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Disclinations dynamics in confined nematic liquid crystals: strong anchoring

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We have investigated the dynamics of pair annihilation of disclination lines in strong anchoring. This work is based on the Frank free energy. The director angle, $\phi(x, y, z)$, is obtained by the continuous theory. We show that the form of the viscous force in a confined nematic liquid crystal and in strong anchoring is a function of the initial distance between the two disclination lines. The asymptotic velocity, v_{asy}, is also a function of the initial distance. Our theoretical result on the asymptotic velocity is in good agreement with previous experimental results.

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1. Introduction

Nematic liquid crystals are systems which are positionally disordered, but reveal a long range orientational order. This property is described on a mesoscopic level by a unit vector field $\mathbf{n}(r)$, the director. Due to the absence of a permanent polarization in the nematic phase, the director indicates the orientation, but has neither head nor tail. This particular feature yields interesting defect structures in nematic liquid crystals. For example, the director field shows line defects in three dimensions (or, equivalently, point defects in two dimensions), called disclinations. Disclinations with topological charge $\pm\frac{1}{2}$ are possible and stable in nematics. Disclinations are never isolated, being subject to the anchoring forces arising from the substrates of the cell containing the liquid crystal. As a consequence, in a confined geometry, the substrate anchoring is expected strongly to influence the interactions between defect lines.

To our knowledge, there have been only a few papers published on the dynamics of disclination lines in the bulk or in a confined geometry. The disclination line near substrates has been studied. The force between the disclnation line and the glass plate was calculated by de Gennes [1]. The forces between the disclination line and concave lens in strong anchoring and in weak anchoring were studied by Biscari *et al.* [2]. Two parallel disclination lines of opposite strengths have been broadly investigated in the literature. Denniston *et al.* used a lattice Boltzmann algorithm to simulate liquid crystal hydrodynamics [3]. The pair annihilation of straight line defects with strength $\pm\frac{1}{2}$ in a bulk nematic system was studied by Svensek and Zumer [4]. Toth *et al.* showed that the annihilation velocity for two parallel and isolated line defects would depend on the topological charge of the defects [5]. The relaxation dynamics of a dipole of $+1/2$ and $-1/2$ disclination lines in a confined geometry was studied by Bogi *et al.* [6]. In their experimental set-up, the nematic liquid crystal 5CB (pentylcyanobiphenyl) was sandwiched between a planar glass plate and a convex spherical lens. The sample was placed in an oven kept at $\Delta T=0.2^{\circ}\mathrm{C}$ below the nematic clearing temperature. They then injected a short pulse of hot air into the oven to heat the liquid crystal to the isotropic phase. Shortly after the pulse, the sample temperature decreased to the oven temperature and the nematic phase was restored. The transition from the high symmetry isotropic phase $[O(3)]$ to the lower symmetry nematic phase $(D_{\infty \mathrm{h}})$ generated topological line defects. Bogi *et al.* investigated the dipole annihilation dynamics experimentally. They obtained the asymptotic velocity, v_{asy}, versus the thickness of the cell, d, experimentally and theoretically. In their theoretical consideration, the form of *bulk* viscous force was taken into account. In this paper, we wish to calculate the viscous force and driving force in the presence of the surface contribution.

The aim of this paper is to present the solution to the pair annihilation of straight disclination lines with strengths $\pm 1/2$ in confined nematic liquid crystals and in strong anchoring. In the first stage we will find the director field by minimizing the total energy. In § two, the driving force is obtained from the total free energy. In § three, we solve the equations of nematodynamics to

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obtain the viscous force in the confined state and in strong anchoring (in the absence of fluid flow). Writing an equation of motion, we derive the velocity of disclinations in the final section and introduce a critical thickness of the cell, d_c, in which the dominant role of the bulk and the anchoring forces will change.

2. Driving force

As a first step, we define the coordinate frame (x', y', z') used in this work (figure 1). We assume that two substrates are fixed at $z' = \pm \frac{d}{2}$. The easy axis on the two substrates is along the y'-axis. Now, consider a disclination line which is located in $x'=0$ with a strength $m=\frac{1}{2}$, and another in $x'=x'_0$ with a strength $m=-\frac{1}{2}$ (at zero time, $t=0$). Each disclination line is perpendicular to the substrate, i.e. parallel to the z'-axis. We restrict our attention to the planar configuration and strong anchoring. Consequently, the director field lies in planes parallel to the substrates (in the $x'y'$-plane). The director, $\mathbf{n}$, make an angle ϕ with the y'-axis; this angle is a function of x', y' and z'. Far from the disclinations, $\mathbf{n}$ is uniformly oriented along the anchoring easy axis $\phi=\phi_0=0$. Hence we can write

$$n=(\sin\phi, \cos\phi, 0). \tag{1}$$

During the annihilation of defects, we see two different regimes. In the first, the asymptotic velocity of disclinations is constant [6]. In this regime, the distance between the two disclination lines along the x'-axis is larger than the distance between the extinction branches, ζ_0, along the y'-axis. In the second regime, this distance is smaller than ζ_0 and the distance between defects follows a square-root time law [1, 6]. In this paper, we wish to investigate the dynamics of two disclination lines in the first regime.

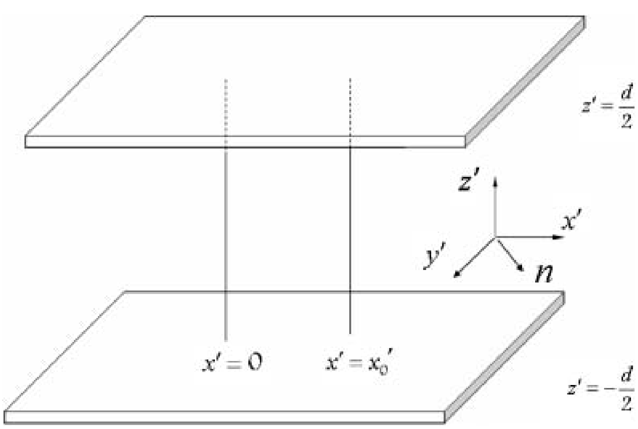

Figure 1. Schematic view of the cell configuration studied in this article. The bottom and top plates are situated at $z'=-d/2$ and $z'=d/2$. The anchoring at the plates is such that the director at the surface is aligned along the y'-axis. Two disclination lines are located in $x'=0$ with strength $m=1/2$ and in $x'=x'_0$ with strength $m=-1/2$.

The free elastic energy may be written as

$$\mathcal{F}'=\frac{1}{2}\int\left[K_1(\nabla.\mathbf{n})^2+K_2(\mathbf{n}.\nabla\times\mathbf{n})^2+K_3(\mathbf{n}\times\nabla\times\mathbf{n})^2\right]\mathrm{d}x'\,\mathrm{d}y'\,\mathrm{d}z' + \frac{K_2}{2L}\int(\sin^2\phi_s)\,\mathrm{d}x'\,\mathrm{d}y' \tag{2}$$

where K_1, K_2 and K_3 are, respectively, the splay, twist, and bend elastic constants; ϕ_s is the surface director angle with the y'-axis and L is the anchoring extrapolation length. The first integral in equation (2) describes the bulk elastic energy, while the second term represents the Rapini–Papoular anchoring energy [1]. We only consider the twist elastic constant for surface energy because the director field lies in the plane parallel to the substrates. To simplify the calculation we will use the two constant approximation, $K_1=K_3=K$, of the free energy. By inserting equation (1) into equation (2) we obtain

$$\mathcal{F}'=\frac{Kd}{4\pi}\int\left[\left(\frac{\partial\phi}{\partial x}\right)^2+\left(\frac{\partial\phi}{\partial y}\right)^2+\left(\frac{\partial\phi}{\partial z}\right)^2\right]\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z+\frac{Kd^2}{8\pi^2L}\int(\sin^2\phi_s)\,\mathrm{d}x\,\mathrm{d}y \tag{3}$$

where according to Bogi *et al.* [6], for strong anchoring we may define $z=\frac{2\pi}{d}z'$, $y=\left(\frac{K_2}{K}\right)^{\frac{1}{2}}\frac{2\pi}{d}y'$ and $x=\left(\frac{K_2}{K}\right)^{\frac{1}{2}}\frac{2\pi}{d}x'$. It is mentioned by Bogi *et al.* [6] that in the weak anchoring case the length l, which is related to the extrapolation length L, appeared instead of d in the dimensionless variables x, y and z. It is noted that the new domains of integrations contain the coefficient K_2, (see equation 9).

By minimizing the free energy with respect to ϕ, we can find $\phi(x, y, z)$. By using the Euler–Lagrange equations we get

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}=0. \tag{4}$$

Consider a disclination line which is located in $x'=0$ and another in $x'=x'_0$ at zero time, $t=0$. The director field around and between the two disclination lines can be obtained from the above Laplace equation by applying the boundary condition. As already mentioned, far from disclination lines the director $\mathbf{n}$ is uniformity oriented along the easy axis; thus if $\rho=(x, y)$ is the point from the disclinations in the xy-normalized plane, then

$$\mathbf{n}\to(0, 1, 0) \qquad \text{as} \qquad \rho\to\infty. \tag{5}$$

The solution of the Laplace equation, equation (4), is

$$\phi=\frac{1}{2}\arctan\left(\frac{2\sinh y\sin z}{\sinh^2 y-\sin^2 z}\right)+\frac{1}{2}\arctan\left(\frac{x}{y}\right)-\frac{1}{2}\arctan\left(\frac{x-x_0}{y}\right). \tag{6}$$

This angle, $\phi(r)$, has the following properties:

(1) $\phi(r)$ satisfies equation (4) and is regular except on the two lines.

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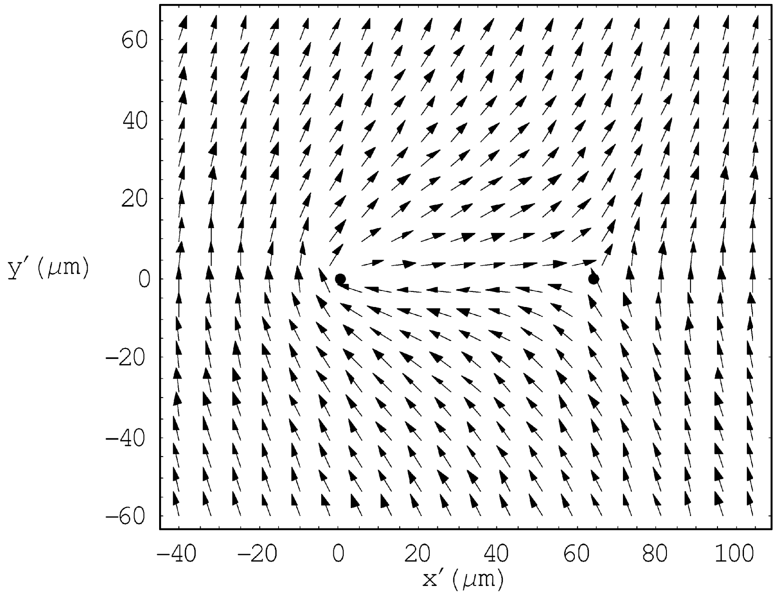

Figure 2. The director field of two annihilation topological line defects with strength $m=\pm 1/2$ in the middle of the slab.

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(2) $\phi(r)$ does not diverge far from the lines.
(3) $\phi(r)$ increases by π if, starting from point **r**, we make one turn around the line and come back to **r**.

It is noted that in the weak anchoring, the extrapolation length appear in the ϕ implicitly [1]. We show a two-dimensional cross-section of the two line defects, equation (6), for $z'=0$ and $x'_0=64\,\mu\mathrm{m}$ in figure 2.

The surface director angle in equation (2), ϕ_s, can be derived from the balance between the elastic and surface torques [1]:

$$\left.\frac{\partial\phi}{\partial z}\right|_{z=\pi}=\frac{d}{4\pi L}\sin(2\phi_s). \tag{7}$$

By using equation (6) in the above equation we have

$$\phi_s=\frac{1}{2}\arcsin\left[\frac{4\pi L}{d\sinh y}\right]. \tag{8}$$

Finally, by using equations (6) and (8) in equation (3), and after some straightforward calculations we obtain

$$\begin{aligned}\mathcal{F}'=&\frac{Kd}{16\pi}\int_{\frac{2\pi\xi'}{d}\left(\frac{K_2}{K}\right)^{\frac{1}{2}}}^{\frac{2\pi(x'_0-a')}{d}\left(\frac{K_2}{K}\right)^{\frac{1}{2}}}\mathrm{d}x\int_{-\infty}^{\infty}\mathrm{d}y\int_{-\pi}^{\pi}\mathrm{d}z\left\{\frac{1}{x^2+y^2}+\frac{1}{(x_0-x)^2+y^2}+\right.\\&\left.\frac{4}{\sinh^2 y+\sin^2 z}-\frac{2y^2}{[x^2+y^2]\left[(x_0-x)^2+y^2\right]}+\frac{2x(x_0-x)}{[x^2+y^2]\left[(x_0-x)^2+y^2\right]}\right\}\\&+\frac{Kd^2}{8\pi^2L}\int_{\frac{2\pi\xi'}{d}\left(\frac{K_2}{K}\right)^{\frac{1}{2}}}^{\frac{2\pi(x'_0-a')}{d}\left(\frac{K_2}{K}\right)^{\frac{1}{2}}}\mathrm{d}x\int_{-\infty}^{\infty}\mathrm{d}y\sin^2\left\{\frac{1}{2}\arcsin\left[\frac{4\pi L}{d\sinh y}\right]\right\}.\end{aligned} \tag{9}$$

Our numerical investigation, figure 2, on the distortion of the director field indicates that the elastic distortion is mostly confined in the region between the two disclination lines. Since the distance between these lines is of the order of a micrometer and the width of substrate is of the order of a centimeter, one can choose the integration boundaries on dimensionless y as $-\infty$ and ∞. Now, the integration on x' is performed on the first regime of annihilation dynamics, from ξ' to x'–a'; in dimensionless units, $x=\frac{2\pi\xi'}{d}\left(\frac{K_2}{K}\right)^{\frac{1}{2}}$ to $x=\frac{2\pi(x'_0-a')}{d}\left(\frac{K_2}{K}\right)^{\frac{1}{2}}$. a' is the core radius of the disclination line, x'_0 is the initial distance between the disclination lines and $\xi'=x'_0$–u', where u' is a distance within which the velocity of the disclinations is constant [1].

By performing the integrations in the above equation we obtain the total free energy

$$\begin{aligned}\mathcal{F}'=&\frac{K\pi d}{8}\left\{\ln\left(\frac{x'_0-a'}{\xi'}\right)-\ln\left(\frac{a'}{x'_0-\xi'}\right)\right\}+\\&4(K_2K)^{\frac{1}{2}}(x'_0-\xi')\left\{C+\frac{\pi}{2}\ln\left(\frac{d}{\pi L}\right)+\frac{\pi}{2}-\arctan\left(\frac{L\pi}{d}\right)\right\}\end{aligned} \tag{10}$$

where $C=\int_0^1\frac{1}{t}\arctan(t)\mathrm{d}t=0.916$ is the Catalan number.

The driving force, F_d, can be calculated from the total free energy

$$F_d=-\frac{\partial\mathcal{F}'}{\partial x'_0}. \tag{11}$$

The core radius of the disclination line, a', is much smaller than x'_0, so

$$F_d\simeq-\frac{K\pi d}{8x'_0}-\frac{K\pi d}{8\left(x'_0-\xi'\right)}-F_e \tag{12}$$

where

$$F_e = 4(KK_2)^{\frac{1}{2}}\left[\frac{\pi}{2} - \arctan\left(\frac{L\pi}{d}\right) + C + \frac{\pi}{2}\ln\left(\frac{d}{\pi L}\right)\right]. \quad (13)$$

The first two terms of the above equation arise from the anchoring energy, while the last two terms come from the bulk energy. The total driving force is an attractive force.

In strong anchoring, $L \ll d$, F_e may be written as

$$F_e \simeq 4(KK_2)^{\frac{1}{2}}\left[\frac{\pi}{2} - \frac{L\pi}{d} + C + \frac{\pi}{2}\ln\left(\frac{d}{\pi L}\right)\right]. \quad (14)$$

3. Viscous force

We intend to calculate the viscous force acting on two disclination lines with strength $m = \pm\frac{1}{2}$ moving with constant velocity v_{asy} along the x'-axis in strong anchoring. According to Blank *et al.* and Oswald *et al.* [7, 8], there is no backflow effect in strong anchoring. In the absence of fluid flow, $\mathbf{V}' = 0$, the dissipation of energy created by the rotation of the director in a nematic liquid crystal may written as [4]

$$T\dot{S} = \int \mathbf{h}.\mathbf{N} d^3 r'. \quad (15)$$

The dissipation of energy has an additional term which relates to dissipation by shear flow. This term is zero in the absence of fluid flow. $\mathbf{h}$ and $\mathbf{N}$ in equation (15) are defined as follows: the molecular field, $\mathbf{h}$, may be written as

$$h_\mu = \gamma_2 n_\alpha A_{\alpha\mu} + \gamma_1 N_\mu \quad (16)$$

together with the relationships

$$A_{\alpha\beta} = \frac{1}{2}\left[\frac{\partial V'_\beta}{\partial x'_\alpha} + \frac{\partial V'_\alpha}{\partial x'_\beta}\right] \quad (17)$$

$$\gamma_1 = \alpha_3 - \alpha_2 \quad (18)$$

$$\gamma_2 = \alpha_2 + \alpha_3 = \alpha_6 - \alpha_5 \quad (19)$$

and the rate of change of the director with respect to the back ground fluid, $\mathbf{N}$, may be written as [4]

$$\mathbf{N} = \dot{\mathbf{n}} - \omega \times \mathbf{n} \quad (20)$$

where $\omega = \frac{1}{2}\nabla' \times \mathbf{V}'$ and $\dot{\mathbf{n}} = \mathrm{d}n/\mathrm{d}t$.

The coefficients α_i are usually called the Leslie coefficients [4].

In the absence of fluid flow, the second term of equation (20) is zero. By inserting equations (1) and (6) into (20) we get

$$\mathbf{N} = v_{asy}[\cos\phi\mathbf{i}' - \sin\phi\mathbf{j}']\left(\frac{\partial\phi}{\partial x'}\right) \quad (21)$$

where $\mathbf{i}'$ and $\mathbf{j}'$ are unit vectors along the x' and y'-axes, respectively. In the absence of fluid flow, the first term in equation (16) is zero and the molecular field, $\mathbf{h}$, is obtained by inserting equation (21) into (16).

By substituting the expressions for $\mathbf{h}$ and $\mathbf{N}$ into equation (15) we have

$$T\dot{S} = \gamma_1 v_{asy}^2 \frac{d}{8\pi}\int_{2\pi\frac{\xi'}{d}\left(\frac{K_2}{K}\right)^{\frac{1}{2}}}^{2\pi\frac{(x'_0 - a')}{d}\left(\frac{K_2}{K}\right)^{\frac{1}{2}}} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}y \int_{-\pi}^{\pi} \mathrm{d}z \left\{\frac{y^2}{(x^2+y^2)^2} + \frac{y^2}{\left[(x_0-x)^2+y^2\right]^2} + \frac{-2y^2}{[x^2+y^2]\left[(x_0-x)^2+y^2\right]}\right\} \quad (22)$$

where the integration boundaries are the same as the integration boundaries of equation (9). By performing the integrations in equation (22) we obtain

$$T\dot{S} = \gamma_1 v_{asy}^2 \frac{\pi d}{4} D \quad (23)$$

where D is a dimonsionless parameter and equal to

$$D = \frac{1}{2}\ln\left(\frac{x'_0}{\xi'}\right) - \frac{1}{2}\ln\left(\frac{a'}{x'_0 - \xi'}\right) - \frac{2}{x'_0}\left(x'_0 - \xi'\right). \quad (24)$$

The viscous force, F_υ, can be obtained from the dissipation of energy. For constant velocity, the total rate of energy dissipation is $F_\upsilon v_{asy}$, so

$$F_\upsilon = \gamma_1 v_{asy}\frac{\pi d}{4} D. \quad (25)$$

It should be noted that the viscous force per unit length of the disclination line, F_υ/d, is independent of the thickness of the cell, d. As is clear from equations (24) and (25), the viscous force is a function of x'_0 and ξ'.

To generalize our method to the case of a disclination line moving in a bulk sample of size R, we should consider only the first term in equation (22). By performing the integrations, the viscous force per unit length, f_υ, is

$$f_\upsilon = \gamma_1 v_{asy}\frac{\pi}{8}\ln\left(\frac{R}{a}\right). \quad (26)$$

This result was obtained by Ryskin and Kremenetsky [9], Imura and Okano [10] and de Gennes [11]. Ryskin *et al.* have also shown that in the quasi-static picture, this force does not diverge with sample size, R. The divergence with sample size in equation (26) is, as shown

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already by Ryskin *et al.*, an artifact of the quasi-static approximation.

4. Asymptotic velocity

The equation of motion of the two disclination lines, in static equilibrium and in the coordinate frame where one of them is at rest, is given by

$$\mathbf{F}_\mathrm{d}+\mathbf{F}_\mathrm{v}=0. \tag{27}$$

By inserting equations (12) and (25) into (27) we obtain

$$v_\mathrm{asy}=\frac{K}{2Dx_0'\gamma_1}+\frac{K}{2D(x_0'-\xi')\gamma_1}+\frac{4F_\mathrm{e}}{\gamma_1 d\pi D}. \tag{28}$$

The asymptotic velocity is a function of x'_0, ξ' and d. In the cases in which ξ' and d are constant, our theory shows that the velocity decreases with increasing initial distance, x'_0.

The calculated asymptotic velocity is consistent with the experimental result of Bogi *et al*. The nematic liquid crystal in their experiments is 5CB; its parameters are $K_2=2.4\times10^{-12}\,\mathrm{N}$, $K=1\times10^{-12}\,\mathrm{N}$, $a'=10\,\mathrm{nm}$ [6] and $L=0.2\,\mu\mathrm{m}$ [12]. The experimental and calculated values of v_asy with $d=13\,\mu\mathrm{m}$, $x'_0=64\,\mu\mathrm{m}$, $\xi'=13\,\mu\mathrm{m}$ [1] are 29 and $29.02\,\mu\mathrm{m\,s^{-1}}$, respectively. We see good agreement with experimental and theoretical results.

Let us examine our result in equation (28) for the bulk case, $d\to\infty$. In this case we obtain

$$v_\mathrm{asy}^\mathrm{bulk}=\frac{K}{2Dx_0'\gamma_1}+\frac{K}{2D(x_0'-\xi')\gamma_1}. \tag{29}$$

As predicted intuitively by de Gennes [11], equation (29) indicates that in the quasi-static picture, there is a one-to-one relationship between the velocity and the distance.

By deriving the velocity with respect to d we can find the critical thickness, d_c, which obeys the following equation

$$\frac{L\pi d_\mathrm{c}}{\pi^2L^2+d_\mathrm{c}^2}-\frac{\pi}{2}\ln\left(\frac{d_\mathrm{c}}{\pi L}\right)+\arctan\left(\frac{L\pi}{d_\mathrm{c}}\right)=C \tag{30}$$

where C is the Catalan number. This critical thickness, d_c, occurs at almost $0.75\,\mu\mathrm{m}$ for planar anchoring SiO with anchoring extrapolation length of $L=0.2\,\mu\mathrm{m}$. We predict that this critical thickness is independent of the elastic constants of the liquid crystal, Leslie coefficients and initial distance, and depends only on the extrapolation length L. If we increase the extrapolation length, the critical thickness will also increase.

In cases in which ξ' and x'_0 are constant, our theory shows that for $d<d_\mathrm{c}$, the asymptotic velocity increases with increasing thickness of the cell, d; it is noted that our theory cannot be applied for $d<L$. But for $d>d_\mathrm{c}$ the asymptotic velocity decreases with increasing d. Then the velocity has a maximum value at the critical thickness. As we show, in thicknesses between L and d_c, the important role of the anchoring force [the first two terms in equation (13)] can be seen, whereas for $d>d_\mathrm{c}$ the dominant role of the bulk force should be considered.

5. Conclusion

The free energy provides one way of investigating problems in nematic liquid crystals. This energy contains two terms: bulk and anchoring. The director field is calculated by minimizing the free energy together with applying the boundary condition for strong anchoring. This is a function of x', y' and z'. By examining the dissipation of energy, the viscous force acting between two disclination lines in the confined state is obtained. Bogi *et al.* have considered the director field to be independent of the variable x'. If one follows this idea, the density of dissipation of energy would be zero. We cannot accept this result since we have a rotation of director during motion of the disclination lines. By using the equation of motion, the asymptotic velocity is calculated. We find that the asymptotic velocity increases with increasing d until a critical thickness, d_c is reached. This critical thickness depends only on the extrapolation length L. It is independent of Leslie coefficients, elastic constants of the liquid crystals and initial distance. This critical thickness occurs where the dominant role of the bulk and the anchoring terms in the equation of motion changes. The asymptotic velocity depends on the initial distance between two disclination lines. It is smaller for two widely separated disclination lines than for lines close together. This effect must therefore be considered in experiment investigations.

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