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The influence of homeotropic and planar boundary conditions on the field induced cholesteric-nematic transition

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Résumé. — On étudie la transition cholestérique-nématique induite par un champ électrique dans le cas où l'axe hélicoïdal est parallèle aux parois. On obtient des solutions approchées pour la valeur critique du champ électrique pour des conditions d'ancrage homéotropes et planaires.

Abstract. — The field induced cholesteric-nematic transition is discussed for the case where the helical axis is parallel to the plane of the sample. Approximate solutions for the critical field are presented for both homeotropic and planar boundary conditions.

1. **Introduction.** — The field induced cholesteric-nematic transition (helix-unwinding) for an infinite medium has been described by de Gennes [1]; for a discussion see [2, 3]. The corresponding boundary-value problem for the case where the helical axis is perpendicular to the bounding surfaces has been described by Dreher [4]. Here we should like to discuss the boundary-value problem for the helix-unwinding when the helical axis is parallel to the surfaces of a finite sample for both homeotropic and planar boundary conditions. In order to do so we shall formulate and solve the boundary value problem without field in section 3. There after in section 4 these results will be used in an approximate way by introducing a surface field acting in the same way as the applied external field. So the solution of the problem is after all along the lines discussed in [1, 2, 3], which therefore are described first in section 2. Finally a discussion of the results is presented in section 5.

2. **General formulation.** — Consider a finite cholesteric liquid crystal confined between two glass plates and subject to an external electric field E. The director dependent part of the free energy density F is given by :

$$2F = K_{11}(\operatorname{div}\mathbf{n})^2 + K_{22}(\mathbf{n}.\operatorname{rot}\mathbf{n} + q_0)^2 + K_{33}(\mathbf{n}\wedge\operatorname{rot}\mathbf{n})^2 - \varepsilon_a(\mathbf{n}.\mathbf{E})^2 \quad (1)$$

where $q_0 = 2\pi/p_0$ and p_0 the natural pitch of the helix, directed along the z-axis.

The sample is bounded at $x = \pm d/2$ and is translationally invariant along the y-axis. The field is along the x-axis and therefore perpendicular to both the helical axis and the sample. The director configuration is described by :

$$n_x = \sin\varphi(x,z)\,,\quad n_y = \cos\varphi(x,z)\,,\quad n_z = 0 \quad (2a)$$

$$n_x = \cos\varphi(x,z)\,,\quad n_y = \sin\varphi(x,z)\,,\quad n_z = 0 \quad (2b)$$

together with the constraint $\varphi(z, x = \pm d/2) = \pi/2$. The above configurations then correspond to homeotropic and planar boundary conditions respectively.

With $K_{11} = K_{33} = K$, $\gamma^2 = K_{22}/K$; $\tilde{x} = \gamma x$ and

$$\xi_{(0)}^{-2} = \varepsilon_a E^2/K_{22}\,,\quad \varepsilon_a > 0\,,$$

equation (1) becomes :

$$\frac{2F}{K_{22}} = \varphi_{,\tilde{x}}^2 + (\varphi_{,z} - q_0)^2 - \xi_{(0)}^{-2}.g(\varphi) \quad (3)$$

where $g(\varphi)$ is $\sin^2\varphi$ or $\cos^2\varphi$ depending on the configuration. Here we use the notation $\varphi_{,z} = \dfrac{\partial\varphi}{\partial z}$, $\varphi_{,zz} = \dfrac{\partial^2\varphi}{\partial z^2}$. Minimizing the free energy one finds :

$$\varphi_{,zz} + \varphi_{,\tilde{x}\tilde{x}} + \frac{1}{2}\xi_{(0)}^{-2}\frac{\partial}{\partial\varphi}g(\varphi) = 0\,. \quad (4)$$

For later use we here recall the usual expressions for the actual pitch of the helix and for the free energy density f averaged over one period.

$$p = 4 \int_0^{\pi/2} \mathrm{d}\varphi . \varphi_{,z}^{-1} \tag{5}$$

$$f = \frac{4}{p} \int_0^{\pi/2} \mathrm{d}\varphi . \varphi_{,z}^{-1} . F . \tag{6}$$

In order to show how the boundary conditions can be fitted in, we shall first recapitulate in brief the derivation of the critical field for the helix-unwinding for the infinite medium. In that case $\varphi = \varphi(z)$ and consequently $\varphi_{,\tilde{x}\tilde{x}} = 0$. Then equation (4) can be integrated to give :

$$\varphi_{,z}^2 = c_0 - \xi_{(0)}^{-2} . g(\varphi) . \tag{7}$$

The integration constant c_0 can be found by minimizing the free energy density f with respect to c_0. After substituting equation (7) into equation (3) we find from equation (6) :

$$\frac{f}{2 K_{22}} = (q_0^2 - c_0) + \frac{8}{p} \left(\left[\int_0^{\pi/2} \mathrm{d}\varphi . \varphi_{,z} \right] - \frac{\pi}{2} q_0 \right) . \tag{8}$$

Since

$$2 \frac{\partial}{\partial c_0} \left(\int_0^{\pi/2} \mathrm{d}\varphi . \varphi_{,z} \right) = \int_0^{\pi/2} \mathrm{d}\varphi . \varphi_{,z}^{-1} = \frac{p}{4},$$

the conditions $\partial f / \partial c_0 = 0$ and $\partial p / \partial c_0 \neq 0$ yield the following equation,

$$\frac{\pi}{2} q_0 = \int_0^{\pi/2} \mathrm{d}\varphi \cdot \varphi_{,z} = c_0^{1/2} \cdot \int_0^{\pi/2} \mathrm{d}\varphi \cdot \left(1 - \frac{g(\varphi)}{c_0 \xi_{(0)}^2} \right)^{1/2}, \tag{9}$$

which defines c_0 as a function of $\xi_{(0)}^2$ i.e. of E^2.

The dependence of the actual pitch on c_0 is found by substituting equation (7) into equation (5) :

$$p = 4 c_0^{-1/2} \cdot \int_0^{\pi/2} \mathrm{d}\varphi \cdot \left(1 - \frac{g(\varphi)}{c_0 \xi_{(0)}^2} \right)^{-1/2} . \tag{10}$$

We now consider the two limits $c_0 \xi_{(0)}^2 = \infty$, i.e. $E^2 = 0$, and $c_0 \xi_{(0)}^2 = 1$.

When $c_0 \xi_{(0)}^2 = \infty$, equation (9) gives $c_0 = q_0^2$; the equations (7) and (10) then yield $\varphi = q_0 z$ and $p = 2 \pi / q_0 = p_0$. On the other hand when $c_0 \xi_{(0)}^2 = 1$ we find from equation (10) with $g(\varphi)$ equal to $\sin^2 \varphi$ or $\cos^2 \varphi$ that p diverges at $\varphi = \pi/2$ or at $\varphi = 0$. The field for which this divergency of p occurs, is found from equation (9). With $c_0 \xi_{(0)}^2 = 1$, $c_0 = \xi_{(0)}^{-1}$ we find :

$$\frac{\pi}{2} q_0 = \xi_{(0)}^{-1} = \left(\frac{\varepsilon_a}{K_{22}} \right)^{1/2} \cdot E , \tag{11}$$

which determines the critical field for the cholesteric-nematic transition.

3. **The boundary-value problem.** — We now return to equation (4) for the bounded medium, which will be solved approximately by considering the term $\varphi_{,\tilde{x}\tilde{x}}$ as a perturbation term to be described as a function of φ. We therefore first consider the perturbation of the helical structure in a finite sample due to the constraints on the director at the surfaces. Consider therefore equation (4) without the field term i.e. :

$$\varphi_{,zz} + \varphi_{,\tilde{x}\tilde{x}} = 0 , \tag{12}$$

subject to the constraint that at the boundaries, defined by $x = \pm d/2$, $| \varphi | = \pi/2$, whereas for $x = 0$, φ should approach its bulk value qz for $qd > 1$. The actual value of q introduced here is in principle not equal to q_0, but has to be determined as a function of q_0 and d by minimizing the averaged elastic free energy density, defined as a function of q. Since $\varphi(x) = \varphi(-x)$ it is convenient to introduce the variable $k = \gamma . (d/2 - x)$ which is zero for $x = \pm d/2$ and equal to $\gamma d/2$ when $x = 0$; moreover $\varphi_{,\tilde{x}\tilde{x}} = \varphi_{,kk}$. The boundary-value problem can then be defined as $\varphi(k, z = \pm \pi/2 q) = \pm \pi/2$ and $\varphi(k, z = 0) = 0$ when $k > 0$, whereas for $k = 0$, $\varphi(k, z = \pm 0) = \pm \pi/2$; here φ jumps by angle π. This problem for φ can be solved analytically in the domain $0 \leqslant k \leqslant \gamma d/2$, $-\pi/2 q \leqslant z \leqslant +\pi/2 q$ (since $\varphi(z) = -\varphi(-z)$ it is sufficient to consider $0 \leqslant z \leqslant \pi/2 q$) using the technique of conformal mapping. The procedure is essentially the same as that described in references [5] and [6] and will therefore be discussed only in brief. The point is that $\varphi(k, z)$ can be considered as the imaginary part of a complex function $w(s) = \chi + i\varphi$, which is holomorphic when considered as a function of the complex variable $s = k + iz$ in the strip $0 \leqslant \mathrm{Im}\, s \leqslant \pi/2 q$. Then the transformation $\sigma = \cosh 2 qs$ maps the strip $0 \leqslant \mathrm{Im}\, s \leqslant \pi/2 q$ of the complex s-plane upon the upperhalf of the complex σ-plane, while $w(s)$ is transformed into $v(\sigma) = w(s(\sigma))$. The solution of the corresponding boundary-value problem for $v(\sigma)$ in the complex σ-plane is easily found to be $v(\sigma) = 1/2 . \log(\sigma - 1)$. Backwards transformation yields :

$$w(s) = \frac{1}{2} \log (2 \sinh^2 qs) . \tag{13}$$

Taking real and imaginary parts one obtains :

$$\chi = \frac{1}{2} \log \left(\frac{2(\alpha^2 + \beta^2)}{(1 + \alpha^2)(1 - \beta^2)} \right) \tag{14}$$

$$\varphi = \arctan \left(\frac{\alpha}{\beta} \right) \tag{15}$$

where $\alpha = \tan qz$ and $\beta = \tanh kq$. Now we have :

$$\varphi_{,k} = \mathrm{Im} \left(\frac{\partial w}{\partial s} \right), \quad \varphi_{,z} = \mathrm{Re} \left(\frac{\partial w}{\partial s} \right),$$
$$\varphi_{,kk} = -\varphi_{,zz} = \mathrm{Im} \left(\frac{\partial^2 w}{\partial s^2} \right), \tag{16}$$

where $\partial w/\partial s$ is found to be :

$$\frac{\partial w}{\partial s} = q.(1 + 2\,e^{-2w})^{1/2} \tag{17}$$

$$= q.(1 + u\cos 2\varphi - iu\sin 2\varphi)^{1/2}.$$

Consequently one finds :

$$\frac{\partial^2 w}{\partial s^2} = -2\,q^2\,e^{-2w} = -q^2\,u(\cos 2\varphi - i\sin 2\varphi) \tag{18}$$

$$\varphi_{,kk} = q^2\,u\sin 2\varphi. \tag{19}$$

Here we have replaced the variable χ by the variable u defined as $u = 2\,e^{-2\chi}$; from equation (14) it follows :

$$u = \frac{(1+\alpha^2)(1-\beta^2)}{\alpha^2+\beta^2} = (1-\beta^2)\left(1+\sum_{n=1}^{\infty}\left(\frac{1-\beta^2}{1+\alpha^2}\right)^n\right). \tag{20}$$

Before continuing with equation (4), we now first determine q as function of q_0 and d. Therefore we calculate the elastic free energy density averaged over the thickness d and the period $p = 2\pi/q$. Since $dk\,dz = d\chi\,d\varphi(\varphi_{,k}^2 + \varphi_{,z}^2)^{-1}$ and $d\chi = -du/2u$ we find in a first approximation

$$\frac{\bar{f}}{2K_{22}} = (q - q_0)^2 + \frac{2}{\gamma d}\,\frac{4}{p}\int_0^{u_0}\frac{du}{u}\times$$

$$\times\int_0^{\pi/2} d\varphi\,\varphi_{,k}^2(\varphi_{,k}^2 + \varphi_{,z}^2)^{-1}. \tag{21}$$

The upperbound u_0 stems from the fact that we have to exclude the singular region at $k = 0$, $z = 0$, where the orientation of the director is undetermined [6]. This region, known as a disclination, can be assumed to have a cylindrical shape with a core radius a of a few molecular lengths. From equation (20) we find with $\beta(k = 0) = 0$ that $u_0 = \sin^{-2} qa$. The calculation of equation (21) is done in the appendix. The result there obtained is :

$$\frac{\bar{f}}{2K_{22}} = (q - q_0)^2 + \frac{q}{2\gamma d}\cdot(1 - 2\log 2qa). \tag{22}$$

Minimizing $\bar{f}$ with respect to q we find :

$$q = q_0\left(1 - \frac{|1 + 2\log 2qa|}{4\gamma dq_0}\right) \tag{23}$$

which in principle is the same result as presented and discussed in reference [7]. Equation (23) implies that in a finite sample q is smaller than q_0; so the actual pitch $p = 2\pi/q$ is greater then the equilibrium value $p_0 = 2\pi/q_0$. Moreover in order that p remains finite, $q_0\,\gamma d$ should be greater then $1/4 * |1 + 2\log 2qa|$, which gives a lower limit to the thickness d. Though we may estimate qa to be in the order of 10^{-2} up to 10^{-1}, we will for the moment not discuss the quantitative aspects of this condition. This point will be considered in section 5.

We now return to our main problem. Though we have found solutions for all relevant derivatives of $\varphi(\tilde{x}, z)$ in terms of the new variables u and φ, with q as known parameter, the actual solution of equation (4) in terms of both these variables is still very cumbersome.

As a first step therefore we shall seek a solution for the critical field for helix-unwinding in the bulk, i.e. for $x = 0$, $k = \gamma d/2$. The term $\varphi_{,\tilde{x}\tilde{x}}$ in equation (4) can then be considered as a fixed surface field of strength $2\,q^2\,u(k = \gamma d/2)$, acting on the helical structure in the same way as the external electric field, both contributions being defined as a function of φ only. This approximation is motivated by the behaviour of u as a function of $\beta = \tanh qk$. At the surfaces $\beta(k = 0) = 0$, u is maximal and p, that is $\varphi_{,z}^{-1}$ diverges at $z = \pi/2q$ as $(1 - u)^{-1} = \alpha^2(z = \pi/2q)$, giving rise to the above mentioned disclination at $z = 0$. Away from the surface however, where qk and $\beta(qk)$ are greater then zero, u is mainly determined by β; for qk only somewhat greater then one, u can already be approximated by $1 - \beta^2 = \cosh^{-2} qk$. Note that for $\gamma qd \gg 1$, $\beta = 1$ and $u = 0$. Then the influence of the boundaries on the bulk becomes negligible and we are left with the unperturbed problem described above.

4. **The cholesteric-nematic transition.** — We now consider the cholesteric-nematic transition in a finite sample. According the discussion in the previous section the procedure is straight forward. Substitution of equation (19) into equation (4) yields :

$$\varphi_{,zz} = -\frac{1}{2}\,\xi_{(0)}^{-2}\,\frac{\partial}{\partial\varphi}\,g(\varphi) + \frac{1}{2}\,q^2\,u\,\frac{\partial}{\partial\varphi}\cos 2\varphi \tag{24}$$

which can be integrated to give :

$$\varphi_{,z}^2 = c_0 - \xi_{(0)}^{-2}\,g(\varphi) + q^2\,u\cos 2\varphi. \tag{25}$$

Here we take u equal to $\cosh^{-2}(\gamma qd/2)$. Now we discriminate between the two configurations described by (2a) and (2b) corresponding to homeotropic and planar boundary conditions respectively. In the first case, where $g(\varphi) = \sin^2\varphi$, equation (25) is written as :

$$\varphi_{,z}^2 = c_1 - \xi_{(1)}^{-2}\sin^2\varphi,\quad \xi_{(1)}^{-2} = \xi_{(0)}^{-2} + 2\,q^2\,u \tag{26}$$

whereas in the second case, where $g(\varphi) = \cos^2\varphi$, we have :

$$\varphi_{,z}^2 = c_2 - \xi_{(2)}^{-2}\cos^2\varphi,\quad \xi_{(2)}^{-2} = \xi_{(0)}^{-2} - 2\,q^2\,u. \tag{27}$$

We then follow the derivation described above with c_0 and $\xi_{(0)}$ replaced by c_i and $\xi_{(i)}$ with $i = 1, 2$. Equation (11) which describes the condition for the divergence of p then reads $q_0 \pi/2 = 1/\xi_{(i)}$, where $\xi_{(i)}$, $i = 1, 2$, is defined in equations (26) and (27) respectively. So we find that the critical field for the cholesteric-nematic transition in the bulk is given by :

$$E_{1,2}^2 = \frac{K_{22}}{\varepsilon_a}\left[\left(\frac{q_0 \pi}{2}\right)^2 \mp 2\, q^2 . \cosh^{-2}\left(\frac{\gamma q d}{2}\right)\right] \quad (28)$$

corresponding to homeotropic and planar boundary conditions respectively. In the limit $\gamma qd \gg 1$, this equation reduces to equation (11) for the unperturbed problem. Moreover it should be noted that the correction term in equation (28) is expressed in terms of $q(d)$, defined in equation (23).

5. **Discussion.** — Our main result is equation (28), which gives the threshold field for the cholesteric-nematic transition in a finite sample with the pitch of the helix parallel to the surfaces, for both homeotropic and planar boundary conditions. It shows that the threshold field for homeotropic or planar boundary conditions is lower or higher then that for an infinite medium. This result is exactly what one would expect on physical grounds ; with homeotropic boundary conditions, the director at the surfaces is already along the field direction, whereas with planar boundary conditions, the director at the surfaces is forced to stay perpendicular to the field direction. Experimental evidence for these facts has already been presented [8, 9, 10].

There remains the question whether the two dimensional director configuration used in the derivation of equation (28) is suited for that purpose. Indeed it is clear that the variety of textures encountered in practice, dependent on $q_0\, d$ and the boundary conditions, cannot be described in all details by equation (2). However we are not aiming at that ; moreover we can't. In literature already many topological models have been proposed and discussed to account for the various experimental, observations. A discussion of these can be found f.i. in references [11] and [12]. These models have in common that, in order to adapt the director to the boundary conditions without singularities at the surfaces, the director configuration is three dimensional ; however they are not exclusive, neither do they give an analytical description. The refinement of – and the differences between these models are rather important for an adequate description of the various optical observations, but don't give rise to great variations in the free energy density. This last point is brought afore more clearly in reference [13], where computer calculations have been done on realistic, rather complicated models for the fingerprint texture. Therefore it seems realistic to accept that the above calculated elastic free energy density is a fairly good approximation to calculate the threshold field for the cholesteric-nematic transition, subject to the prescribed boundary conditions ; for our director configuration accounts for the overall helical configuration adapted to these boundary conditions, which in fact is the most essential feature of all topological models with, grosso modo, the same free energy.

In connection with the latter statement we like to discuss the condition $\gamma d q_0 > 1/4 * \mid 1 + 2 \log 2\, qa \mid$, necessary to have a properly defined two dimensional helical structure with a finite $p = 2\, \pi/q$. In reference [6] disclination lines in twisted nematics have been studied. From the experimental data it was derived that the quantity $\pi b/2\, h$, where b is the radius of the core of the disclination and $2\, h$ is the thickness over which the director is rotated by an angle $\pi/2$, had a constant value 4.8×10^{-2}, independent of the thickness $2\, h$ of three different samples. Since $2\, qa$ is equivalent to $\pi b/2\, h$, we may accept the above value for $2\, qa$. We then obtain

$$\gamma d q_0 > 1/4 * \mid 1 + 2 \log 0.048 \mid \cong 1 ,$$

which defines the validity of the model. Since equation (28) holds for $\gamma qd > 2$ both conditions are consistent for $q_0/2 \leqslant q \leqslant q_0$.

Appendix. — Equation (21) for the averaged elastic free energy density is written as :

$$\frac{\overline{f}}{2\, K_{22}} = (q - q_0)^2 + \frac{f^{(1)}}{2\, K_{22}} . \quad (A.1)$$

From equations (16), (17) and (21) we then find :

$$\begin{aligned}\frac{f^{(1)}}{2\, K_{22}} &= \frac{2}{\gamma\, dp} \cdot \int_0^{u_0} \frac{du}{u} \int_0^{\pi/2} d\varphi \left(\frac{[(1 + u)^2 - 4\, u \sin^2 \varphi]^{1/2} - [1 + u - 2\, u \sin^2 \varphi]}{[(1 + u)^2 - 4\, u \sin^2 \varphi]^{1/2}} \right) \\ &= \frac{2}{\gamma\, dp} \int_0^{u_0} \frac{du}{u} \int_0^{\pi/2} d\varphi \left(1 - \left(\frac{1 - u}{2}\right)\left(1 - \frac{4\, u \sin^2 \varphi}{(1 + u)^2}\right)^{-1/2} - \left(\frac{1 + u}{2}\right)\left(1 - \frac{4\, u \sin^2 \varphi}{(1 + u)^2}\right)^{1/2} \right) \\ &= \frac{2}{\gamma\, dp} \int_0^{u_0} \frac{du}{u} \left(\frac{\pi}{2} - \left(\frac{1 - u}{2}\right) \cdot K(k) - \left(\frac{1 + u}{2}\right) E(k) \right) .\end{aligned} \quad (A.2)$$

$K(k)$ and $E(k)$ are the usual notations for the complete elliptic integrals of the first and second kind respectively. Here the modulus $k = k(u)$ is defined by :

$$k^2 = \frac{4\,u}{(1+u)^2}. \tag{A.3}$$

Since $k(u) = k(u^{-1})$, equation (A.2) can be transformed into,

$$\frac{f^{(1)}}{2\,K_{22}} = \frac{2}{\gamma\, dp}\int_0^1 \frac{\mathrm{d}u}{u}\left(\frac{\pi}{2} - \left(\frac{1-u}{2}\right)K(k) - \left(\frac{1+u}{2}\right)E(k)\right) + \frac{2}{\gamma\, dp}\int_v^1 \frac{\mathrm{d}u}{u}\left(\frac{\pi}{2} + \left(\frac{1-u}{2\,u}\right)K(k) - \left(\frac{1+u}{2\,u}\right)E(k)\right) \tag{A.4}$$

where $v = u_0^{-1}$.

Since the complementary modulus k', defined by $(k')^2 = 1 - k^2$, is equal to $(1-u)/(1+u)$ and therefore $u = (1-k')/(1+k')$ with $u \leqslant 1$, Gauss transformation for the complete elliptic integrals then reads [14] :

$$K(u) = \frac{1}{1+u}K(k), \quad E(u) = \frac{1+u}{2}E(k) + \frac{1-u}{2}K(k). \tag{A.5}$$

Substituting for $K(k)$ and $E(k)$ into equation (A.4) we obtain :

$$\frac{f^{(1)}}{2\,K_{22}} = \frac{2}{\gamma\, dp}\int_0^1 \frac{\mathrm{d}u}{u}\left(\frac{\pi}{2} - E(u)\right) + \frac{2}{\gamma\, dp}\int_v^1 \frac{\mathrm{d}u}{u}\left(\frac{\pi}{2} - \left(\frac{E(u) - K(u)}{u}\right) - uK(u)\right). \tag{A.6}$$

From reference [14] we find,

$$\int_0^1 \frac{\mathrm{d}u}{u}\left(\frac{\pi}{2} - E(u)\right) = \frac{\pi}{2}(1 - \log 4) - 1 + \int_0^1 \mathrm{d}u\, K(u) \tag{A.7}$$

and :

$$\int_v^1 \frac{\mathrm{d}u}{u^2}(K(u) - E(u)) = \left(\frac{E(u) - (1-u^2)\,K(u)}{u}\right)\Bigg|_v^1 = 1 - \left(\frac{E(v) - (1-v^2)\,K(v)}{v}\right). \tag{A.8}$$

Substituting these equations in equation (A.6) and collecting terms, we are left with,

$$\frac{f^{(1)}}{2\,K_{22}} = \frac{2}{\gamma\, dp}\left(\frac{\pi}{2}(1 - \log 4\,v) - \left(\frac{E(v) - (1-v^2)\,K(v)}{v}\right) + \int_0^v \mathrm{d}u\, K(u)\right), \tag{A.9}$$

where $v = u_0^{-1} = \sin^2 qa \cong (qa)^2 \ll 1$.

Neglecting therefore in equation (A.9) those terms in between the brackets which are of order v^n, $n \geqslant 1$, [14], we then obtain from equations (A.1) and (A.9),

$$\frac{\bar{f}}{2\,K_{22}} = (q - q_0)^2 + \frac{q}{2\,\gamma d}(1 - 2\log 2\,qa), \tag{A.10}$$

which is the result presented in equation (22). Equation (A.10) does not include the contribution of the core of the disclinations, which is hard to calculate quantitatively ; it can be estimated however to be of the order of K per unit length [2]. When taken into account, it would give a slight change in $f^{(1)}$, which indeed is of minor importance for the equations (22) and (23).

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