Dynamics of nematic loop disclinations

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The shrinking of defect loops under the influence of boundary conditions in a confined geometry is studied. Using a suitable model for a nematic disclination, we calculate a director field that minimizes the Frank-Oseen free energy [F. C. Frank, Discuss. Faraday Soc. **25**, 19 (1958); C. W. Onseen, Trans. Faraday Soc. **29**, 883 (1933)]. With this static model we find by means of a dissipation principle a linear dependence of the loop radius on time, explaining recent measurements performed on polymeric liquid crystals.
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I. INTRODUCTION

The continuum theory of liquid crystals usually employs a director field $\boldsymbol{n}$ indicating the local mean orientation of the molecules. Equilibrium configurations are obtained by minimizing the well-known Frank-Oseen elastic free energy [1,2]. In an actual physical situation the director field is not smooth everywhere, but it exhibits various kinds of discontinuities, called *disclinations*. Nematic liquid crystals even owe their name to the typical threadlike defects, the *line* disclinations often found in this state of matter [3,4].

Similar structures can also be observed in various biological patterns [5] and ferromagnets [6] and they have been adopted by cosmologists in models explaining the distribution of matter in the early universe [7]. Consequently, the dynamics of disclinations has attracted wide interest and a mathematical theory concerned with the *flow by curvature* [8] and, in the higher-dimensional case, with the *motion by mean curvature* [9] has been developed.

A major advantage that nematic liquid crystals yield for the study of disclinations stems from the experimental point of view. The preparation of liquid-crystal cells with various boundary alignments is technically well understood and typical relaxation times range from seconds for small-molecule liquid crystals to several hours for polymeric liquid crystals. Furthermore, due to the birefringence depending on the alignment, the dynamical process can easily be observed optically.

Experiments on the shrinking of defect loops [10] have been known for a long time and some years ago even quantitative measurements were performed using the small-molecule nematic liquid crystal 4-cyano-4′-*n*-pentylbiphenyl. The major result, in agreement with theoretical considerations, is that the radius of the defect loop scales with time as $r \propto (t_0 - t)^{\alpha}$, where $\alpha = 0.5$ [11,12].

More recent experiments with poly(1,4-phenylene-2,6-benzobisthiazole) have yielded a different result: The defect loops vanish following a linear decay law, for which $\alpha = 1$ [13,14]. The alignment at the boundary of the cell was along a prescribed direction and the area enclosed by the loop, when viewed under crossed polarizers, appeared to be homogeneous, precisely as the region outside it. This is compatible with a closed twist disclination loop.

We show that this behavior can be explained by taking into account not only the elastic energy associated with the actual thread and proportional to its radius R, but also a contribution due to the twist of the director field in the loop's interior that is proportional to R^2. Such a contribution is important for large loops in thin cells, where this part of the energy cannot be neglected with respect to the energy of the disclination line.

In this paper we proceed as follows. In Sec. II we introduce a coordinate system fit to describe disclination lines. In this framework we produce a director field that minimizes the elastic free energy of a circular loop disclination in the limit of long threads and within a special class of admissible fields that we show to be meaningful. Starting from the static model thus obtained, in Sec. III we apply a dissipation principle, whence we arrive at an ordinary differential equation for the loop radius. In Sec. IV we compare our results to the experimental evidence and discuss the connection with previous predictions. We do not restrict attention to circular loops, though our analysis mainly focuses on them. For loops of arbitrary shape, our model predicts an evolution law different from the flow by curvature of a plane curve, whose properties still remain to be fully understood.

II. STATIC MODEL

A. System of coordinates for the loop

There are essentially two types of line disclinations in nematic liquid crystals (see [15], Sec. 7.1): namely, the *axial* and the *twist* disclinations. The disclinations of the first type are characterized by a director field perpendicular to the direction of the line. If the disclination is supposed to lie along the z axis, the orientation can be given in the form $\boldsymbol{n} = \cos\varphi \boldsymbol{e}_x + \sin\varphi \boldsymbol{e}_y$ and φ is found to be

$$\varphi = m\psi + \varphi_0, \tag{1}$$

where ψ is the polar angle in cylindrical coordinates, φ_0 is a constant, and the winding number m takes the values

$\pm\frac{1}{2},\pm 1,\pm\frac{3}{2},\pm 2,\ldots$ [1]. The occurrence of half-integer winding numbers is a consequence of the nematic symmetry, i.e., the physical identity of the alignments $\boldsymbol{n}$ and $-\boldsymbol{n}$.

In this paper we are concerned with the second type of defect lines. Here the director field has components only along the line itself and one fixed direction perpendicular to the disclination. Minimizing the Frank-Oseen elastic free energy gives again the solutions (1), with φ the angle designating the director in the appropriate plane.

More specifically, we consider a liquid crystal between two parallel orienting layers. Cartesian coordinates are chosen so that the plane of the cell coincides with the x-y plane and the origin is selected so that the upper and lower bounding plates have z coordinates $-H$ and $+H$, respectively. The disclination loop is supposed to lie entirely in the midplane between the two plates and it is described by a smooth, unknotted curve. A curve parallel to it, in the interior of the plane region it encloses, will play a central role in our model: We call it the *thread* and represent it as $\boldsymbol{q}(s)=x(s)\boldsymbol{e}_x+y(s)\boldsymbol{e}_y$, where s is taken to be the arc length of the curve.

Since we consider pure twist disclinations, we further assume that the orientation is parallel to the bounding plates everywhere, thus allowing for a description of the alignment in terms of a single angle φ with $\boldsymbol{n}=\cos\varphi\boldsymbol{e}_x+\sin\varphi\boldsymbol{e}_y$. The anchoring conditions on the plates are then prescribed in the form

$$\varphi(x,y,\pm H)=0. \tag{2}$$

The Frank-Oseen elastic free-energy density is calculated in the one-constant approximation as

$$f=\frac{K}{2}(\nabla\boldsymbol{n})^2=\frac{K}{2}(\nabla\varphi)^2. \tag{3}$$

An analytic expression for the equilibrium structure satisfying the Euler-Lagrange equation

$$\Delta\varphi=0 \tag{4}$$

is known for circular loops [10]. It is given as the sum of a Fourier series whose coefficients are evaluated in terms of the hyperbolic Bessel functions of index 0 and 1: It is represented in closed form only at distances from the z axis large compared with the cell thickness. Unlike [10], our paper aims at a description of the shrinking dynamics of loops of arbitrary shape; thus we need a simpler model, which will be based on an approximate equilibrium solution fit to mimic that in [10], but such to be represented explicitly.

First, we assume that the distortion of the director field caused by the disclination takes place only in the vicinity of the thread in a more or less tubular region $\mathcal{T}$. Outside $\mathcal{T}$ the alignment is supposed to be homogeneous: In the outer region we have simply $\varphi\equiv 0$, while inside the thread φ twists by the angle π between the two plates.

We introduce the angle $\theta(s)$ to describe both the unit tangent to the curve $\boldsymbol{q}(s)$

$$\boldsymbol{\tau}(s)=x'(s)\boldsymbol{e}_x+y'(s)\boldsymbol{e}_y=\cos(\theta)\boldsymbol{e}_x+\sin(\theta)\boldsymbol{e}_y \tag{5}$$

and the unit normal

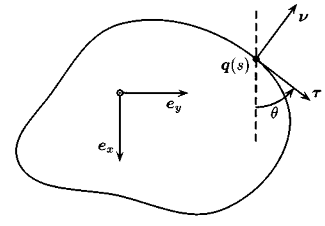

FIG. 1. Coordinate system for a disclination loop. Each point in the vicinity of the thread is uniquely determined by specifying s, which parametrizes the curve $\boldsymbol{q}(s)$, and its position in the local coordinate frame $\{\boldsymbol{\nu},\boldsymbol{e}_z\}$.

$$\boldsymbol{\nu}(s)=-\sin(\theta)\boldsymbol{e}_x+\cos(\theta)\boldsymbol{e}_y, \tag{6}$$

which points outward. Since $\boldsymbol{\tau}'(s)=-\theta'\sin(\theta)\boldsymbol{e}_x+\theta'\cos(\theta)\boldsymbol{e}_y=\theta'\boldsymbol{\nu}(s)$, we have that the curvature σ of the curve is given by

$$\sigma(s)=\theta'(s). \tag{7}$$

Each point $\boldsymbol{p}$ in $\mathcal{T}$ has a unique description in the form

$$\boldsymbol{p}(s,\xi,z)=\boldsymbol{q}(s)+\xi\boldsymbol{\nu}+z\boldsymbol{e}_z, \quad \xi\geqslant 0, \tag{8}$$

provided $\sigma\xi<1$. The equation of the thread is clearly $\xi\equiv 0$, $z\equiv 0$. (See Fig. 1.)

We record here for later use the expressions for both the Jacobi determinant of the change of variables $(x,y,z)\mapsto(s,\xi,z)$ and the gradient of a smooth scalar-valued function f of (s,ξ,z). They are

$$\frac{\partial(x,y,z)}{\partial(s,\xi,z)}=1-\sigma\xi \tag{9}$$

and

$$\nabla f=\frac{1}{1-\sigma\xi}\frac{\partial f}{\partial s}\boldsymbol{\tau}+\frac{\partial f}{\partial\xi}\boldsymbol{\nu}+\frac{\partial f}{\partial z}\boldsymbol{e}_z. \tag{10}$$

B. Simple model for a straight disclination line

To construct the director field in the vicinity of the defect line, we consider a cross section $\mathcal{C}$ through $\mathcal{T}$. Since the thread is supposed to lie in the midplane between the two plates, the problem is symmetric in z and it suffices to look at the upper half of the cell where the director makes half of the total twist.

We first attack a two-dimensional problem in the plane (ξ,z), which corresponds to a straight disclination line. The region where the director is simply twisted by the angle π and has no defect lies in the half plane with $\xi<0$; the defect is found at $z=0$ and $\xi=d$ and the highest point of $\mathcal{T}$ is at $z=h$. This means that the following conditions are prescribed on the angle φ:

$$\varphi=\begin{cases}0, & \xi=0, \quad z\geqslant h\\ \dfrac{\pi}{2}, & z=0, \quad 0\leqslant\xi<d\\ 0, & z=0, \quad \xi>d,\end{cases} \tag{11}$$

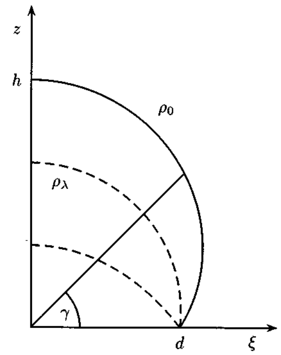

FIG. 2. Coordinate system in terms of the lines of equal alignment. Only the upper half is depicted. The lines of equal alignment meet at the defect with ρ_0, corresponding to $\varphi=0$, indicating the outer boundary of the tubular region $\mathcal{T}$.

where d and h are parameters to be determined.

We find it convenient to introduce the new system of coordinates (γ,λ) in the quadrant $\xi>0$, $z>0$ as follows: $\gamma=\arctan(z/\xi)\in[0,\pi/2]$ is the angle between the ξ axis and the straight line connecting the origin to the point (γ,λ). The other coordinate λ parametrizes the lines of equal alignment for the director in such a way that as λ ranges in $[0,\infty]$, $\varphi=\phi(\lambda)$ ranges in $[0,\pi/2]$ and

$$\phi|_{\lambda=0}=0, \quad \lim_{\lambda\to\infty}\phi(\lambda)=\frac{\pi}{2}. \tag{12}$$

The new coordinate lines are then the straight lines emanating from the origin, along which γ is constant, and the lines of equal alignment for the director, along which both λ and φ are constant. In this system of coordinates a curve along which φ is constant is labeled by a value of λ: In polar coordinates (γ,ρ), it can be represented as $\rho=\rho_\lambda(\gamma)$ and so

$$\xi=\rho_\lambda(\gamma)\cos(\gamma) \tag{13}$$

and

$$z=\rho_\lambda(\gamma)\sin(\gamma), \tag{14}$$

with

$$\rho_\lambda(0)=d, \quad \rho_0\left(\frac{\pi}{2}\right)=h, \quad \lim_{\lambda\to\infty}\rho_\lambda\left(\frac{\pi}{2}\right)=0 \tag{15}$$

(see Fig. 2). Our endeavor with the new coordinates has the effect of replacing φ as a function of (γ,ρ) with the pair of functions $\phi(\lambda)$ and $\rho_\lambda(\gamma)$, which suffice to describe a large class of twisted director alignments in a cross section of the tubular region $\mathcal{T}$.

To compute the elastic free energy, we need to know both the Jacobi determinant of the change of variables $(\xi,z)\mapsto(\gamma,\lambda)$ and the gradient in the new coordinates of a scalar-valued function f. The former is

$$\frac{\partial(\xi,z)}{\partial(\gamma,\lambda)}=-\rho_\lambda\frac{\partial\rho_\lambda}{\partial\lambda}. \tag{16}$$

Introducing the local pair of orthogonal unit vectors $\{\boldsymbol{e}_r,\boldsymbol{e}_\gamma\}$ as

$$\boldsymbol{e}_r=\cos(\gamma)\boldsymbol{e}_\xi+\sin(\gamma)\boldsymbol{e}_z \tag{17}$$

and

$$\boldsymbol{e}_\gamma=-\sin(\gamma)\boldsymbol{e}_\xi+\cos(\gamma)\boldsymbol{e}_z, \tag{18}$$

the gradient of f takes the form

$$\nabla f=\frac{1}{\partial\rho_\lambda/\partial\lambda}\frac{\partial f}{\partial\lambda}\boldsymbol{e}_r+\left(\frac{1}{\rho_\lambda}\frac{\partial f}{\partial\gamma}-\frac{\partial\rho_\lambda/\partial\gamma}{\rho_\lambda(\partial\rho_\lambda/\partial\lambda)}\frac{\partial f}{\partial\lambda}\right)\boldsymbol{e}_\gamma. \tag{19}$$

Since, by the very definition of ϕ, φ depends on λ only, we get

$$(\nabla\varphi)^2=\left(\frac{\phi'}{\partial\rho_\lambda/\partial\lambda}\right)^2\left[1+\left(\frac{\partial\rho_\lambda/\partial\gamma}{\rho_\lambda}\right)^2\right], \tag{20}$$

where $\phi':=d\phi/d\lambda$. Insering this into Eq. (3) and integrating in both γ and λ yields the elastic free energy stored in $\mathcal{T}$ per unit length of the disclination:

$$F_t=2\frac{K}{2}\int_0^{\pi/2}\int_0^\infty-\phi'^2\frac{\rho_\lambda}{\partial\rho_\lambda/\partial\lambda}\left[1+\left(\frac{\partial\rho_\lambda/\partial\gamma}{\rho_\lambda}\right)^2\right]d\gamma\, d\lambda. \tag{21}$$

The minimization of this energy in the general case seems to be intractable. Thus we choose a special form for ρ_λ, namely,

$$\rho_\lambda(\gamma)=e^{-(4\lambda/\pi^2)\gamma(\pi-\gamma)}\rho_0(\gamma), \tag{22}$$

which relates all lines of equal alignment to that with $\lambda=0$. For $\lambda>0$ the curve ρ_λ appears as an exponential retraction of ρ_0, done in such a way that ρ_λ crosses at right angles the line $\gamma=\pi/2$ for all $\lambda>0$, whenever ρ_0 does so. Such a requirement will ensure that all lines of equal alignment in $\mathcal{T}$ can be smoothly joined to those in the region that is surrounded by $\mathcal{T}$ when we shall no longer consider a straight disclination. We have clearly restricted the class of admissible director fields around the disclination, but not too severely: Still the curve ρ_0 that determines the shape of $\mathcal{T}$ is left free; moreover, once this is known, all other curves of equal alignment are known as well, but the values the function ϕ takes upon them are still to be determined. Thus we believe that our ansatz, though special, is fit to be applied to a wide variety of alignment fields.

It follows from Eq. (22) that

$$\frac{\partial\rho_\lambda}{\partial\gamma}=e^{-(4\lambda/\pi^2)\gamma(\pi-\gamma)}\rho_0'+\frac{4\lambda}{\pi}\left(\frac{2}{\pi}\gamma-1\right)\rho_\lambda \tag{23}$$

and

$$\frac{\partial\rho_\lambda}{\partial\lambda}=-\frac{4}{\pi^2}\gamma(\pi-\gamma)\rho_\lambda, \tag{24}$$

where $\rho_0':=d\rho_0/d\gamma$. Hereafter, in addition to Eq. (15), we also require

$$\rho_0'\left(\frac{\pi}{2}\right)=0, \tag{25}$$

which ensures that the lines of equal alignment in $\mathcal{T}$ can be matched in a differentiable way to those in the region of simple twist ($\xi<0$). These equations reduce F_t to a functional of both ϕ and ρ_0:

$$F_t=K\int_0^{\pi/2}\int_0^{\infty}\frac{\phi'^2}{\frac{4}{\pi^2}\gamma(\pi-\gamma)}\left\{1+\left[\frac{4\lambda}{\pi}\left(\frac{2}{\pi}\gamma-1\right)+\frac{\rho_0'}{\rho_0}\right]^2\right\}d\gamma\, d\lambda. \tag{26}$$

Letting

$$\eta:=\frac{2}{\pi}\gamma \tag{27}$$

and

$$y_0(\eta):=\ln\rho_0\left(\frac{\pi}{2}\eta\right) \tag{28}$$

leads to

$$F_t=\frac{2}{\pi}K\int_0^1\int_0^{\infty}\frac{\phi'^2}{\eta(2-\eta)}\left[\frac{\pi^2}{4}+[2\lambda(\eta-1)+y_0']^2\right]d\eta\, d\lambda. \tag{29}$$

Further defining

$$I_0:=\int_0^{\infty}\phi'^2d\lambda,\quad I_1:=\int_0^{\infty}\lambda\phi'^2d\lambda,$$

$$I_2:=\int_0^{\infty}\lambda^2\phi'^2d\lambda, \tag{30}$$

we easily perform the integration with respect to λ, arriving at

$$F_t=\frac{2}{\pi}K\int_0^1\frac{1}{\eta(2-\eta)}\times\left[\frac{\pi^2}{4}I_0+4(\eta-1)^2I_2+I_0y_0'^2+4(\eta-1)I_1y_0'\right]d\eta. \tag{31}$$

Since the integrand does not depend on y_0 explicitly, the Euler-Lagrange equation for F_t in this form can readily be integrated once (see [16], Chap. IV) and then it reads

$$2I_0y_0'+4I_1(\eta-1)=c\,\eta(2-\eta), \tag{32}$$

c being an arbitrary constant. In terms of y_0, the boundary conditions for ρ_0 become

$$y_0(0)=\ln d,\quad y_0(1)=\ln h, \tag{33}$$

and

$$y_0'(1)=0. \tag{34}$$

Using the latter in Eq. (32), we see that $c=0$ and thus

$$y_0'=-\frac{2I_1}{I_0}(\eta-1). \tag{35}$$

Integrating this and taking care of Eq. (33) yields

$$\frac{d}{h}=e^{-I_1/I_0} \tag{36}$$

and

$$y_0(\eta)=\ln h+(\eta-1)^2\ln\frac{d}{h}. \tag{37}$$

This leads to

$$\rho_0(\gamma)=h\left(\frac{d}{h}\right)^{(2\gamma/\pi-1)^2}. \tag{38}$$

Evaluating Eq. (31) on the minimizer, we obtain the following expression for the energy per unit length of a straight disclination:

$$F_t=\frac{\pi}{4}K\left\{F_d\left[I_0+\frac{16}{\pi^2}\left(I_2-\frac{I_1{}^2}{I_0}\right)\right]-2\frac{16}{\pi^2}\left(I_2-\frac{I_1{}^2}{I_0}\right)\right\}, \tag{39}$$

where

$$F_d:=\ln\frac{\pi d}{r_c}=2\int_{\eta_c}^1\frac{d\eta}{\eta(2-\eta)} \tag{40}$$

is obtained by excluding from the integration of otherwise divergent integrals a *core* region with radius $r_c=d\gamma_c=(\pi/2)d\eta_c$. As customary, the energy of the core can be taken into account by adjusting r_c appropriately (see [3], p. 171).

Still the task of determining $\phi(\lambda)$ remains to be achieved. In principle, this can be done by minimizing the expression for the free energy in Eq. (39), where I_0, I_1, and I_2 are functionals of ϕ. We postpone this problem to the following subsection, where we take a further step towards the construction of our static model by considering a circular disclination loop. Requiring that the function ϕ in $\mathcal{T}$ matches that defined in the disk-shaped region surrounded by $\mathcal{T}$ will allow us to find the director field that minimizes the free energy within our class.

C. Model for a circular loop

The alignment in the interior of the thread is such that the director somehow twists from the angle $\pi/2$ with $\boldsymbol{e}_x$ to 0 as z goes from 0 to h. In order to give the alignment in terms of $\phi(\lambda)$, note that, by Eqs. (22) and (24), for $\gamma=\pi/2$ to each λ in $[0,\infty]$ there corresponds a value of z given by

$$z(\lambda)=\rho_\lambda\left(\frac{\pi}{2}\right)=he^{-\lambda}. \tag{41}$$

Since the director twist is the same function of z throughout the region enclosed by the thread, a contribution proportional to the area $\mathcal{A}$ of this region is to be added to the elastic free energy stored in $\mathcal{T}$: By Eq. (41), it becomes

$$F_{\mathcal{A}}=2\mathcal{A}\frac{K}{2}\int_0^h\left(\frac{\partial\varphi}{\partial z}\right)^2dz=\mathcal{A}\frac{K}{h}\int_0^\infty\phi'^2e^{\lambda}d\lambda. \quad (42)$$

The Euler-Lagrange equation of this functional is easy to solve: It yields

$$\phi(\lambda)=\frac{\pi}{2}(1-e^{-\lambda}), \quad (43)$$

which describes a linear twist [see again Eq. (41)]. Using this, we find that for a given h the minimum of $F_{\mathcal{A}}$ is

$$F_{\mathcal{A}}=\frac{\pi^2}{4}\mathcal{A}\frac{K}{h}. \quad (44)$$

This conclusion applies whatever the shape of the region enclosed by $\mathcal{T}$ may be. Let us further consider the case of a circular thread of radius R. More precisely, this curve is to be thought of as the locus where $\xi\equiv0$, $z\equiv0$ in the coordinate system (s,ξ,z). Since the loop shrinks without leaving a defect point after it, we take $\partial\varphi/\partial s=0$. Also with aid of Eq. (9), the total free energy then becomes

$$\begin{aligned}\mathcal{F}=&\frac{\pi KR^2}{h}\int_0^\infty\phi'^2e^{\lambda}d\lambda\\&+\frac{K}{2}\int_0^L\int\int_{\mathcal{C}}(\nabla\varphi)^2(1-\sigma\xi)d\xi\, dz\, ds\\=&\frac{\pi KR^2}{h}\int_0^\infty\phi'^2e^{\lambda}d\lambda+\pi K\int\int_{\mathcal{C}}(\nabla\varphi)^2(R+\xi)d\xi\, dz,\end{aligned} \quad (45)$$

where $L=2\pi R$ is the length of the thread and $\sigma=-1/R$ is its curvature, as in our parametrization $\boldsymbol{\nu}$ is the outward normal. For $R\gg H$, the largest contribution is from the area inside the thread. Thus we take ϕ as in Eq. (43), so that this part of the energy is minimized. Since $F_{\mathcal{A}}$ is proportional to h^{-1} and $h\leqslant H$, for large loops the minimum of $F_{\mathcal{A}}$ is attained when $h=H$. Note that having found ϕ as a function of λ does not amount to knowing the free-energy density stored in $\mathcal{T}$, which also depends on the lines of equal alignment [see Eq. (20)].

The energy contribution arising from the tubular region $\mathcal{T}$ bears an integrand proportional to $R+\xi$. In minimizing this part, we neglect ξ with respect to R, which amounts to omitting the influence of the thread curvature on the disclination's structure. This is certainly reasonable for large values of R and leads to the solution found in Sec. II B. With ϕ as in Eq. (43), we have

$$I_0=\frac{\pi^2}{8}, \quad I_1=I_2=\frac{\pi^2}{16}, \quad (46)$$

which by Eq. (36) yields

$$d=\frac{h}{\sqrt{e}}, \quad (47)$$

which is the distance between the thread and the disclination loop. Inserting this into Eq. (38) and using Eq. (22), for this model we easily express the curves of equal alignment as functions of η:

$$\rho_\lambda(\eta)=de^{(\eta^2-2\eta)(\lambda-1/2)}=he^{(\eta^2-2\eta)(\lambda-1/2)-1/2}. \quad (48)$$

To compute the total free energy, we still have to evaluate the integral

$$F_\sigma:=\int\int_{\mathcal{C}}(\nabla\varphi)^2\xi\, d\xi\, dz. \quad (49)$$

By use of Eqs. (43) and (48) and the change of variables $(\xi,z)\mapsto(\eta,\lambda)$, F_σ can also be written as

$$\begin{aligned}F_\sigma=&\frac{\pi^3}{4\sqrt{e}}h\int_0^1\frac{e^{\eta-\eta^2/2}\cos\frac{\pi}{2}\eta}{\eta(2-\eta)}\left\{\frac{1}{2+2\eta-\eta^2}\right.\\&+\left(\frac{2(\eta-1)}{\pi}\right)^2\left[\frac{8}{(2+2\eta-\eta^2)^3}-\frac{4}{(2+2\eta-\eta^2)^2}\right.\\&\left.\left.+\frac{1}{2+2\eta-\eta^2}\right]\right\}d\eta,\end{aligned} \quad (50)$$

where the integration in λ has already been performed. This integral, which is too complicated for an analytical approach, cannot even be computed numerically because of the divergence at $\eta=0$. We treat it in the following way: We write the integrand as a linear combination of nondivergent terms and $1/\eta(2-\eta)$, making use of the identities $\cos\alpha=1-2\sin^2\alpha$ and $e^x=(e^x-1)+1$ and decomposition into partial fractions. The divergent part is thus isolated, and by exclusion of the core region from the integration, we obtain a contribution proportional to $F_d=\ln(\pi d/r_c)$. The remaining convergent parts are then evaluated numerically. We finally get

$$F_\sigma=h\left(\frac{\pi^3+4\pi}{16\sqrt{e}}F_d-2.13\right). \quad (51)$$

Collecting all above contributions, within our model we give the total free energy of a ring disclination the form

$$\begin{aligned}\mathcal{F}=&\frac{\pi^3KR^2}{4h}+2\pi RF_t+\pi KF_\sigma\\=&\frac{\pi^2}{4}K\left\{\frac{\pi R^2}{h}+\left(\frac{\pi^2+4}{4}F_d-2\right)R\right.\\&\left.+\left(\frac{\pi^2+4}{4\sqrt{e}}F_d-2.71\right)h\right\},\end{aligned} \quad (52)$$

where h is still a free parameter. Minimizing this energy with respect to R/h, we would arrive at

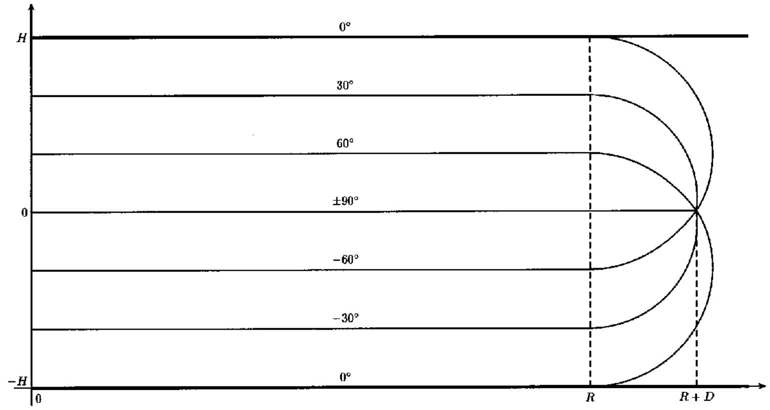

FIG. 3. Curves of equal alignment for the complete model. The circular thread is located in the plane $z=0$. The twist region has a radius R and the defect is found at a distance $R+D$ from the loop's center.

$$\frac{R}{h}=0.55+\sqrt{0.11+0.67\ln\frac{\pi h}{r_c\sqrt{e}}}. \tag{53}$$

The logarithm being typically of order 10, this gives $R\approx 3h$. For long threads this requirement cannot be met because h cannot exceed the cell's thickness. Thus we take $h=H$, as for the minimum of $F_{\mathcal{A}}$, which makes the distortion fill the entire cell. The director field we have constructed is depicted in Fig. 3, where $D:=H/\sqrt{e}$ is the equilibrium distance between the thread and the loop.

D. Model for a noncircular loop

Our model is also fit to describe a noncircular disclination loop. To see this, first recall that Eq. (42) expresses the free energy $F_{\mathcal{A}}$ stored in the region inside the thread, regardless of the shape of this curve. As to the energy stored in $\mathcal{T}$, the same argument leading to the first line in Eq. (45) shows that it can be given the form

$$F_{\mathcal{T}}:=\frac{K}{2}\int_0^L\int\int_{\mathcal{C}}(\nabla\varphi)^2(1-\sigma\xi)d\xi\, dz\, ds, \tag{54}$$

where the length L of the thread is now a functional of $\boldsymbol{q}(s)$. Since this is a closed curve, in our parametrization it satisfies

$$\int_0^L\sigma(s)ds=-2\pi. \tag{55}$$

Thus here we replace Eq. (45) by

$$\mathcal{F}=\frac{K\mathcal{A}}{h}\int_0^\infty\phi'^2e^\lambda d\lambda+\frac{K}{2}\int\int_{\mathcal{C}}(\nabla\varphi)^2(L+2\pi\xi)d\xi\, dz. \tag{56}$$

If then the approximation $\mathcal{A}/H\gg L\gg H$ is valid, repeating *verbatim* the line of thought followed in Sec. II C, for all $h\leqslant H$ we arrive at

$$\mathcal{F}=\frac{\pi^2}{4}K\left\{\frac{\mathcal{A}}{h}+\frac{1}{2\pi}\left(\frac{\pi^2+4}{4}F_d-2\right)L+\left(\frac{\pi^2+4}{4\sqrt{e}}F_d-2.71\right)h\right\}, \tag{57}$$

whence $h=H$, as in the above approximation $\mathcal{F}$ turns out to be a decreasing function of h.

III. DYNAMICS

A. Dissipation principle

To describe the dynamics of our model, we start from a dissipation principle [17], which, when flow effects are neglected, takes the form

$$\dot{\mathcal{F}}+\mathcal{W}=0 \tag{58}$$

and states that the rate of change in the elastic free energy $\dot{\mathcal{F}}$ in a fixed region in space is compensated for by the energy $\mathcal{W}$ dissipated in the same region by the viscous torque acting on the director. In the absence of flow and with the usual approach of neglecting the inertia of the molecular reorientation, the dissipation per unit volume has the simple form

$$w=\gamma_1\left(\frac{\partial\varphi}{\partial t}\right)^2, \tag{59}$$

where γ_1 is the rotational viscosity.

Making the further assumption that during the time evolution the system traverses only equilibrium configurations as described by Eqs. (43) and (48), the dissipation principle (58) leads to an evolution equation for the disclination loop, which we first derive for a circle and then extend to a general shape.

B. Dissipation for a circular loop

The first problem to be faced in calculating the dissipation is to obtain an expression for $\partial\varphi/\partial t$. As time elapses, the alignment changes only inside the tubular region $\mathcal{T}$, which follows the motion of the circular thread. The shape of its cross section $\mathcal{C}$ remains unaltered as it slides radially towards the loop center: Both h and d retain the same equilibrium values obtained above, which do not depend on the thread radius R. Consider the value of the alignment φ at the point in $\mathcal{T}$ represented by

$$\boldsymbol{p}(s,\xi,z)=\boldsymbol{q}(s)+\xi\boldsymbol{\nu}(s)+z\boldsymbol{e}_z. \tag{60}$$

It is conveyed unchanged as $\mathcal{T}$ shrinks, so that along the trajectory followed by $\boldsymbol{p}$

$$0=\frac{d\varphi}{dt}=\frac{\partial\varphi}{\partial t}+\nabla\varphi\cdot\dot{\boldsymbol{p}}. \tag{61}$$

Now, for a given s, $\dot{\boldsymbol{p}}$ is the same for all ξ and z, as every cross section of $\mathcal{T}$ moves with velocity $v_\nu=\dot{R}$:

$$\dot{\boldsymbol{p}}=\dot{R}\boldsymbol{\nu}(s). \tag{62}$$

Computing the gradient of φ as indicated in Eq. (10), we thus have

$$\frac{\partial\varphi}{\partial t}=-\dot{R}\frac{\partial\varphi}{\partial\xi}. \tag{63}$$

When expressed as a function of (η,λ), φ does not depend on η; to compute the partial derivative of φ with respect to ξ, we solve the linear system of equations

$$\frac{\partial\varphi}{\partial\lambda}=\phi'=\frac{\partial\varphi}{\partial\xi}\frac{\partial\xi}{\partial\lambda}+\frac{\partial\varphi}{\partial z}\frac{\partial z}{\partial\lambda},$$

$$\frac{\partial\varphi}{\partial\eta}=0=\frac{\partial\varphi}{\partial\xi}\frac{\partial\xi}{\partial\eta}+\frac{\partial\varphi}{\partial z}\frac{\partial z}{\partial\eta}, \tag{64}$$

where it is again understood that $\partial\varphi/\partial s=0$ because the loop shrinks to a homogeneous alignment. The solution of Eq. (64) is

$$\frac{\partial\varphi}{\partial\xi}=\frac{2\phi'}{\pi\rho_\lambda\dfrac{\partial\rho_\lambda}{\partial\lambda}}\left(\rho_\lambda\frac{\pi}{2}\cos\frac{\pi}{2}\eta+\frac{\partial\rho_\lambda}{\partial\eta}\sin\frac{\pi}{2}\eta\right),$$

$$\frac{\partial\varphi}{\partial z}=\frac{2\phi'}{\pi\rho_\lambda\dfrac{\partial\rho_\lambda}{\partial\lambda}}\left(\rho_\lambda\frac{\pi}{2}\sin\frac{\pi}{2}\eta-\frac{\partial\rho_\lambda}{\partial\eta}\cos\frac{\pi}{2}\eta\right). \tag{65}$$

Making use in Eq. (65) of ρ_λ and $\phi(\lambda)$ as derived in our static model, we arrive at

$$\left(\frac{\partial\varphi}{\partial t}\right)^2=\frac{\phi'^2\dot{R}^2}{\rho_\lambda\dfrac{\partial\rho_\lambda}{\partial\lambda}(\eta^2-2\eta)}\times\left[\cos^2\frac{\pi}{2}\eta+\left(\frac{2}{\pi}(2\lambda-1)(\eta-1)\sin\frac{\pi}{2}\eta\right)^2+\frac{4}{\pi}(2\lambda-1)(\eta-1)\sin\frac{\pi}{2}\eta\cos\frac{\pi}{2}\eta\right]. \tag{66}$$

The total dissipation $\mathcal{W}$ is then obtained by integration over $\mathcal{T}$:

$$\begin{aligned}\mathcal{W}&=2\pi\gamma_1\int\int_{\mathcal{C}}\left(\frac{\partial\varphi}{\partial t}\right)^2(R+\xi)d\xi\,dz\\&=-4\pi\gamma_1\int_0^{\pi/2}\int_0^\infty\left(\frac{\partial\varphi}{\partial t}\right)^2\rho_\lambda\frac{\partial\rho_\lambda}{\partial\lambda}(R+\rho_\lambda\cos\gamma)d\gamma\,d\lambda\\&=2\pi^2\gamma_1\dot{R}^2\int_0^1\int_0^\infty\frac{\dfrac{\pi^2}{4}e^{-2\lambda}}{\eta(2-\eta)}\\&\quad\times\left[\cos^2\frac{\pi}{2}\eta+\left(\frac{2}{\pi}(2\lambda-1)(\eta-1)\sin\frac{\pi}{2}\eta\right)^2+\frac{4}{\pi}(2\lambda-1)(\eta-1)\sin\frac{\pi}{2}\eta\cos\frac{\pi}{2}\eta\right]\\&\quad\times\left(R+d\,e^{(\eta^2-2\eta)(\lambda-1/2)}\cos\frac{\pi}{2}\eta\right)d\eta\,d\lambda.\end{aligned} \tag{67}$$

Again the integration in λ is easily done, while that in η requires the same skill applied to Eq. (50): The singular part needs to be isolated and the convergent remainder is integrated numerically. The result is

$$\mathcal{W}=\frac{\pi^4}{8}\gamma_1\dot{R}^2\left((F_D-1.13)R+(F_D-1.23)\frac{H}{\sqrt{e}}\right), \tag{68}$$

with $F_D:=\ln(\pi D/r_c)=\ln(\pi H/r_c\sqrt{e})$ analogous to F_d in Eq. (40).

C. Shrinking circles

Inserting the energy (52) and the dissipation (68) into the dissipation principle (58), we obtain the following differential equation for $r:=R/H$:

$$r+a_1=-\tau\dot{r}(a_2r+a_3), \tag{69}$$

where the coefficients are defined by

$$a_1=\frac{\pi^2+4}{8\pi}F_D-\frac{1}{\pi}, \tag{70}$$

$$a_2=F_D-1.13, \tag{71}$$

$$a_3=\frac{1}{\sqrt{e}}(F_D-1.23) \tag{72}$$

and τ is a relaxation time depending on both the material and the cell size:

$$\tau=\frac{\pi\gamma_1H^2}{4K}. \tag{73}$$

This equation is easily integrated by separation of variables to yield

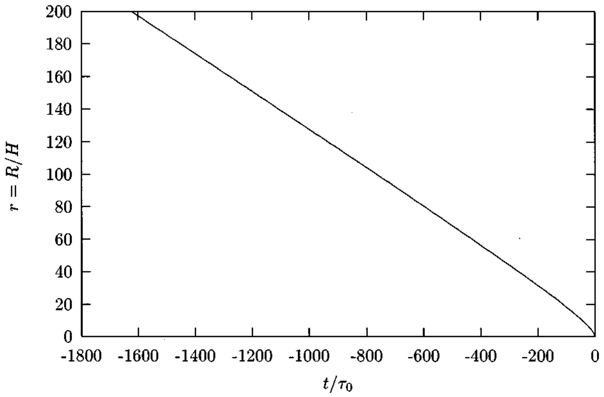

FIG. 4. Time evolution of the thread radius R scaled to H. Here $t_0 = 0$.

$$\frac{t_0 - t}{\tau} = a_2 r - (a_1 a_2 - a_3) \ln\left(1 + \frac{r}{a_1}\right). \tag{74}$$

Clearly for large values of r this implies a linear dependence of the thread radius on time, which amounts to the same conclusion for the loop radius, as in our model the two differ by a constant. For $F_D = 10$ we give a plot of the solution in Fig. 4 and we represent in Fig. 5 the scaling exponent

$$\alpha := \frac{d \ln t}{d \ln r} = \frac{r}{t(r)} \frac{dt}{dr}$$

as a function of r. It must be noted that the assumptions made in deriving Eq. (69) render the solution valid only for values of $r \gtrsim 3$.

D. General evolution equation

When the disclination loop fails to be circular, we may apply essentially the same arguments as in Sec. III B to compute the total dissipation. Now, however, at any given time, the cross sections of $\mathcal{T}$ do not slide all with the same velocity: That through the point $\boldsymbol{q}(s)$ on the thread moves along $\boldsymbol{\nu}(s)$ with the normal velocity of the thread at that point $v_\nu := \dot{\boldsymbol{q}} \cdot \boldsymbol{\nu}$, which in general changes with s. Thus, in Eq. (66) we need only substitute v_ν^2 for $\dot{R}^2$ to get the appropriate expression for $(\partial\varphi/\partial t)^2$. Using this in the integral

$$\mathcal{W} = \gamma_1 \int_0^L ds \int \int_{\mathcal{C}} \left(\frac{\partial \varphi}{\partial t}\right)^2 (1 - \sigma\xi) d\xi \, dz, \tag{75}$$

we readily arrive at

$$\mathcal{W} = \frac{\pi^3 \gamma_1}{16} \int_0^L (a_2 - a_3 \sigma H) v_\nu^2 ds, \tag{76}$$

where a_2 and a_3 are as in Eqs. (71) and (72) and L is the actual length of the thread. Clearly, Eq. (76) is valid, provided that $a_2 - a_3\sigma H > 0$ along the curve, as is required by the inequality $1 - \sigma\xi > 0$, which follows from Eq. (9): A convex curve, for which $\sigma < 0$, would satisfy both of these equations.

The total free energy $\mathcal{F}$ is given by Eq. (57) with $h = H$ and $d = D$. To compute its time derivative we observe that

$$\dot{\mathcal{A}} = \int_0^L v_\nu ds \tag{77}$$

and

$$\dot{L} = -\int_0^L \sigma v_\nu ds, \tag{78}$$

to conclude that

$$\dot{\mathcal{F}} = \frac{\pi^2 K}{4H} \int_0^L (1 - a_1 \sigma H) v_\nu ds, \tag{79}$$

where a_1 is as in Eq. (70). The dissipation principle then reads as

$$\int_0^L v_\nu \left\{ \frac{\pi^3 \gamma_1}{16} (a_2 - a_3 \sigma H) v_\nu + \frac{\pi^2 K}{4H} (1 - a_1 \sigma H) \right\} ds = 0 \tag{80}$$

and it is satisfied along any portion of the curve, provided this evolves in time according to the equation

$$v_\nu = \frac{H}{\tau} g(\sigma H), \tag{81}$$

with

$$g(\sigma H) := \frac{a_1 \sigma H - 1}{a_2 - a_3 \sigma H}, \tag{82}$$

where τ is the relaxation time defined by Eq. (73).

Since g fails to be linear, the evolution described by this equation is different from the flow by curvature of a plane curve, which applies when $v_\nu \propto \sigma$. We conjecture, however, that the same qualitative properties of this motion apply to that described by Eq. (81), as long as the function g is increasing. As made precise in [8], where previous results valid only for convex curves [18–20] were first extended to all plane curves, the flow by curvature shrinks a curve to a point, making it round in the limit. In other words, a nonconvex curve becomes convex as it shrinks. We expect the same

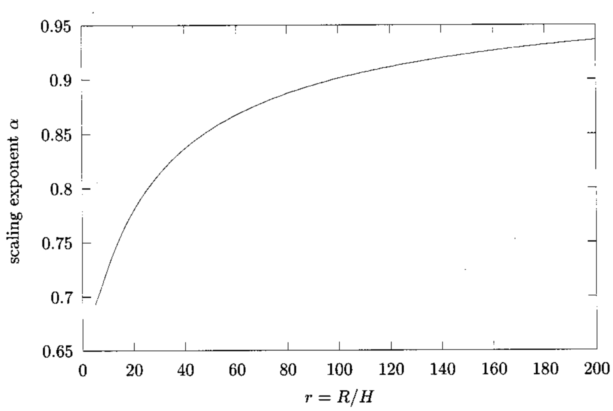

FIG. 5. Scaling exponent of the solution depending on the radius. The scalar $\alpha = d \ln t(r)/d \ln r$ is the slope of t versus r in a bilogarithmic plot.

conclusion to apply to the flow predicted by our model, provided the normal velocity v_ν is higher at points with higher curvature. It is easily seen that the function g is increasing whenever $a_1 a_2 - a_3 > 0$: A direct computation resorting to Eqs. (70)–(72) shows that this inequality is satisfied for all values of H/r_c, the only parameter on which the coefficients a_i depend.

Finally, there is a distinctive feature of the flow described by Eq. (81) that the flow by curvature does not possess: Since $g(0) < 0$, also a point where the curvature is infinitesimal would have a finite velocity. This requires care in dealing with the singularities, such as corners and points of self-contact, that a curve may develop in its evolution. It is known from [8] that no singularity arises in the flow by curvature: We do not know whether the same theorem applies also to the flow we have derived.

IV. CONCLUSIONS

We have constructed a model director field that describes a twist disclination line confined to a thin cell with planar boundary anchoring. First the case of a closed circular disclination loop has been treated via a dissipation principle. Our main result was to show that for large threads the loop radius shrinks linearly with time. Then, within a suitable approximation, we also treated noncircular loops: For them the dissipation principle led to a flow that formally differs from the flow by curvature of a plane curve, though we expect the qualitative properties of both flows to be the same.

The linear shrinking law is in qualitative agreement with recent measurements on polymeric liquid crystals. The experimental setup, however, differed in one respect from our model. While we assumed the loop to lie in the midplane of a thin cell, in the experiment the disclinations were found in the proximity of the plates such that ''the distance of the loops from a surface [was] smaller than their size'' (see [13], p. 206).

This observation is consistent with what is known about twist disclination loops, namely, that though the minimal energy is attained if the loop lies in the midplane, since the minimum is not very pronounced, threads may be found away from the center [10]. As, according to our model, the ratio of the loop diameter to the cell's thickness determines the shrinking law, a direct quantitative comparison to experiments requires a well-defined distance between the loop and the boundary.

The case of small loops without confining boundaries cannot be treated directly within our model because of the assumptions made in deriving the minimizing configuration. Nevertheless, it is easy to obtain the correct shrinking law via the dissipation principle. The free energy connected with the disclination is then proportional to the length of the thread

$$\mathcal{F} \propto R \tag{83}$$

since the contribution stemming from the enclosed area is proportional to R^2/H, which becomes negligible both for large cells $(H \to \infty)$ and small loops $(R \to 0)$. A similar argument holds for the dissipation, which is proportional to the length of the disclination and the square of its shrinking velocity $\dot{R}$,

$$\mathcal{W} \propto \dot{R}^2 R. \tag{84}$$

Consequently, by Eq. (58),

$$\dot{R}R = \text{const}, \tag{85}$$

which yields $R \propto (t_0 - t)^{0.5}$ in agreement with the experimental evidence.

ACKNOWLEDGMENTS

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