations of Guyon *et al.* Further comparison between experimental results and accurate solutions for a wide variety of nematic materials would be useful as a check on the predictions of the continuum theory. Also a theoretical investigation incorporating non-Boussinesq effects would be well worth while provided such an analysis is manageable.

Appendix

In the appendix we derive the linear systems of equations (4.8) and (4.9) associated with the even solution and we give the analogous systems associated with the odd solution. If the expansions (4.7) are substituted in (3.12) the coefficients of $T_n(\zeta)$ may be equated, by virtue of the orthogonality properties of the Chebyshev polynomials. This process yields

$$\phi_n^{(4)}+\mu_1\phi_n^{(2)}+\mu_2\phi_n+\mu_3\eta_n+ik[\delta_1\phi_n^{(2)}+\delta_2\phi_n+\delta_3\theta_n^{(2)}+\delta_4\theta_n] = 0,$$

$$\phi_n^{(2)}+\mu_4\phi_n+\mu_5\theta_n^{(2)}+\mu_6\theta_n+ik[\delta_5\theta_n] = 0,$$

$$\eta_n^{(2)}+\mu_7\eta_n+\mu_8\theta_n+\mu_9\phi_n+ik[\delta_6\eta_n] = 0,$$

where $\phi_n \equiv \phi_n^{(0)}$, $\eta_n = \eta_n^{(0)}$ and $\theta_n = \theta_n^{(0)}$. The coefficients with superscripts 2 and 4 may be expressed in terms of the basic coefficients using (4.5) and (4.6), with the summations over p truncated at N. This reduction process leads to the linear system of algebraic equations

$$\left.\begin{aligned}
&\frac{1}{24}\sum_{p=n+4}^{N} F_{pn}[(p-n)^2-4]\,[(p+n)^2-4]\,\phi_p+\mu_1\sum_{p=n+2}^{N} F_{pn}\phi_p+\mu_2 c_n\phi_n\\
&\quad+\mu_3 c_n\eta_n+ik\left[\delta_1\sum_{p=n+2}^{N} F_{pn}\phi_p+\delta_2 c_n\phi_n+\delta_3\sum_{p=n+2}^{N} F_{pn}\theta_p+\delta_4 c_n\theta_n\right]=0,\\
&\sum_{p=n+2}^{N} F_{pn}\phi_p+\mu_4 c_n\phi_n+\mu_5\sum_{p=n+2}^{N} F_{pn}\theta_p+\mu_6 c_n\theta_n+ik\delta_5 c_n\theta_n=0,\\
&\sum_{p=n+2}^{N} F_{pn}\eta_p+\mu_7 c_n\eta_n+\mu_8 c_n\theta_n+\mu_9 c_n\phi_n+ik\delta_6 c_n\eta_n=0,
\end{aligned}\right\}\tag{A 1}$$

for $0 \leqslant n \leqslant N$, where $F_{pn} = p(p^2-n^2)$ and summations over p are restricted such that $p \equiv n \,(\mathrm{mod}\, 2)$. If the expansions (4.7) are used in the boundary conditions (3.13) one finds, on using the properties $T_n(\pm 1) = (\pm 1)^n$ and $T_n'(\pm 1) = (\pm 1)^{n-1} n^2$, that

$$\sum_{n=0}^{N}\phi_n = 0, \quad \sum_{n=0}^{N} n^2\phi_n = 0, \quad \sum_{n=0}^{N}\eta_n = 0, \quad \sum_{n=0}^{N}\theta_n = 0, \tag{A 2}$$

and

$$\sum_{n=1}^{N}\phi_n = 0, \quad \sum_{n=1}^{N} n^2\phi_n = 0, \quad \sum_{n=1}^{N}\eta_n = 0, \quad \sum_{n=1}^{N}\theta_n = 0, \tag{A 3}$$

with $n \equiv 0 \,(\mathrm{mod}\,2)$ in (A 2) and $n \equiv 1\,(\mathrm{mod}\,2)$ in (A 3). The equations (A 1)–(A 3) separate into two sets with no coupling between the odd-subscript coefficients and the even-subscript coefficients. There are solutions of the algebraic equations in which all the coefficients with odd subscripts are identically zero and these solutions yield approximations to $\bar{v}$, $\bar{s}$ and $\bar{n}$ which are even functions of ζ. In another set of solutions of (A 1)–(A 3) all the coefficients with even subscripts are zero and this set yields solutions for $\bar{v}$, $\bar{s}$ and $\bar{n}$ which are odd functions of ζ. To examine the even solution it is convenient to replace N by $2M$. On introducing the transformations $n = 2m$, $p = 2q$, $c_n = c_m$, $\phi_{2m} = \hat{\phi}_m$, $\eta_{2m} = \hat{\eta}_m$, $\theta_{2m} = \hat{\theta}_m$ the even equations in (A 1) readily transform to equations (4.8). The boundary equations (A 2) give rise to the system (4.9).

In an analogous manner, the odd solution is simplified by means of the transformation $N = 2M+1$, $n = 2m+1$, $p = 2q+1$, $c_n = 1$, $\phi_{2m+1} = \hat{\phi}_m$, $\eta_{2m+1} = \hat{\eta}_m$, $\theta_{2m+1} = \hat{\theta}_m$. The odd equations in (A 1) yield the system

$$\left.\begin{aligned}
&\frac{8}{3}\sum_{q=m+2}^{M} G_{qm}[(q-m)^2-1]\,[(q+m+1)^2-1]\,\hat{\phi}_q+4\mu_1\sum_{q=m+1}^{M} G_{qm}\hat{\phi}_q+\mu_2\hat{\phi}_m+\mu_3\hat{\eta}_m\\
&\quad+ik\left[4\delta_1\sum_{q=m+1}^{M} G_{qm}\hat{\phi}_q+\delta_2\hat{\phi}_m+4\delta_3\sum_{q=m+1}^{M} G_{qm}\hat{\theta}_q+\delta_4\hat{\theta}_m\right]=0,\\
&4\sum_{q=m+1}^{M} G_{qm}\hat{\phi}_q+\mu_4\hat{\phi}_m+4\mu_5\sum_{q=m+1}^{M} G_{qm}\hat{\theta}_q+\mu_6\hat{\theta}_m+ik\delta_5\hat{\theta}_m=0,\\
&4\sum_{q=m+1}^{M} G_{qm}\hat{\eta}_q+\mu_7\hat{\eta}_m+\mu_8\hat{\theta}_m+\mu_9\hat{\phi}_m+ik\delta_6\hat{\eta}_m=0,
\end{aligned}\right\}\tag{A 4}$$

where $G_{qm} = (2q+1)(q+m+1)(q-m)$ and $m = 0, 1, \ldots, M$. Equations (A 3) become

$$\sum_{q=0}^{M} \hat{\phi}_q = 0, \quad \sum_{q=0}^{M} (2q+1)^2 \hat{\phi}_q = 0, \quad \sum_{q=0}^{M} \hat{\theta}_q = 0, \quad \sum_{q=0}^{M} \hat{\eta}_q = 0. \tag{A 5}$$

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