On the Field-Induced Cholesteric-Nematic Transition in Cholesteric Liquid Crystals with Homeotropic Boundary Conditions

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Z. Naturforsch. **38a**, 1–9 (1983); received August 28, 1982

The influence of homeotropic boundary conditions on the cholesteric-nematic transition is discussed, starting from the assumption that the director field consists of only components perpendicular to the helix axis, which is directed parallel to the boundary planes. Attention is paid to the solution of Cladis and Kléman for the simpler case without magnetic field. Their solution, consisting of regularly spaced line singularities, is derived in another more transparent way. Besides it is shown that even director fields without singularities are possible. The presence of a magnetic field complicates the solution considerably. Now the relevant Euler-Lagrange equation is solved in an approximate way by partly resorting to the difference method. The usefulness of the method is demonstrated by applying this technique to the nematic-cholesteric transition and the Fréedericksz transition in nematics.

1. Introduction

The cholesteric-nematic transition is brought about by a magnetic (electric) field. This field is applied perpendicular to the helix axis. As soon as the field strength reaches a certain threshold value the system becomes a nematic, i.e. the period (pitch) λ of the helix diverges. This type of transition was discussed by de Gennes [1] and Meyer [2] for a cholesteric without boundary conditions. The corresponding transition and its counter part, the nematic-cholesteric transition, in a cholesteric with homeotropic boundary conditions were considered by Greubel [3] and Fischer [4]. According to Greubel the twist axis may be thought to be parallel to the boundary layers near the cholesteric-nematic transition and the threshold value of the applied field may be approximated by the corresponding one without boundary conditions. Cladis and Kléman [5] studied a similar situation without magnetic field. They obtained a solution describing a twisted configuration with periodically distributed disclinations on the boundaries.

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It is the purpose of this paper to discuss the cholesteric-nematic transition in the presence of homeotropic boundary conditions. A prerequisite for the appearance of this transition is the existence of a helix-like director field beneath the threshold value of the magnetic field. Such a type of director field was proposed by Cladis and Kléman [5]. This director field is the starting point of our analysis. First, for clearness sake, attention is paid to the simple case without magnetic field. Several types of solution are discussed. The solution of Cladis and Kléman is derived in a more transparent way. Even solutions without line singularities appear to be possible. Next the general case is discussed, where the resulting Euler-Lagrange equation is non-linear due to the presence of the magnetic field. The Euler-Lagrange equation is solved in an approximate way by changing it partly into a difference equation. In order to get an idea about the merits of this approximation the nematic-cholesteric transition is calculated in an analogous way. The Appendix is devoted to the usefulness of the difference method in the case of the Fréedericksz transition [6] in nematics. A simple relation is obtained for the distortion induced by sufficiently large magnetic fields.

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2. The Euler-Lagrange Equation

Consider a cholesteric layer of thickness d with homeotropic boundary conditions. The normal to the layer is taken to be parallel to the z-axis. Consequently the x and y components of the director $\boldsymbol{n}$ are zero at the boundaries. Next a magnetic field parallel to the z-axis is applied. The Frank free energy for a cholesteric in a magnetic field is given by

$$F = \tfrac{1}{2} \int \mathrm{d}\boldsymbol{r} \, [K_{11} (\operatorname{div} \boldsymbol{n})^2 + K_{22} (\boldsymbol{n} \cdot \operatorname{rot} \boldsymbol{n} - t_0)^2 + K_{33} (\boldsymbol{n} \times \operatorname{rot} \boldsymbol{n})^2 - \Delta\chi (\boldsymbol{n} \cdot \boldsymbol{H})^2], \quad (2.1)$$

where K_{11}, K_{22} and K_{33} are the Frank elastic constants for the basic distortions, splay, twist and bend, respectively, $\Delta\chi$ is the diamagnetic anisotropy and $\boldsymbol{H}$ denotes the magnetic field. The natural twist t_0 is related to the natural pitch p_0 through $t_0 = 2\pi/p_0$.

In order to investigate the cholesteric-nematic transition brought about by the magnetic field a helix-like solution is sought, where the helix axis is assumed to lie along the x-axis. This means that the director field is described by

$$n_x = 0, \quad n_y = \sin\theta(x, z), \quad n_z = \cos\theta(x, z), \quad (2.2)$$

where θ is the angle between the director and its projection on the z-axis. The function $\theta(x, z)$ satisfies the boundary conditions

$$\theta(x, 0) = \theta(x, d) = 0. \quad (2.3)$$

The functional dependence on x and z is determined by requiring that the Frank free energy must be stationary with respect to variations of θ. In order to avoid unnecessarily complicated mathematics most of the calculations are done assuming

$$K_{11} = K_{22} = K_{33} = K.$$

Substitution of (2.2) in the expression for the Frank free energy gives

$$F = \frac{K}{2} \int \mathrm{d}\boldsymbol{r} \, [\theta_z^2 + (\theta_x - t_0)^2 - \Lambda \cos^2\theta], \quad (2.4)$$

where

$$\Lambda = \frac{\Delta\chi H^2}{K}$$

and

$$\theta_k = \frac{\partial\theta}{\partial k}; \quad \theta_{kl} = \frac{\partial^2\theta}{\partial k \, \partial l}, \quad k, l = x, y, z.$$

The function $\theta(x, z)$ satisfies the Euler-Lagrange equation

$$\theta_{zz} + \theta_{xx} - \Lambda \cos\theta \sin\theta = 0. \quad (2.5)$$

Up to the present an explicit general solution of this non-linear partial differential equation is not available.

3. The Case $H = 0$

In order to find a director field of the form (2.2), that is periodic in the x-coordinate, with period λ say, and satisfies the homeotropic boundary conditions at $z = 0$ and $z = d$, one may wish to minimize the Frank free energy over a periodic region R: $0 \leqq x \leqq \lambda$, $0 \leqq z \leqq d$, subject to the boundary conditions (2.3) and the periodicity condition

$$\theta(0, z) = \theta(\lambda, z), \quad 0 \leqq z \leqq d. \quad (3.1)$$

As a consequence of the variational principle it follows that θ has to satisfy Laplace's equation

$$\theta_{zz} + \theta_{xx} = 0 \quad (3.2)$$

in the interior of R, together with the natural boundary condition

$$\theta_x(0, z) = \theta_x(\lambda, z), \quad 0 \leqq z \leqq d. \quad (3.3)$$

This natural boundary condition allows a continuation of the solution, defined for $0 \leqq x \leqq \lambda$, in a continuous differentiable way to a solution that is periodic in x. The only solution obtained in this way, however, is the trivial one $\theta = 0$, corresponding to a constant director field in the z-direction. This is a simple consequence of Green's Theorem

$$\iint_R \mathrm{d}x \, \mathrm{d}z \, \theta(\theta_{zz} + \theta_{xx}) = -\iint_R \mathrm{d}x \, \mathrm{d}z \, [\theta_z^2 + \theta_x^2] + \int_C \theta \frac{\partial\theta}{\partial n} \mathrm{d}s, \quad (3.4)$$

where $\partial/\partial n$ denotes differentiation with respect to the outward-drawn normal to the boundary curve C of the region R and $\mathrm{d}s$ is a line element of that curve. The conditions (2.3), (3.1) and (3.3) imply directly that the boundary integral vanishes, so that on account of (3.2) it is found that

$$\iint_R \mathrm{d}x \, \mathrm{d}z \, [\theta_z^2 + \theta_x^2] = 0, \quad (3.5)$$

i.e. θ is a constant, necessarily zero because of (2.3).

The lesson to be learned from this argument is that, if a helix-like solution of the form (2.2) has to be found, the function θ cannot be a smooth, periodic solution of Laplace's equation. The next-best thing to do is to look for a non-smooth periodic function that satisfies Laplace's equation everywhere except at a discrete set of values of x, where the solution or its derivatives may have discontinuities.

For that purpose solutions of Laplace's equation are looked for by separation of variables. Putting

$$\theta(x,z) = \psi(x)\,\varphi(z) \tag{3.6}$$

gives

$$\frac{\psi_{xx}}{\psi} = m^2 = -\frac{\varphi_{zz}}{\varphi}. \tag{3.7}$$

The separation constant m^2 follows from the boundary conditions (2.3), which imply

$$m^2 = n^2 q^2, \quad n = 1, 2, \dots \quad (\text{with } q = \pi/d) \tag{3.8}$$

and give rise to solutions

$$\theta_n(x,z) = \psi_n(x)\,\varphi_n(z) = \psi_n(x)\sin(nqz), \quad n = 1, 2, 3, \dots, \tag{3.9}$$

where $\psi_n(x)$ is an arbitrary linear combination of $\sinh(nqx)$ and $\cosh(nqx)$. The general solution of Laplace's equation satisfying the boundary conditions (2.3) then reads

$$\theta(x,z) = \sum_{n=1}^{\infty} a_n\,\psi_n(x)\sin(nqz). \tag{3.10}$$

As has already been pointed out, such a function is not periodic in x. A periodic structure, however, may be forced by allowing discontinuities.

First attention is payed to the particular solution $\theta_n(x,z)$. Two out of several ways are discussed to implement such a periodic structure.

The first way is obtained by restricting the possibilities to the following three reasonable requirements:

(1) at $z = d/2$ the director field must complete one full turn of 2π over one period.
(2) the discontinuities are spaced at distances equal to λ.
(3) the period λ is optimized in such a way that the Frank free energy density, obtained by dividing the Frank free energy per periodic cell by the volume of that cell, is minimized.

The function $\psi_n(x)$, defined by

$$\psi_n(x) = \alpha_n \sinh(nqx) \quad \text{for} \quad x \in (-\tfrac{1}{2}\lambda, \tfrac{1}{2}\lambda) \tag{3.11}$$

with

$$|\alpha_n| = \frac{\pi}{\sinh\left(nq\dfrac{\lambda}{2}\right)} \tag{3.12}$$

and continued periodically with period λ, gives rise to a director field that can be interpreted as a helix and satisfies (1) and (2), the discontinuities being found at

$$x = \tfrac{1}{2}(2k+1)\lambda, \quad k = 0, \pm 1, \pm 2, \dots.$$

The sign of the coefficient α_n and the length of the period can then be determined from requirement (3). The Frank free energy density is given by

$$\begin{aligned} f_n &= \frac{K}{2\lambda d}\int_0^d dz \int_{-\frac{1}{2}\lambda}^{+\frac{1}{2}\lambda} dx\,[(\varphi_n \psi_{n_x} - t_0)^2 + \varphi_{n_z}^2 \psi_n^2] \\ &= \frac{1}{2}Kt_0^2 + \frac{K}{2\lambda}\int_{-\frac{1}{2}\lambda}^{+\frac{1}{2}\lambda} dx\,[\tfrac{1}{2}\psi_{n_x}^2 + \tfrac{1}{2}n^2 q^2 \psi_n^2] \\ &\quad - \frac{2Kt_0}{n\pi\lambda}[\psi_n(\tfrac{1}{2}\lambda) - \psi_n(-\tfrac{1}{2}\lambda)]\,\delta_{n,\mathrm{odd}}, \end{aligned} \tag{3.13}$$

where

$$\delta_{n,\mathrm{odd}} = \begin{cases} 1 & \text{if } n \text{ is odd}, \\ 0 & \text{if } n \text{ is even}. \end{cases}$$

In order to find the minimum value of f_n as a function of λ the sign of α_n must be taken positive if $t_0 > 0$ for odd n, and can be taken to be positive for n even: the direction of the rotation of the helix then fits the natural rotation, thus

$$\psi_n(\tfrac{1}{2}\lambda) - \psi_n(-\tfrac{1}{2}\lambda) = 2\pi \tag{3.14}$$

and

$$f_n = \frac{1}{2}Kt_0^2 + \frac{K}{2\lambda}\int_{-\frac{1}{2}\lambda}^{+\frac{1}{2}\lambda} dx\,[\tfrac{1}{2}\psi_{n_x}^2 + \tfrac{1}{2}n^2 q^2 \psi_n^2] - \frac{4Kt_0}{n\lambda}\,\delta_{n,\mathrm{odd}}. \tag{3.15}$$

Note that (3.14) implies

$$\theta_n(\tfrac{1}{2}\lambda, z) - \theta_n(-\tfrac{1}{2}\lambda, z) = 2\pi\sin(nqz), \tag{3.16}$$

which shows that the discontinuities in these particular solutions are not disclinations but sheet singularities.

In order to determine λ the expression (3.15) must be minimized. Here only the case $n = 1$ is considered. The simplest way to proceed is to note that $\psi_1 = \psi$ satisfies

$$\psi_x^2 = C + q^2 \psi^2 \tag{3.17}$$

with $C = q^2 \alpha^2$ and that the dependence of C on λ can be expressed by

$$\lambda = \int_{-\pi}^{+\pi} [C + q^2 \psi^2]^{-1/2} \, d\psi . \tag{3.18}$$

Then f_1 can be written as

$$f_1 = \frac{1}{2} K t_0^2 - \frac{4 K t_0}{\lambda} - \frac{KC}{4} + \frac{K}{2\lambda} \int_{-\pi}^{+\pi} [C + q^2 \psi^2]^{1/2} \, d\psi \tag{3.19}$$

and $\partial f_1 / \partial \lambda$ reduces to

$$\frac{\partial f_1}{\partial \lambda} = \frac{4 t_0 K}{\lambda^2} - \frac{K}{2\lambda^2} \int_{-\pi}^{+\pi} [C + q^2 \psi^2]^{1/2} \, d\psi . \tag{3.20}$$

Hence there exists a unique optimal period λ, given implicitly by

$$8 t_0 = \int_{-\pi}^{+\pi} [C + q^2 \psi^2]^{1/2} \, d\psi , \tag{3.21}$$

provided that

$$8 t_0 > \int_{-\pi}^{+\pi} q \, |\psi| \, d\psi = q \pi^2 , \tag{3.22}$$

i.e.

$$d/p_0 > \pi^2/16 . \tag{3.23}$$

Clearly the appearing discontinuities are sheet singularities.

It is of interest to note that with the aid of the solutions (3.9) a non-singular director field can be composed. For that purpose consider the general solution

$$\theta(x, z) = \pi \sum_{n=1}^{\infty} a_n \frac{\sinh(nqx)}{\sinh(\frac{1}{2} n q \lambda)} \sin(nqz) \tag{3.24}$$

and require that $\theta(x, z)$ satisfies the relation

$$\theta\left(\frac{\lambda}{2}, z\right) - \theta\left(-\frac{\lambda}{2}, 2\right) = 2\pi \tag{3.25}$$

for all z with $0 < z < d$.

This requirement determines the coefficients α_n uniquely. It follows

$$\sum_{n=1}^{\infty} a_n \sin(nqz) = 1 \tag{3.26}$$

or

$$a_n = \frac{4}{n\pi} \delta_{n,\mathrm{odd}} . \tag{3.27}$$

Consequently the solution

$$\theta(x, z) = \sum_{k=0}^{\infty} \frac{4}{(2k+1)} \frac{\sinh((2k+1) q x)}{\sinh(\frac{1}{2}(2k+1) q \lambda)} \cdot \sin((2k+1) q z) \tag{3.28}$$

does not have a sheet singularity but only line singularities at $(x = -\frac{1}{4}\lambda, z = 0)$, $(x = -\frac{1}{4}\lambda, z = d)$, $(x = \frac{1}{4}\lambda, z = 0)$ and $(x = \frac{1}{4}\lambda, z = d)$. The corresponding jump is π. This means that, although $\theta(x, z)$ possesses singularities, the corresponding director field does not contain singularities because of the head-tail symmetry of the director.

The second way of implementing a periodic structure in the particular solution θ_n is to restrict the possibilities to the following three also reasonable requirements:

(1) at $z = d/2$ the director field must complete a turn of π over half a period;
(2) the discontinuities are spaced at distances equal to $\frac{1}{2}\lambda$;
(3) the period λ is optimized in such a way that the Frank free energy density of the smooth director field in a cell of half a period is minimized. This means that, considering a cell with the full period, the contribution due to the discontinuity of the director field half-way the period is neglected in minimizing the density per periodic cell.

The function $\psi_n(x)$, defined by

$$\psi_n(x) = \alpha_n \sinh(nqx) \quad \text{for} \quad x \in (-\tfrac{1}{4}\lambda, \tfrac{1}{4}\lambda) \tag{3.29}$$

with

$$|\alpha_n| = \frac{\pi}{2 \sinh\left(nq \dfrac{\lambda}{4}\right)} \tag{3.30}$$

and continued periodically with period $\lambda/2$, gives rise to a director field that can be interpreted as a helix with period λ due to the absence of head-tail effects. Such a director field satisfies (1) and (2), the discontinuities being found at

$$x = \tfrac{1}{4}(2k+1)\lambda, \quad k = 0, \pm 1, \pm 2, \ldots .$$

The sign of α_n and the length of the period are determined by requirement (3). The Frank free energy density over one period, neglecting the contribution due to the discontinuity, reads

$$f_n = \frac{K}{\lambda d} \int_0^d dz \int_{-\frac{1}{4}\lambda}^{+\frac{1}{4}\lambda} dx \, [(\varphi_n \psi_{n_z} - t_0)^2 + \varphi_{n_z}^2 \psi_n^2]$$

$$= \frac{1}{2} K t_0^2 + \frac{K}{\lambda} \int_{-\frac{1}{4}\lambda}^{+\frac{1}{4}\lambda} \mathrm{d}x \, [\tfrac{1}{2} \psi_{n_x}^2 + \tfrac{1}{2} n^2 q^2 \psi_n^2] - \frac{4 K t_0}{\pi \lambda n} [\psi_n(\tfrac{1}{4}\lambda) - \psi_n(-\tfrac{1}{4}\lambda)] \, \delta_{n,\text{odd}} \,. \tag{3.31}$$

Again, α_n is taken to be positive if $t_0 > 0$. Because of

$$\psi_n(\tfrac{1}{4}\lambda) - \psi_n(-\tfrac{1}{4}\lambda) = \pi \tag{3.32}$$

it is found that

$$f_n = \frac{1}{2} K t_0^2 + \frac{K}{\lambda} \int_{-\frac{1}{4}\lambda}^{+\frac{1}{4}\lambda} \mathrm{d}x \, [\tfrac{1}{2} \psi_{n_x}^2 + \tfrac{1}{2} n^2 q^2 \psi_n^2] - \frac{4 K t_0}{n \lambda} \delta_{n,\text{odd}} \,. \tag{3.33}$$

Note that (3.32) implies

$$\theta_n(\tfrac{1}{4}\lambda, z) - \theta_n(-\tfrac{1}{4}\lambda, z) = \pi \sin(n q z) \,, \tag{3.34}$$

which again shows that the discontinuities are walls. By way of example f_n is minimized for $n = 1$. Analogous to the previous calculation use is made of (3.17) with $\psi_1 = \psi$, where the dependence of C on λ reads in the underlying case

$$\tfrac{1}{2}\lambda = \int_{-\pi/2}^{+\pi/2} [C + q^2 \psi^2]^{-1/2} \, \mathrm{d}\psi \,. \tag{3.35}$$

Then f_1 can be written in the form

$$f_1 = \frac{1}{2} K t_0^2 - \frac{4 K t_0}{\lambda} - \frac{K C}{4} + \frac{K}{\lambda} \int_{-\pi/2}^{+\pi/2} [C + q^2 \psi^2]^{1/2} \, \mathrm{d}\psi \tag{3.36}$$

and $\partial f_1 / \partial \lambda$ reduces to

$$\frac{\partial f_1}{\partial \lambda} = \frac{4 K t_0}{\lambda^2} - \frac{K}{\lambda^2} \int_{-\pi/2}^{+\pi/2} [C + q^2 \psi^2]^{1/2} \, \mathrm{d}\psi \,. \tag{3.37}$$

Hence there exists a unique optimal period λ determined by

$$4 t_0 = \int_{-\pi/2}^{+\pi/2} [C + q^2 \psi^2]^{1/2} \, \mathrm{d}\psi \tag{3.38}$$

provided that

$$4 t_0 > \int_{-\pi/2}^{+\pi/2} q \, |\psi| \, \mathrm{d}\psi = q \frac{\pi^2}{4} \,, \tag{3.39}$$

i.e.

$$d/p_0 > \pi^2/32 \,. \tag{3.40}$$

Comparing this result with the previous result (3.21) it must be concluded that the second way of implementing a helix-like director field gives rise to a lower d/p_0 ratio for the appearance of this type of structure, if any.

So far for the investigation of the particular solution $\theta_n(z)$. By construction, for each n, θ_n has sheet singularities at well defined planes.

It is known that Cladis and Kléman [5] constructed a solution of Laplace's equation which satisfies the boundary conditions (2.3) and has only disclinations (i.e. line singularities) at regularly spaced intervals. More precisely, they showed that (in the underlying notation)

$$\theta_{\text{CK}}(x, z) = \frac{2\pi}{\lambda} x + \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \frac{\cosh\left(\frac{4\pi n}{\lambda}\left(z - \frac{d}{2}\right)\right)}{\cosh\left(\frac{2\pi n d}{\lambda}\right)} \sin\left(\frac{4\pi n x}{\lambda}\right) \tag{3.41}$$

satisfies

$$\theta_{xx} + \theta_{zz} = 0, \quad -\frac{\lambda}{4} < x < \frac{\lambda}{4}, \quad 0 < z < d, \tag{3.42}$$

$$\theta(x, 0) = \theta(x, d) = 0 \quad \text{for} \quad -\frac{\lambda}{4} < x < \frac{\lambda}{4}, \tag{3.43}$$

$$\theta\left(\frac{\lambda}{4}, z\right) - \theta\left(-\frac{\lambda}{4}, z\right) = \pi \quad \text{for} \quad 0 < z < d. \tag{3.44}$$

Note that in the expression for θ_{CK} there appear particular solutions of Laplace's equation viz. $(2\pi/\lambda) x$ and

$$\hat{\theta}_n(x, z) = \cosh\left(\frac{4\pi n}{\lambda}\left(z - \frac{d}{2}\right)\right) \sin\left(\frac{4\pi n}{\lambda} x\right).$$

Each of these solutions does not satisfy the boundary conditions (3.43), but in θ_{CK} they are taken together in such a way that the boundary conditions and the periodicity condition (3.44) are satisfied. It is also possible to construct the Cladis-Kléman solution with the particular solutions (3.29) considered above:

$$\theta_n(x, z) = \frac{\pi}{2} \frac{\sinh(n q x)}{\sinh\left(n q \frac{\lambda}{4}\right)} \sin(n q z) \,. \tag{3.45}$$

For that purpose consider

$$\theta(x, z) = \sum_{n=1}^{\infty} a_n \theta_n(x, z) \tag{3.46}$$

and require that $\theta(x, z)$ satisfies (3.44), i.e.

$$\sum_{n=1}^{\infty} a_n \sin(n q z) = 1 \quad \text{for} \quad z \in (0, d) \,. \tag{3.47}$$

This requirement determines a_n uniquely and gives

$$a_n = \frac{4}{\pi n}\,\delta_{n,\mathrm{odd}}\,. \tag{3.48}$$

Consequently

$$\theta(x,z) = \sum_{k=0}^{\infty} \frac{2}{(2k+1)} \frac{\sinh((2k+1)\,q x)}{\sinh\left((2k+1)\,q\,\frac{\lambda}{4}\right)} \cdot \sin((2k+1)\,q z) \tag{3.49}$$

is a solution of (3.42), (3.43) and (3.44). The solution (3.49) and that of Cladis-Klêman coincide because this boundary value problem is uniquely solvable.

4. The Cholesteric-Nematic Transition

First of all it must be remarked that minimization of the Frank free energy with $\theta(x,z)$ satisfying the boundary conditions (2.3) and (3.1) together with the natural boundary condition (3.3) gives rise to $\theta(x,z) = 0$. It can be proven that non-trivial solutions of (2.5) satisfying these boundary conditions do not exist. Consequently periodic structures must be imposed as discussed in the previous section.

The influence of the homeotropic boundary conditions on the cholesteric-nematic transition can be reasonably approximated by resorting partly to the difference method. This method boils down to the following approximation of θ_z and θ_{zz}:

$$\theta_z\,(x,z) = \frac{1}{2h}\,[\theta(x,z+h) - \theta(x,z-h)], \tag{4.1 a}$$

$$\theta_{zz}(x,z) = \frac{1}{h^2}\,[\theta(x,z+h) + \theta(x,z-h) - 2\theta(x,z)] \tag{4.1 b}$$

with $h = d/N$ and $z = dj/N$, $j = 1, 2, \ldots, N-1$. Clearly this difference method makes explicitly use of the symmetry of the problem and the boundary conditions. In order to gain an insight into the effect of the boundary conditions it suffices to study the case $N = 2$ in a first approximation, i.e. only the middle of the layer, $z = d/2$, is considered. Then it holds

$$\theta_z\left(x, \frac{d}{2}\right) = 0, \tag{4.2 a}$$

$$\theta_{zz}\left(x, \frac{d}{2}\right) = -\frac{8}{d^2}\,\theta\left(x, \frac{d}{2}\right). \tag{4.2 b}$$

Next consider the non-linear partial differential equation (2.5) at $z = d/2$. Substitution of (4.2) gives rise to the non-linear differential equation

$$-\frac{8}{d^2}\,\theta + \theta_{xx} - \Lambda \sin\theta\cos\theta = 0, \tag{4.3}$$

where $\theta = \theta\left(x, \frac{d}{2}\right)$, i.e. θ depends only on the coordinate x.

In order to obtain a helix-like solution the second way of implementing a helix-like structure, as mentioned in Sect. 3, is followed. This means that again discontinuities are allowed in the form of walls. The differential equation (4.3) is solved in exactly the same way as the one concerning the cholesteric-nematic transition without boundary conditions [1]. For that purpose multiply (4.3) with θ_x and integrate. This gives

$$K\theta_x^2 - \frac{8}{d^2}\,K\theta^2 + \Delta\chi\,H^2\cos^2\theta = C\,. \tag{4.4}$$

The pitch $\lambda(H)$ of the helix is determined by

$$\lambda(H) = 4\sqrt{K}\int_0^{\pi/2}\left[C + \frac{8}{d^2}\,K\theta^2 - \Delta\chi H^2\cos^2\theta\right]^{-1/2} \mathrm{d}\theta. \tag{4.5}$$

Next it is important to know the dependence of C on H. For that purpose the free energy density associated with the differential equation (4.3) must be minimized with respect to C. This Frank free energy density reads

$$f = \frac{2}{\lambda(H)}\int_0^{\frac{1}{4}\lambda(H)} \mathrm{d}x\left[K(\theta_x - t_0)^2 + \frac{8}{d^2}\,K\theta^2 - \Delta\chi\,H^2\cos^2\theta\right]. \tag{4.6}$$

Substitution of (4.4) in (4.6) gives

$$f = \frac{1}{2}\,K t_0^2\left[1 - \frac{4\pi}{t_0\,\lambda(H)} - \frac{C}{K t_0^2} + \frac{8}{\lambda(H)\,t_0^2\sqrt{K}} \cdot \int_0^{\pi/2}\left(C + \frac{8}{d^2}\,K\theta^2 - \Delta\chi\,H^2\cos^2\theta\right)^{1/2} \mathrm{d}\theta\right]. \tag{4.7}$$

Minimization of f with respect to C results into

$$\frac{\partial f}{\partial C} = \left[\frac{4\pi}{t_0\,\lambda^2(H)} - \frac{8}{\lambda^2(H)\,t_0^2\sqrt{K}} \cdot \int_0^{\pi/2}\left(C + \frac{8}{d^2}\,K\theta^2 - \Delta\chi\,H^2\cos^2\theta\right)^{1/2} \mathrm{d}\theta\right]\frac{\mathrm{d}\lambda}{\mathrm{d}C}$$

$$-\frac{1}{K t_0^2}+\frac{4}{\lambda(H)\, t_0^2 \sqrt{K}} \cdot \int_0^{\pi/2}\left[C+\frac{8}{d^2} K \theta^2-\Delta\chi\, H^2 \cos^2\theta\right]^{-1/2} \mathrm{d}\theta=0. \tag{4.8}$$

This means, using Eq. (4.5),

$$\frac{\pi}{2} t_0 \sqrt{K}=\int_0^{\pi/2}\left[C+\frac{8}{d^2} K \theta^2-\Delta\chi\, H^2 \cos^2\theta\right]^{+1/2} \mathrm{d}\theta. \tag{4.9}$$

The critical field H_1 inducing the cholesteric-nematic transition is obtained in the following way. At the transition it holds $\lambda(H_1) \rightarrow \infty$. According to (4.5) this means that

$$\left[C_1+\frac{8}{d^2} K \theta^2-\Delta\chi\, H_1^2 \cos^2\theta\right]^{-1/2}$$

must diverge at $\theta=0$, where $C_1=C(H_1)$. It follows immediately that

$$C_1=\Delta\chi\, H_1^2. \tag{4.10}$$

The equation that determines H_1 is obtained by substituting (4.10) in (4.9). It results

$$\frac{\pi}{2} t_0 \sqrt{K}=\int_0^{\pi/2}\left[\Delta\chi\, H_1^2 \sin^2\theta+\frac{8}{d^2} K \theta^2\right]^{1/2} \mathrm{d}\theta. \tag{4.11}$$

Analytical expressions for H_1 can be obtained for small p_0/d ratios. Then the critical field H_1 appears to be given by

$$\Delta\chi\, H_1^2=\frac{\pi^2}{4} t_0^2 K\left[1-\frac{8}{\pi^4} a\left(\frac{p_0}{d}\right)^2\right], \tag{4.12}$$

where

$$a=\int_0^{\pi/2} \mathrm{d}\theta \frac{\theta^2}{\sin\theta} \cong 1.56\,. \tag{4.13}$$

Expression (4.12) reduces to the result of de Gennes [1] and Meyer [2] in the limit $p_0/d \rightarrow 0$. In that limit the appearing sheet discontinuities disappear as well.

It should be remarked here that the difference method used, $N=2$, amounts to an approximation of the solution by a quadratic function of z:

$$\theta(x, z) \approx \theta\left(x, \frac{d}{2}\right) \cdot 4 \frac{z}{d}\left(1-\frac{z}{d}\right).$$

An approximation of the same status can be obtained by taking the first Fourier component only:

$$\theta(x, z) \approx \psi(x) \sin q z\,. \tag{4.14}$$

Inserting (4.14) into (2.5), and then taking $z=d/2$, shows that (4.3) changes into

$$-q^2 \psi+\psi_{xx}-\Lambda \sin\psi \cos\psi=0, \tag{4.15}$$

i.e. all subsequent calculations remain valid provided that $8/d^2$ is replaced by q^2.

The general case with mutually differing elastic constants can be dealt with in an analogous way. Now the critical field H_1 is determined by the equation

$$\frac{\pi}{2} t_0 \sqrt{K_{22}}=\int_0^{\pi/2} \mathrm{d}\theta\left[\Delta\chi\, H_1^2 \sin^2\theta+\frac{4}{d^2}(K_{33}+K_{11})\, \theta^2 +\frac{4}{d^2}(K_{33}-K_{11})(\theta \sin 2\theta-\sin^2\theta)\right]^{1/2}. \tag{4.16}$$

For small p_0/d ratios an analytical expression for H_1 can be obtained reading

$$\Delta\chi\, H_1^2=\frac{\pi^2}{4} t_0^2 K_{22}\left[1-\frac{4}{\pi^4}\left(\frac{K_{33}+K_{11}}{K_{22}} a +\frac{K_{33}-K_{11}}{K_{22}}(\pi-3)\right)\left(\frac{p_0}{d}\right)^2\right], \tag{4.17}$$

where the constant a is given by (4.13). In the limit $(p_0/d) \rightarrow 0$ this expression reduces to the well-known result.

5. The Nematic-Cholesteric Transition

In order to calculate the nematic-cholesteric transition the director field is described by

$$n_x=\sin\theta \sin\varphi, \quad n_y=\sin\theta \cos\varphi, \quad n_z=\cos\theta, \tag{5.1}$$

where θ is the angle between the director and its projection on the z-axis, being perpendicular to the layer, and φ is the angle between the projection of $\boldsymbol{n}$ on the xy-plane and the y-axis. The functions θ and φ are assumed to be only dependent on z. The resulting Frank free energy density is now given by

$$\begin{aligned} f=\frac{1}{2d} \int_0^d \mathrm{d}z\, [&(K_{11} \sin^2\theta+K_{33} \cos^2\theta)\, \theta_z^2 \\ &+(K_{22} \sin^2\theta+K_{33} \cos^2\theta) \sin^2\theta\, \varphi_z^2 \\ &-2 K_{22}\, t_0 \sin^2\theta\, \varphi_z+K_{22}\, t_0^2-\Delta\chi\, H^2 \cos^2\theta]. \end{aligned} \tag{5.2}$$

The functions $\varphi(z)$ and $\theta(z)$ are determined by the requirement that they must minimize f. This means that they satisfy the following Euler-Lagrange equations:

$$\frac{d}{dz}\,[\sin^2\theta\,[(K_{22}\sin^2\theta + K_{33}\cos^2\theta)\,\varphi_z - K_{22}\,t_0]] = 0\,, \tag{5.3 a}$$

$$\begin{aligned}&(K_{11}\sin^2\theta + K_{33}\cos^2\theta)\,\theta_{zz} + (K_{11}-K_{33})\sin\theta\cos\theta\,\theta_z^2\\ &\quad - (K_{22}\sin^2\theta + K_{33}\cos^2\theta)\sin\theta\cos\theta\,\varphi_z^2\\ &\quad - (K_{22}-K_{33})\sin^3\theta\cos\theta\,\varphi_z^2 + 2K_{22}\,t_0\sin\theta\cos\theta\,\varphi_z\\ &\quad - \Delta\chi\,H^2\sin\theta\cos\theta = 0\,.\end{aligned} \tag{5.3 b}$$

It follows directly from (5.3 a) that

$$\varphi_z = \frac{K_{22}\,t_0}{K_{22}\sin^2\theta + K_{33}\cos^2\theta}\,. \tag{5.4}$$

Substitution of (5.4) in (5.3 b) gives the equation for θ:

$$\begin{aligned}&(K_{11}\sin^2\theta + K_{33}\cos^2\theta)\,\theta_{zz} + (K_{11}-K_{33})\sin\theta\cos\theta\,\theta_z^2\\ &\quad + K_{33}K_{22}^2\,t_0^2\,\frac{\sin\theta\cos\theta}{[K_{22}\sin^2\theta + K_{33}\cos^2\theta]^2}\\ &\quad - \Delta\chi\,H^2\sin\theta\cos\theta = 0.\end{aligned} \tag{5.5}$$

The critical field H_2 is obtained by linearizing this equation. Such a procedure is allowed, because θ is very small just below the critical field H_2. Then the following equation results:

$$K_{33}\,\theta_{zz} = \left(\Delta\chi\,H^2 - \frac{K_{22}^2}{K_{33}}\,t_0^2\right)\theta\,. \tag{5.6}$$

In order to compare the resulting critical field H_2 with the corresponding critical field H_1 that is characteristic for the cholesteric-nematic transition, (5.6) is solved by making use of the difference method (4.2) with $N = 2$. Then it holds

$$\Delta\chi\,H_2^2 = \frac{K_{22}^2}{K_{33}}\,t_0^2 - K_{33}\,\frac{8}{d^2}\,. \tag{5.7}$$

It should be remarked here that the exact expression for the critical field H_2 can be rather easily determined from (5.6). The first non-trivial solution, satisfying the boundary conditions $\theta(0) = \theta(d) = 0$, is given by $\theta(z) = \sin(\pi/d)\,z$. This solution appears as soon as the field strength becomes smaller than the value given by

$$\Delta\chi\,H_2^2 = \frac{K_{22}^2}{K_{33}}\,t_0^2 - K_{33}\left(\frac{\pi}{d}\right)^2. \tag{5.8}$$

This result was first obtained by Greubel [3] in a slightly different way. Later on the complete solution of the set of Eqs. (5.3) was given by Fischer [4]. Comparing the expressions (5.7) and (5.8) it may be concluded that the simplest difference method, i.e. $N = 2$, gives quite satisfactory answers in a first approximation.

6. Conclusion

A helix-like director field satisfying homeotropic boundary conditions and having only components perpendicular to the helix axis, which is directed parallel to the boundary planes, can be a smooth periodic function, although the solutions of Laplace's equation always contain singularities in that case. According to Cladis and Kléman such a director field must contain line singularities. However, the analysis in this paper shows clearly that non-singular solutions can be constructed. In this context it is worth-while to remark that the relevance of the singular and non-singular solutions cannot be compared, because the energy density at singularities is not well-defined.

In the case of the one-constant approximation a lower bound for the critical field H_1 can be easily obtained by approximating θ by $(\pi/2)\sin\theta$. Then it follows

$$\Delta\chi\,H_1^2 = K\,\frac{\pi^2}{4}\left[t_0^2 - \frac{8}{d^2}\right]. \tag{6.1}$$

This means that a helix-like solution is certainly impossible as soon as

$$\frac{p_0}{d} > \frac{1}{2}\,\pi\sqrt{2}\,. \tag{6.2}$$

Clearly the existence of a critical width of the layer in order to allow for a helix with its axis along the x-direction is in total conformity with expectations based upon physical reasoning. An analogous conclusion can be drawn for the appearance of a helix with its axis along the z-axis using the result concerning the nematic-cholesteric transition. The estimation (6.2) is qualitatively confirmed by the exact result (3.12).

Finally the question remains, also in view of the rather artificial construction of the director field, whether this type of cholesteric-nematic transition is actually observed in displays [5, 7]. With respect to that it should be remarked that Cladis and Kléman pointed out that the assumption, $n_x = 0$, is not obeyed in the absence of a magnetic field. Similar remarks have been made by Wahl [8], who studied cholesteric inversion structures generated by torsional shear flow. Clearly it would be of interest to study the director field (5.1) with θ and φ being functions of both x and z. The resulting mathematical problem, however, is quite difficult and up to now unsolved.

Appendix

In order to gain insight into the usefulness of the difference method it is quite instructive to apply this method to the Fréedericksz transition [6]. Consider e.g. a nematic planar layer of thickness d with rigid boundary conditions. The normal to the layer is taken to be parallel to the z-axis. The components of the director are given by

$$n_x = \cos\theta(z); \quad n_y = \sin\theta(z); \quad n_z = 0. \qquad \text{(A.1)}$$

The boundaries of the layers are defined by $z = 0$ and $z = d$. Because of the planar boundary conditions it holds

$$\theta(0) = \theta(d) = 0. \qquad \text{(A.2)}$$

Next a magnetic field is applied in the y-direction. The Frank free energy per unit area reads

$$F = \tfrac{1}{2}\int_0^d [K_{22}\,\theta_z^2 - \Delta\chi\, H^2 \sin^2\theta]\, \mathrm{d}z, \qquad \text{(A.3)}$$

where $\theta(z)$ is determined by the Euler-Lagrange equation

$$\frac{K_{22}}{\Delta\chi\, H^2}\,\theta_{zz} = -\sin\theta\cos\theta. \qquad \text{(A.4)}$$

In terms of the simplest difference method, i.e. $N = 2$, expression (A.4) changes into

$$-\frac{8K_{22}}{d^2\Delta\chi\, H^2}\,\theta\left(\frac{d}{2}\right) = -\sin\theta\left(\frac{d}{2}\right)\cos\theta\left(\frac{d}{2}\right). \qquad \text{(A.5)}$$

Just above the threshold $\theta(d/2)$ is small. This means that $\sin\theta(d/2)\cos\theta(d/2)$ may be approximated by $\theta(d/2)$. Consequently the threshold value of the critical field follows from

$$\frac{8K_{22}}{d^2\Delta\chi\, H_{cr}^2} = 1 \quad \text{or} \quad H_{cr} = \frac{2\sqrt{2}}{d}\sqrt{\frac{K_{22}}{\Delta\chi}}. \qquad \text{(A.6)}$$

The exact value, as follows from (A.4), is given by $\frac{\pi}{d}\sqrt{\frac{K_{22}}{\Delta\chi}}$. This means that the simplest difference method approximates the real threshold value already up to 90%. The distortion, induced by a magnetic field, $H > H_{cr}$, can be easily estimated using (A.5). It follows, putting $\theta(d/2) = \frac{1}{2}\pi(1-\varepsilon)$,

$$\left(\frac{H_{cr}}{H}\right)^2 \pi(1-\varepsilon) = \sin\pi\varepsilon. \qquad \text{(A.7)}$$

If H is large compared to H_{cr}, $\sin\pi\varepsilon$ may be approximated by $\pi\varepsilon$, and ε is given by

$$\varepsilon = \alpha^2/(1+\alpha^2), \quad \alpha = H_{cr}/H. \qquad \text{(A.8)}$$

Putting $H = 2H_{cr}$ and $H = 4H_{cr}$ one finds $\varepsilon = \frac{1}{5}$ and $\varepsilon = \frac{1}{17}$, respectively. These values are quite close to the exact values obtained by numerical integration on the computer [9].

According to the remark in Sect. 4 this result can also be obtained by putting $\theta(z) = b\sin qz$. Then (A.5) reads

$$-q^2\frac{K_{22}}{\Delta\chi\, H^2}\, b = -\frac{1}{2}\sin 2b. \qquad \text{(A.9)}$$

This relation determines the exact value of H_{cr}; approximate values for the amplitude b can be obtained according to the procedures mentioned above.

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