Minimizers of disclinations in nematic liquid crystals

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Abstract

In this work, we revisit the important problem of disclinations for nematic liquid-crystals in the variational theory of Oseen-Zöcher-Frank. Using the framework of dynamical system theory, the Frank's energy functional among a class of special director fields for both the elastically isotropic and anisotropic cases are examined. The existence result on the critical points of the energy functional is reproduced in a much simpler and intuitive way. With the help of a new observation, the (local) minimality of all critical points within the class of director fields is established.

Key words. Nematics, disclination, minimizer

AMS subject classifications. 76A15, 49K15, 34K21

Running head. Minimizers of disclinations in nematics

1 Introduction

Liquid-crystals are intermediate phases between solid states and liquid states ([14, 9, 5, 7, 11, 3]). They have capability of flow but also possess a certain degree of crystal structures. Nematics are the simplest liquid crystals that consist of rod-like molecules: at each location x in the region Ω occupied by the nematic liquid crystals, a unit vector $\mathbf{n}(x) \in \mathbb{S}^2$ is introduced to characterize the average preferred alignment of the rod-like elements near x. The static theory of Oseen-Zöcher-Frank ([14, 9, 7]) for nematic liquid crystals looks for *director fields* $\mathbf{n} : \Omega \to \mathbb{S}^2$ that minimize the elastic energy

$$\mathcal{F}(\mathbf{n}) = \int_\Omega \mathcal{W}(\mathbf{n}, \nabla\mathbf{n})dx, \qquad (1) \quad \{\texttt{Energy}\}$$

where $\mathcal{W}(\mathbf{n}, \nabla\mathbf{n})$ is the Frank's energy function ([9, 7, 11]) given by

$$\begin{aligned}\mathcal{W}(\mathbf{n}, \nabla\mathbf{n}) =& \frac{K_1}{2}(\operatorname{div}\mathbf{n})^2 + \frac{K_2}{2}(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 \\ &+ \frac{K_3}{2}|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2 + \frac{K_2+K_4}{2}\left(\operatorname{tr}(\nabla\mathbf{n})^2 - (\operatorname{div}\mathbf{n})^2\right),\end{aligned} \qquad (2) \quad \{\texttt{FrankE}\}$$

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where K_j's are the Frank's constants with the properties

$$2K_1 \geq K_2 + K_4,\ K_2 \geq |K_4|,\ K_3 \geq 0.$$

The four terms on the right-hand-side of (2) are, respectively, the splay, twist, bend, and saddle-splay modes (see, for example, [17, 16]).

The existence, regularity and the nature of defects of a *global* minimizer $\mathbf{n}$ for general smooth domain $\Omega \subset \mathbb{R}^3$ under a strong anchoring boundary condition $\mathbf{n}|_{\partial\Omega} = \mathbf{n}_0$ are established in [1, 2, 10, 12], etc.. In particular, a typical global minimizer exhibits point defects of the form $\pm x/|x|$.

Nevertheless, a special type of line defects – *disclination* – has been examined within the classical continuum theory of Oseen-Zöcher-Frank. This type of defects was observed frequently. An example is the Schlieren texture in a thin film between crossed polarizers. Several forms of disclinations are illustrated in Figure 1. See [15, 3, 17, 16, 5] for more examples. In the figure, the origin represents the disclination line perpendicular to the plane and the curves in the plane are integral curves of director fields $\mathbf{n}$ projected onto the plane.

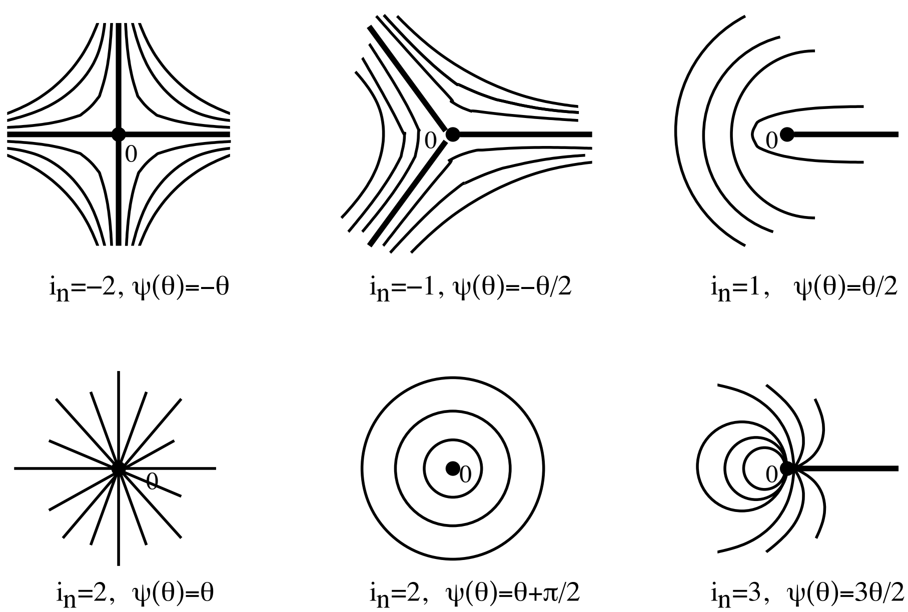

Figure 1: Examples of disclinations: The Frank's index i_n of disclinations is defined in Section 2; θ is the angular component of the polar coordinates, ψ is the angle made by $\mathbf{n}$ from the positive x-axis; The case with $i_n = 2$ can have different structures, one with $\psi(0) = \pi/2$ and the others are equivalent (up to deformations) to that with $\psi(0) = 0$. {sampleDS}

A mathematical examination of these line defects was first given by Oseen ([14]) and later by Frank ([9]) and by Dzyaloshinskii ([6]). In those works, disclinations were described by critical points, solutions of the Euler-Lagrange equation of the energy functional $\mathcal{F}$ among special classes of director fields $\mathbf{n}$, and Frank also introduced an index to further characterize the complexity degrees of disclinations. See also excellent references, for examples, [5, 3, 17, 16], for detailed discussions of this important property of nematic textures. On the other hand, it lacks the study of minimality of these solutions in the literature. The main contribution of this paper is on the minimality of disclination solutions. It turns out the global minimizer of $\mathcal{F}$ does not possess defects but most of other critical points of $\mathcal{F}$ do and are indeed local minimizers within the class of planar director fields $\mathbf{n}$ defined in display (3).

We point out that the minimality of disclination solutions is examined within the special class of director fields in display (3) and one has to exclude the disclination line in order to have a finite energy $\mathcal{F}$ ($r_0 > 0$ in (7)). If one allows general director fields $\mathbf{n}$, then the minimality result may be different. In fact, it has been noticed independently by Cladis and Kléman ([4]) and by Meyer ([13]) that disclination solutions with even Frank's indices can be deformed to other form of solutions (with nontrivial z-components) *without discontinuity* – "Escape of the disclination into the third dimension" (see also [5, 15, 16]). Of course, the escaping solutions having no singularities do not provide an explanation of disclinations. A new theory was proposed by Ericksen ([8], see also [12]) by introducing an order parameter S to resolve the divergence of energy due to singularity. This theory seems to need further development to give a better understanding of line disclinations. We hope to study disclination solutions and their minimality or stability with the new theory in the future.

To end this introduction, we describe the organization of the rest of this paper. Following the books [3, 16, 17], a formulation of disclination problems and the Frank's index will be given in §2. In §3, we re-examine the Euler-Lagrange equation for the energy functional in the framework of dynamical systems, which allows us to establish the existence and properties of solutions of the Euler-Lagrange equation in a much simpler way (Theorem 3.1). The minimality of the solutions will be studied in §4 through the Jacobian equation method. Here an observation makes the Jacobian equation completely solvable and, in turn, we are able to completely determine the local minimality of all critical points of $\mathcal{F}$ within a special class of director fields (Theorem 4.1).

2 Disclinations and Frank's index

{DisIndex}

We start with the setup of the disclination problem following [3, 16, 17] closely. Let

$$\begin{aligned}\Omega =&\{(x,y,z):\ r_0^2 < x^2+y^2 < R_0^2,\ 0<z<L\}\\ =&\{(r,\theta,z):\ r_0 < r < R_0,\ 0<z<L\}\end{aligned}$$

be a hollow cylinder. Denote $\mathbf{e}_r$ and $\mathbf{e}_\theta$ the unit radial and angular vectors in the plane perpendicular to the z-axis, respectively, that is, if $\mathbf{e}_x$, $\mathbf{e}_y$ and $\mathbf{e}_z$ are the unit vectors of Cartesian axes, then

$$\mathbf{e}_r = \cos\theta\,\mathbf{e}_x + \sin\theta\,\mathbf{e}_y, \quad \mathbf{e}_\theta = -\sin\theta\,\mathbf{e}_x + \cos\theta\,\mathbf{e}_y.$$

Consider planar director fields $\mathbf{n}$ that depend on θ only:

$$\mathbf{n}(r,\theta,z) = \cos\phi(\theta)\,\mathbf{e}_r + \sin\phi(\theta)\,\mathbf{e}_\theta. \tag{3}$$ {director}

For $\mathbf{n}$ to be continuous, it is necessary that

$$\phi(2\pi) - \phi(0) = m\pi \ \text{ for some } \ m \in \mathbb{Z} \tag{4}$$ {perbv}

since $\mathbf{n} = -\mathbf{n}$ for nematic liquid crystals. Note that, in terms of the Cartesian axes unit vectors,

$$\mathbf{n} = \cos\psi(\theta)\,\mathbf{e}_x + \sin\psi(\theta)\,\mathbf{e}_y.$$

where the angle between $\mathbf{n}$ and the positive x-axis is

$$\psi(\theta) = \phi(\theta) + \theta \ \text{ and } \ \psi(2\pi) - \psi(0) = \phi(2\pi) - \phi(0) + 2\pi. \tag{5}$$ {angle}

If $\phi(\theta)$ is not constant, then the director field $\mathbf{n}$ defined in (3) becomes discontinuous along the line $\{r = 0\}$ or the z-axis and the line $\{r = 0\}$ is called the line of *disclination* ([9]) or *wedge disclination* in [5]. This is the reason the special form (3) for director fields $\mathbf{n}$ is taken.

The Frank's energy function (2) is reduced to

$$\mathcal{W}(\mathbf{n}, \nabla\mathbf{n}) = \frac{1}{2r^2}(\phi' + 1)^2(K_1\cos^2\phi + K_3\sin^2\phi).$$

The total energy is

$$\mathcal{F}(\phi) := \mathcal{F}(\mathbf{n}) = \frac{L}{2}\ln\frac{R_0}{r_0}\int_0^{2\pi}(\phi'(\theta) + 1)^2(K_1\cos^2\phi(\theta) + K_3\sin^2\phi(\theta))d\theta.$$

Note that the integrand above consists of two terms $K_1(\phi' + 1)^2\cos^2\phi$ and $K_3(\phi' + 1)^2\sin^2\phi$. They correspond to, respectively, the splay mode and bend mode of the Frank's energy function. There are no twist and saddle-splay modes due to the restriction of planar director field $\mathbf{n}$ in (3).

We will denote

$$f(\phi) = K_1\cos^2\phi + K_3\sin^2\phi \ \text{ and } \ W(\phi, \phi') = (\phi' + 1)^2 f(\phi) \tag{6}$$ {energyfun}

so that the total energy is

$$\mathcal{F}(\phi) = \frac{L}{2}\ln\frac{R_0}{r_0}\int_0^{2\pi} W(\phi, \phi')d\theta. \tag{7}$$ {angularF}

It is obvious that $W(\phi, \phi') = 0$ if and only if $\phi' = -1$ or $\phi(\theta) = -\theta + \phi_0$ for some constant ϕ_0. In view of (5), $\psi(\theta) = \phi_0$, that is, $\mathbf{n}$ is a constant vector. If $\phi'(\theta) \neq -1$, then the energy $\mathcal{F}(\phi)$ approaches infinity as $r_0 \to 0$. This particular situation shows a serious drawback of the Oseen-Zöcher-Frank theory in handing line defects of liquid-crystals. In this sense, the results described in this paper within the Oseen-Zöcher-Frank theory provide an "approximation" for an understanding of the disclinations.

To characterize the complexity of disclination defects, Frank introduced an index for director fields $\mathbf{n}$ of form in (3). For such a planar situation, the director $\mathbf{n}$ lies in $\mathbb{S}^1$. Since we don't distinguish $-\mathbf{n}$ from $\mathbf{n}$ for nematic liquid crystals, instead of $\mathbb{S}^1$, we should have taken the projected $\mathbb{S}^1$ by identifying the opposite points of $\mathbb{S}^1$. In particular, as a point moves counterclockwise along a closed curve enclosed the origin, if the director field $\mathbf{n}$ covers k times the unit circle $\mathbb{S}^1$, then it wraps up $2k$ times the projected $\mathbb{S}^1$. This motivates the following definition of Frank's index.

Definition 2.1. For a planar director field $\mathbf{n}$ in (3), the *Frank's index* is

$$i_n = \frac{\psi(2\pi) - \psi(0)}{\pi} = \frac{\phi(2\pi) - \phi(0)}{\pi} + 2. \qquad (8) \quad \{\texttt{FrankInd}\}$$

It follows from the condition $\phi(2\pi) - \phi(0) \in \pi\mathbb{Z}$ in (4) that $i_n \in \mathbb{Z}$.

We end this section with the formulation of the Euler-Lagrange equation for the functional $\mathcal{F}$ in (7) and a brief discussion of Frank's result for the elastically isotropic case.

It is a standard result from calculus of variations that the Euler-Lagrange equation for the functional $\mathcal{F}$ in (7) is

$$\left(\frac{\partial W}{\partial \phi'}\right)' - \frac{\partial W}{\partial \phi} = 0 \ \text{ in } (0, 2\pi) \qquad (9) \quad \{\texttt{ELnew}\}$$

with the boundary requirement, due to the periodic boundary condition (4),

$$\frac{\partial W}{\partial \phi'}(\phi(0), \phi'(0)) = \frac{\partial W}{\partial \phi'}(\phi(2\pi), \phi'(2\pi)). \qquad (10) \quad \{\texttt{ELbv}\}$$

It follows from the expressions of $W(\phi, \phi')$ and $f(\phi)$ in (6) that the Euler-Langrange equation (9) becomes

$$f(\phi)\phi'' + \frac{1}{2} f_\phi(\phi)(\phi'^2 - 1) = 0 \ \text{ in } (0, 2\pi), \qquad (11) \quad \{\texttt{angularEL}\}$$

and the condition (10) is reduced to $(\phi'(2\pi) - \phi'(0)) f(\phi(2\pi)) = 0$, which is equivalent to $\phi'(2\pi) = \phi'(0)$ if $K_1^2 + K_3^2 \neq 0$. In the sequel, we assume that $K_1 > 0$ and $K_3 > 0$.

Frank ([9]) examined the *elastically isotropic* case, that is, $K_1 = K_3 = K$. In this case, equation (11) becomes $\phi'' = 0$, and hence, $\phi(\theta) = c\theta + \phi_0$ for some constants c and ϕ_0. Note that $\phi'(2\pi) = \phi'(0)$ is automatically satisfied. Also, $\phi(2\pi) - \phi(0) = 2c\pi$. Hence, the Frank's index is $i_n = 2c + 2$ and the energy is

$$\mathcal{F}(\phi) = \frac{\pi L K}{4} i_n^2 \ln \frac{R_0}{r_0}.$$

Frank also illustrated the complexity of a director field $\mathbf{n}$ through its "flux lines"; that is, integral curves of the director field $\mathbf{n}$ (see Figure 1). Note that, in terms of ψ, the Frank's solutions are $\psi(\theta) = \dfrac{i_n}{2}\theta + \phi_0$.

Dzyaloshinskii ([6]) late provided a complete result on the existence of solutions for *elastically anisotropic* cases, i.e., $K_1 \neq K_3$.

3 Solutions of Euler-Lagrange equation (11)

{EL}

In this section, we examine the Euler-Lagrange equation (11), reproducing the result of Dzyaloshinskii ([6]) but in the framework of dynamical systems. Note that equation (11) can be rewritten as

$$\phi' = \frac{\rho}{f(\phi)}, \quad \rho' = \frac{f_\phi(\phi)}{2f^2(\phi)}\rho^2 + \frac{1}{2}f_\phi(\phi) \tag{12}$$ {angularsys}

where $f(\phi)$ is defined in (6), and the boundary condition is

$$\phi(2\pi) - \phi(0) \in \pi\mathbb{Z} \ \text{ and } \ \phi'(2\pi) = \phi'(0). \tag{13}$$ {angularBV}

System (12) is a Hamiltonian system with a Hamiltonian function

$$\mathcal{H}(\phi, \rho) = \frac{\rho^2}{2f(\phi)} - \frac{1}{2}f(\phi). \tag{14}$$ {ham}

Remark 3.1. A result from calculus of variations says, if $L(t, y, y') = L(y, y')$ does not depend on t explicitly, the Euler-Lagrange equation for the functional

$$I(y) = \int_\alpha^\beta L(y, y')dt$$

has an integral given by $L - y'L_{y'}$. For the problem at hand, it is $f(\phi)\phi'^2 - f(\phi)$ that agrees with the Hamiltonian function $\mathcal{H}$ above. □

Note that, if we interchange K_1 and K_3 and shift ϕ by $\pi/2$ in system (12), we end up with the same system with the same boundary condition (13). Therefore, we will examine the existence of solutions of (12) and (13) for the case that $K_1 > K_3$ only.

The equilibria of (12) are $(\phi^*, \rho^*) = (k\pi, 0), (k\pi + \pi/2, 0)$ for $k \in \mathbb{Z}$. For $K_1 > K_3$, one finds that the equilibria $(m\pi, 0)$'s are centers with eigenvalues $\pm\sqrt{\frac{K_1-K_3}{K_1}}i$ and the equilibria $(k\pi + \pi/2, 0)$'s are saddles with eigenvalues $\pm\sqrt{\frac{K_1-K_3}{K_3}}$. There are heteroclinic loops between adjacent saddle equilibria. The phase plane portrait is sketched in Figure 2.

We now consider non-equilibrium solutions.

Case 1. Non-equilibrium solutions inside a heteroclinic loop. We may only consider non-equilibrium solutions inside the heteroclinic loop for $\phi \in (-\pi/2, \pi/2)$. The boundary condition (13) implies that $(\phi(2\pi), \rho(2\pi)) = (\phi(0), \rho(0))$; that is,

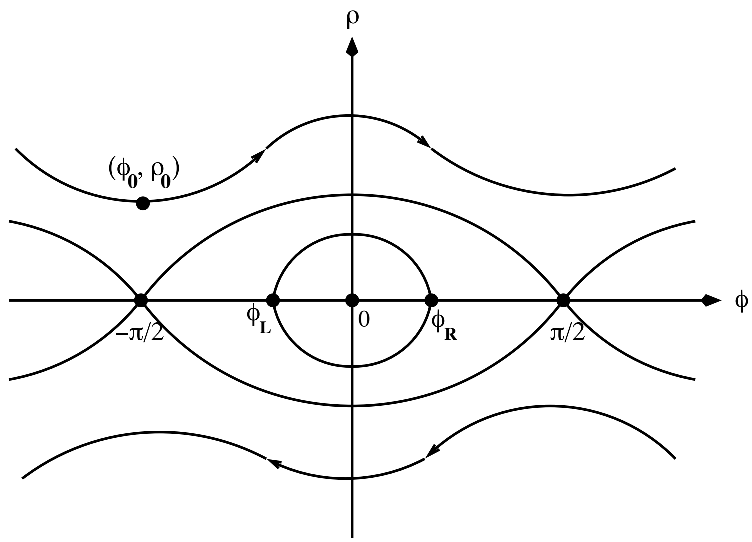

Figure 2: The phase portrait of system (12) for the case of $K_1 > K_3$ {firstfig}

the solution has to be a periodic solution with a period 2π. Since system (12) is autonomous, we may assume that $(\phi(2\pi), \rho(2\pi)) = (\phi(0), \rho(0)) = (\phi_L, 0)$ with $\phi_L \in (-\pi/2, 0)$. Note that, due to the symmetry of system (12), necessarily, $(\phi(\pi), \rho(\pi)) = (\phi_R, 0)$ with $\phi_R = -\phi_L \in (0, \pi/2)$.

Using the Hamiltonian function (14), we have $\mathcal{H}(\phi, \rho) = \mathcal{H}(\phi_R, 0)$; that is,

$$\frac{\rho^2}{f(\phi)} - f(\phi) = -f(\phi_R) \quad \text{or} \quad \phi'^2 = \frac{f(\phi) - f(\phi_R)}{f(\phi)}.$$

Let $\theta_1 > 0$ be the first value so that $(\phi(\theta_1), \rho(\theta_1)) = (\phi_R, 0)$. Then, $\theta_1 = \pi/k$ for some positive integer k, and $\phi'(\theta) > 0$ for $\theta \in (0, \pi/k)$.

Therefore, for $\theta \in (0, \pi/k)$,

$$\frac{d\phi}{d\theta} = \sqrt{\frac{f(\phi) - f(\phi_R)}{f(\phi)}} \quad \text{or} \quad d\theta = \sqrt{\frac{f(\phi)}{f(\phi) - f(\phi_R)}}\, d\phi.$$

Integrate over $\theta \in (0, \pi/k)$ and use the fact that $f(\phi)$ is even in ϕ to get

$$\pi/k = \int_{\phi_L}^{\phi_R} \sqrt{\frac{f(\phi)}{f(\phi) - f(\phi_R)}}\, d\phi = 2\int_0^{\phi_R} \sqrt{\frac{f(\phi)}{f(\phi) - f(\phi_R)}}\, d\phi. \qquad (15)$$ {inside}

With the substitution $\sin\phi = \sin\phi_R \sin\alpha$, we get

$$\int_0^{\phi_R} \sqrt{\frac{f(\phi)}{f(\phi) - f(\phi_R)}}\, d\phi = \frac{1}{\sqrt{K_1 - K_3}} \int_0^{\pi/2} \sqrt{G(\alpha, \phi_R)}\, d\alpha,$$

where

$$G(\alpha, \phi_R) = \frac{K_1 + (K_3 - K_1)\sin^2\phi_R \sin^2\alpha}{1 - \sin^2\phi_R \sin^2\alpha}.$$

It follows from

$$\frac{\partial}{\partial \phi_R} G(\alpha, \phi_R) = \frac{2K_3}{(1 - \sin^2\phi_R \sin^2\alpha)^2} \sin\phi_R \cos\phi_R \sin^2\alpha$$

that $G(\alpha, \phi_R)$ is monotonically increasing in ϕ_R, and hence,

$$T(\phi_R) := 2\int_0^{\phi_R} \sqrt{\frac{f(\phi)}{f(\phi) - f(\phi_R)}}\, d\phi$$

is monotonically increasing in $\phi_R \in (0, \pi/2)$. Note that, as $\phi_R \to \pi/2$, the orbit $(\phi(\theta), \rho(\theta))$ approaches the heteroclinic orbit, and hence, $T(\phi_R) \to \infty$ as $\phi_R \to \pi/2$. Also, $T(\phi_R) \to \pi\sqrt{\frac{K_1}{K_1 - K_3}} > \pi$ as $\phi_R \to 0$, where $\sqrt{\frac{K_1 - K_3}{K_1}}$ is the frequency of the linearization of system (12) at the origin. We conclude that there is no $\phi_R \in (0, \pi/2)$ satisfying (15); that is, there is no non-equilibrum solution $(\phi(\theta), \rho(\theta))$ of (12) and (13) whose orbit is enclosed in the heteroclinic loop.

Case 2. Non-equilibrium solutions outside heteroclinic loops.

Since system (12) is autonomous and is symmetric with respect to the ϕ-axis, we may consider $(\phi(0), \rho(0)) = (-\pi/2, \rho_0)$ with $\rho_0 > 0$ and $(\phi(2\pi), \rho(2\pi)) = (m\pi - \pi/2, \rho_0)$ for some positive integer m. Use the Hamiltonian function to get

$$f(\phi)\phi'^2 = f(\phi) + C_0, \tag{16}$$ {phiprime}

where $C_0 = (\rho_0^2 - K_3^2)/K_3$. Therefore,

$$\sqrt{\frac{f(\phi)}{f(\phi) + C_0}} d\phi = d\theta \quad \text{or} \quad T(C_0) := \int_{-\pi/2}^{m\pi - \pi/2} \sqrt{\frac{f(\phi)}{f(\phi) + C_0}} d\phi = 2\pi.$$

Note that $T(C_0) \to 0$ as $C_0 \to \infty$ (or $\rho_0 \to \infty$), $T(C_0) \to \infty$ as $C_0 \to -K_3$ (or $\rho_0 \to 0$), and $T(C_0)$ is a strictly decreasing function. We conclude that, for any positive integer m, there is a unique $C_0 = C_0(m)$ ($\rho_0 = \rho_0(m)$) that provides a solution of (12) and (13) and $C_0(m)$ (and hence $\rho_0(m)$) is increasing in m. This solution has index $i_n = m + 2$ since $\phi(2\pi) - \phi(0) = m\pi$.

In summary, we have

{angularcase}

Theorem 3.1. *Assume $K_1 > 0$, $K_3 > 0$ and $K_1 \neq K_3$. Then, for any $\phi_0 \in [-\pi/2, \pi/2)$ and $m \in \mathbb{Z}\backslash\{0\}$, there is a unique solution (ϕ_*, ρ_*) of (12) and (13) such that $\phi_*(0) = \phi_0$ and $\phi_*(2\pi) = \phi_0 + m\pi$. For $m = 0$, the only solutions are the equilibrium solutions $(\phi_*, \rho_*) = (0, 0)$ or $(\phi_*, \rho_*) = (-\pi/2, 0)$ (necessarily, $\phi_0 = 0$ or $-\pi/2$). For $m > 0$, $\rho_* > 0$ (and hence $\phi'_* > 0$); for $m < 0$, $\rho_* < 0$ (and hence $\phi'_* < 0$). For each $m \in \mathbb{Z}$, the Frank's index of the corresponding solution(s) is $i_n = m + 2$.*

For the special case $i_n = 0$ or $m = -2$, we note that $\phi' < 0$ and, correspondingly,

$$T(C_0) := \int_{-\pi/2}^{-2\pi-\pi/2} \sqrt{\frac{f(\phi)}{f(\phi)+C_0}} d\phi = -2\pi.$$

The latter is true if and only if $C_0 = 0$. It follows from (16) that $\phi'(\theta) = -1$ or $\phi(\theta) = -\theta + \phi_0$ for some ϕ_0. This gives that $\psi(\theta) = \phi(\theta) + \theta = \phi_0$. We thus conclude that a critical point $\mathbf{n}$ of $\mathcal{F}$ has index $i_n = 0$ if and only if $\mathbf{n}$ is constant. Exactly those constant director fields $\mathbf{n}$ are extendable to the z-axis without defects.

4 Minimizers of the functional $\mathcal{F}(\phi)$

{mini}

In view of (7), the energy $\mathcal{F}(\phi)$ is zero (global minimum value) if and only if $\phi'(\theta) = -1$ or $\mathbf{n}$ is a constant director field. As discussed above, these global minimizers do not exhibit disclinations. We now give a complete result on the (local) minimality of other solutions in Theorem 3.1 as well as the solutions considered by Frank for $K_1 = K_3$ among the director fields $\mathbf{n}$ defined in (3).

{suff_cond}

Theorem 4.1. *Assume $K_1 > 0$ and $K_3 > 0$.*

(i) If $K_1 = K_3$, then all critical points of $\mathcal{F}$ are minimizers.

(ii) If $K_3 < K_1$, then the critical point $\phi(\theta) = m\pi$ (or $\psi(\theta) = \theta + m\pi$, i.e. the pure radial director field $\mathbf{n} = \pm\mathbf{e}_r$) of $\mathcal{F}$ is not a minimizer. All other critical points of $\mathcal{F}$ are minimizers.

(iii) If $K_3 > K_1$, then the critical point $\phi(\theta) = m\pi+\pi/2$ or $\psi(\theta) = \theta+m\pi+\pi/2$ (i.e. the pure angular director field $\mathbf{n} = \pm\mathbf{e}_\theta$) of $\mathcal{F}$ is not a minimizer. All other critical points of $\mathcal{F}$ are minimizers.

Proof. It amounts to examine the second variation $\delta^2\mathcal{F}(\phi_*)$ at a critical point $\phi_*(\theta)$ of $\mathcal{F}$. We first consider a general functional

$$I(y) := \int_\alpha^\beta L(t, y, y')dt, \quad y(\beta) - y(\alpha) = a.$$

Let $y_*(t)$ be a critical point of $I(y)$; that is, $\delta I(y_*) = 0$ and $y_*(\beta)-y_*(\alpha) = a$.

Then, the second variation $\delta^2 I(y_*)$ of I at y_* is given as follows. For any function h with $h(\beta)-h(\alpha) = 0$ so that, for any ε, $(y_*+\varepsilon h)(\beta)-(y_*+\varepsilon h)(\alpha) = a$,

$$\begin{aligned}\delta^2 I(y_*)[h] =& \frac{1}{2}\int_\alpha^\beta \left(L_{yy}h^2 + 2L_{yy'}hh' + L_{y'y'}h'^2\right) dt \\ =& \frac{1}{2}\int_\alpha^\beta \left((L_{yy} - (L_{yy'})')h^2 + L_{y'y'}h'^2\right) dt \\ &+ \frac{1}{2}h^2(\beta)\left(L_{yy'}(\beta, y_*(\beta), y_*'(\beta)) - L_{yy'}(\alpha, y_*(\alpha), y_*'(\alpha))\right).\end{aligned}$$

Now let $\phi_*(\theta)$ be a critical point of the functional $\mathcal{F}$ in (7). Note that,

$$W_{\phi\phi'}(\phi,\phi') = 2f_\phi(\phi)(\phi'+1) = 2(K_3-K_1)\sin(2\phi)(\phi'+1),$$

and $\phi_*(2\pi) = \phi_*(0) + m\pi$ and $\phi_*'(2\pi) = \phi_*'(0)$. We have that

$$W_{\phi\phi'}(\phi_*(0),\phi_*'(0)) = W_{\phi\phi'}(\phi_*(2\pi),\phi_*'(2\pi)),$$

and hence, the boundary term in the second variation $\delta^2\mathcal{F}(\phi_*)[h]$ is zero. Therefore,

$$\delta^2\mathcal{F}(\phi_*)[h] = \frac{L}{2}\ln\frac{R_0}{r_0}\int_0^{2\pi}\left(Ph'^2 + Qh^2\right)d\theta,$$

where

$$\begin{aligned}
P =&P(\theta) = \frac{1}{2}\frac{\partial^2 W}{\partial\phi'\partial\phi'}(\phi_*(\theta),\phi_*'(\theta))\\
=&\frac{1}{2}\frac{\partial^2}{\partial\phi'\partial\phi'}\left((\phi'+1)^2 f(\phi)\right)|_{\phi_*(\theta)} = f(\phi_*(\theta)) > 0,\\
Q =&Q(\theta) = \frac{1}{2}\frac{\partial^2 W}{\partial\phi\partial\phi}(\phi_*(\theta),\phi_*'(\theta)) - \frac{1}{2}\frac{d}{d\theta}\left(\frac{\partial^2 W}{\partial\phi\partial\phi'}(\phi_*(\theta),\phi_*'(\theta))\right)\\
=&\frac{1}{2}(\phi_*'+1)^2 f_{\phi\phi}(\phi_*) - \frac{d}{d\theta}\left((\phi_*'+1)f_\phi(\phi_*)\right)\\
=&\frac{1}{2}(\phi_*'+1)^2 f_{\phi\phi}(\phi_*) - \phi_*'' f_\phi(\phi_*) - (\phi_*'+1)f_{\phi\phi}(\phi_*)\phi_*'\\
=&\frac{1}{2}\phi'^2 f_{\phi\phi} + \phi' f_{\phi\phi} + \frac{1}{2}f_{\phi\phi} + \frac{f_\phi^2}{2f}(\phi'^2-1) - \phi'^2 f_{\phi\phi} - \phi' f_{\phi\phi}\\
=&\frac{1}{2f}(\phi'^2-1)(f_\phi^2 - ff_{\phi\phi}) = \frac{\rho_0^2-K_3^2}{2K_3f^2}(f_\phi^2 - ff_{\phi\phi}) = -\frac{C_0}{2}\left(\frac{f_\phi}{f}\right)_\phi(\phi_*(\theta)).
\end{aligned}$$

For $K_1 = K_3$, we have $Q = 0$, and hence, for all critical points ϕ_* of $\mathcal{F}$, the second variation $\delta^2\mathcal{F}(\phi_*)[h] \geq 0$. Therefore, all critical points of $\mathcal{F}$ are minimizers in the elastically isotropic case examined by Frank ([9]). This establishes statement (i).

We now consider elastically anisotropic case where $K_1 \neq K_3$.

First of all, we consider the special case where $(\phi_*(\theta),\rho_*(\theta))$ is an equilibrium solution; that is, either $(\phi_*(\theta),\rho_*(\theta)) = (\pi/2, 0)$ or $(\phi_*(\theta),\rho_*(\theta)) = (0,0)$. The former corresponds to $\psi(\theta) = \theta + \pi/2$ or the pure angular director field $\mathbf{n} = \mathbf{e}_\theta$, and the latter corresponds to $\psi(\theta) = \theta$ or the pure radial director field $\mathbf{n} = \mathbf{e}_r$.

If $(\phi_*(\theta),\rho_*(\theta)) = (\pi/2, 0)$, then $P = K_3$ and $Q = 1/2 f_{\phi\phi}(\pi/2) = K_1 - K_3$. If $K_1 > K_3$, then $Q > 0$, and hence, $\mathbf{n} = \mathbf{e}_\theta$ is a minimizer of $\mathcal{F}$; if $K_1 < K_3$, then, for nonzero constant functions h,

$$\delta^2\mathcal{F}(\phi_*)[h] = \frac{L}{2}\ln\frac{R_0}{r_0}\int_0^{2\pi}(K_1-K_3)h^2 d\theta < 0,$$

and hence, $\mathbf{n} = \mathbf{e}_\theta$ is not a local minimizer.

If $(\phi_*(\theta), \rho_*(\theta)) = (0,0)$, then $P = K_1$ and $Q = 1/2 f_{\phi\phi}(0) = K_3 - K_1$. If $K_3 > K_1$, then $Q > 0$, and hence, $\mathbf{n} = \mathbf{e}_r$ is a minimizer of $\mathcal{F}$; if $K_3 < K_1$, then, for nonzero constant functions h,

$$\delta^2 \mathcal{F}(\phi_*)[h] = \frac{L}{2} \ln \frac{R_0}{r_0} \int_0^{2\pi} (K_3 - K_1) h^2 d\theta < 0,$$

and hence, $\mathbf{n} = \mathbf{e}_r$ is not a local minimizer.

It remains to show that all other critical points of $\mathcal{F}$ are minimizers.

A necessary condition for nonnegative definiteness of $\delta^2 \mathcal{F}(\phi_*)$ is $P \geq 0$. For Dirichlet boundary conditions $\phi(0) = A$ and $\phi(2\pi) = B$, a sufficient condition is given in terms of *conjugate points* to $\theta = 0$ of the Euler equation for the second variation $\delta^2 \mathcal{F}(\phi_*)$ or the Jacobian equation for the original functional $\mathcal{F}(\phi_*)$. For the boundary condition $\phi(2\pi) - \phi(0) \in \pi\mathbb{Z}$, we will follow the idea for Dirichlet boundary conditions to examine the positive definiteness of $\delta^2 \mathcal{F}(\phi_*)$. Recall the Jacobian equation is, with prime for the derivative with respect to θ,

$$-(Pz')' + Qz = 0 \quad \text{or} \quad - f(\phi_*) z'' - f_\phi(\phi_*) \phi'_* z' - \frac{C_0}{2} \left(\frac{f_\phi}{f} \right)_\phi (\phi_*) z = 0. \quad (17) \quad \{\texttt{Jacbeqn}\}$$

A new observation is crucial for the study of the Jacobian equation (17). Since $(\phi_*(\theta), \rho_*(\theta))$ is now not an equilibrium, Theorem 3.1 implies that $\phi_*(\theta)$ is strictly monotone, and hence, $\phi = \phi_*(\theta)$ is a change of variable. Let $z(\theta) = Z(\phi_*(\theta))$. Then,

$$z' = Z_\phi \phi'_*, \quad z'' = Z_{\phi\phi} \phi'^2_* + Z_\phi \phi''_*.$$

Therefore, the Jacobian equation (17) becomes

$$f \phi'^2_* Z_{\phi\phi} + f \phi''_* Z_\phi + f_\phi \phi'^2_* Z_\phi + \frac{C_0}{2} \left(\frac{f_\phi}{f} \right)_\phi Z = 0. \quad (18) \quad \{\texttt{newJacbeqn}\}$$

It follows from

$$\phi'^2_* = \frac{f(\phi_*) + C_0}{f(\phi_*)} \quad \text{and} \quad f(\phi_*) \phi''_* = -\frac{1}{2} f_\phi(\phi_*) (\phi'^2_* - 1)$$

that

$$\begin{aligned}(f + C_0) Z_{\phi\phi} - \frac{C_0}{2} \frac{f_\phi}{f} Z_\phi + \frac{(f + C_0) f_\phi}{f} Z_\phi + \frac{C_0}{2} \left(\frac{f_\phi}{f} \right)_\phi Z \\ = (f + C_0) Z_{\phi\phi} + f_\phi Z_\phi + \frac{C_0}{2} \frac{f_\phi}{f} Z_\phi + \frac{C_0}{2} \left(\frac{f_\phi}{f} \right)_\phi Z = 0,\end{aligned}$$

or

$$((f + C_0) Z_\phi)_\phi + \frac{C_0}{2} \left(\frac{f_\phi}{f} Z \right)_\phi = 0.$$

Therefore,

$$(f + C_0) Z_\phi + \frac{C_0}{2} \frac{f_\phi}{f} Z = D,$$

and hence, with $\phi_*(0) = \phi_0$,

$$Z(\phi) = S(\phi)Z(\phi_0) + D\int_{\phi_0}^{\phi} S(\phi)S^{-1}(t)(f(t)+C_0)^{-1}dt,$$

where

$$S(\phi) = \exp\left\{-\frac{C_0}{2}\int_{\phi_0}^{\phi}\frac{f_\phi(t)}{f(t)(f(t)+C_0)}dt\right\}.$$

Let $Z(\phi_0) > 0$. With $D = 0$, the particular solution $Z(\phi) = S(\phi)Z(\phi_0) > 0$ for all ϕ. Thus, $z(\theta) = Z(\phi_*(\theta))$ is a nonzero solution of the Jacobian equation (17). We claim that if

$$\begin{aligned} w(\theta) = &-\frac{z'(\theta)}{z(\theta)}P(\theta) = -\frac{Z_\phi(\phi_*(\theta))\phi_*'(\theta)}{Z(\phi_*(\theta))}f(\phi_*(\theta)) \\ =&\frac{C_0\phi_*'(\theta)f_\phi(\phi_*(\theta))}{2(f(\phi_*(\theta))+C_0)}z(\theta), \end{aligned} \tag{19}$$ {w}

then

$$P(\theta)(Q(\theta)+w'(\theta)) = w^2(\theta),\ z(0) = z(2\pi)\ \text{ and }\ w(0) = w(2\pi). \tag{20}$$ {claim}

Assume the claim (20) for the moment. We then have

$$Pz'^2 + Qz^2 + (wz^2)' = Pz'^2 + 2wzz' + (Q+w')z^2 = P\left(z' + \frac{w}{P}z\right)^2.$$

and $(wz^2)(0) = (wz^2)(2\pi)$ so that

$$\begin{aligned} \int_0^{2\pi}\left(Pz'^2 + Qz^2\right)d\theta &= \int_0^{2\pi}\left(Pz'^2 + Qz^2 + (wz^2)'\right)d\theta - w(\theta)z^2(\theta)|_0^{2\pi} \\ &= \int_0^{2\pi} P\left(z' + \frac{w}{P}z\right)^2 d\theta \geq 0. \end{aligned}$$

Since, for any θ_0, the translation $\phi(\theta) = \phi_*(\theta+\theta_0)$ is also a critical point of $\mathcal{F}$ giving the same energy as that of $\phi_*(\theta)$, this produces a one-parameter family of minimizers for $\mathcal{F}$. □

We now complete the proof by establishing the claim (20).
Proof of (20). The first part of the claim (20) follows directly from that $z(\theta)$ is a solution of (17). In view of (19), it suffices to show that $z(0) = z(2\pi)$ or $Z(\phi_*(2\pi)) = Z(\phi_*(0))$. The latter is equivalent to $S(\phi_*(2\pi)) = 1$. Now,

suppose $\phi_*(2\pi) = \phi_*(0) + m\pi$. Then,

$$
\begin{aligned}
\int_{\phi_0}^{\phi_*(2\pi)} \frac{f_\phi(t)}{f(t)(f(t)+C_0)} dt =& \int_{\phi_0}^{\phi_0+m\pi} \frac{(K_3-K_1)\sin(2t)}{f(t)(f(t)+C_0)} dt \\
=& \int_0^{m\pi} \frac{(K_3-K_1)\sin(2t)}{f(t)(f(t)+C_0)} dt \\
=& m\int_0^{\pi} \frac{(K_3-K_1)\sin(2t)}{f(t)(f(t)+C_0)} dt \qquad (21) \quad \{\texttt{est1}\} \\
=& m(K_3-K_1)\int_0^{\pi/2} \frac{\sin(2t)}{f(t)(f(t)+C_0)} dt \\
&+ m(K_3-K_1)\int_{\pi/2}^{\pi} \frac{\sin(2t)}{f(t)(f(t)+C_0)} dt.
\end{aligned}
$$

With the substitution $s = \pi - t$ in the second integral above, we get

$$
\begin{aligned}
\int_{\pi/2}^{\pi} \frac{\sin(2t)}{f(t)(f(t)+C_0)} dt =& \int_{\pi/2}^{0} \frac{\sin(2s)}{f(s)(f(s)+C_0)} ds \\
=& -\int_0^{\pi/2} \frac{\sin(2s)}{f(s)(f(s)+C_0)} ds.
\end{aligned} \qquad (22) \quad \{\texttt{est2}\}
$$

It follows from (21) and (22) that

$$
\int_{\phi_0}^{\phi_*(2\pi)} \frac{f_\phi(t)}{f(t)(f(t)+C_0)} dt = 0
$$

and hence,

$$
S(\phi_*(2\pi)) = \exp\left\{ -\frac{C_0}{2} \int_{\phi_0}^{\phi_*(2\pi)} \frac{f_\phi(t)}{f(t)(f(t)+C_0)} dt \right\} = 1.
$$

This completes the proof. $\square$

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