Constant-angle surfaces in liquid crystals

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Abstract

We discuss some properties of surfaces in $\mathbb{R}^3$ whose unit normal has constant angle with an assigned direction field. The constant angle condition can be rewritten as an Hamilton-Jacobi equation correlating the surface and the direction field. We focus on examples motivated by the physics of interfaces in liquid crystals and of layered fluids, and discuss the properties of the constant-angle surfaces when the direction field is singular along a line (disclination) or at a point (hedgehog defect).

1 Introduction

We discuss below some properties of surfaces in $\mathbb{R}^3$ whose unit normal forms a constant angle with an assigned direction field. The main idea is to show that

the constant angle condition results in an Hamilton-Jacobi equation correlating the surface and the direction field. We discuss examples motivated by the physics of interfaces in liquid crystals and of layered fluids, and discuss the properties of the constant-angle surfaces when the direction field is singular along a line or at a point. A more complete approach to the determination of layered structures in smectics, which allows the director field to vary, can be found in Kidney, McKay and Stewart [5], McKay and Leslie [6], and McKay [7]. Also, constant angle surfaces are of interest in the shape-from-shading problem (cf. e.g., Lions, Rouy and Tourin [9])

A direction field on a domain $\Omega \subset \mathbb{R}^3$ is a smooth map $\boldsymbol{m} : \Omega \to \mathbb{P}^2(\mathbb{R})$, with $\mathbb{P}^2(\mathbb{R})$ the real projective plane, and can be locally described by a unit vector field, which we continue to denote by $\boldsymbol{m}$ (so that $|\boldsymbol{m}| = 1$). Consider a piecewise smooth surface $S \subset \Omega$ whose unit normal $\boldsymbol{n}$ has a constant angle α with $\boldsymbol{m}$:

$$|\boldsymbol{n} \cdot \boldsymbol{m}| = \cos \alpha, \tag{1}$$

for fixed $\alpha \in [0, \frac{\pi}{2}]$.

Viewing the surface S as a level set of a Lipschitz continuous function $f : \Omega \to \mathbb{R}$,

$$S = \{\boldsymbol{x} \in \Omega \,/\, f(\boldsymbol{x}) = \text{const.}\}, \tag{2}$$

and letting $\boldsymbol{n} = \nabla f / |\nabla f|$, (1) is equivalent to the quadratic Hamilton-Jacobi equation

$$\nabla f \cdot \boldsymbol{A}_\alpha \nabla f = 0, \tag{3}$$

with

$$\boldsymbol{A}_\alpha = \boldsymbol{A}_\alpha(\boldsymbol{x}) = \cos^2 \alpha \boldsymbol{1} - \boldsymbol{m}(\boldsymbol{x}) \otimes \boldsymbol{m}(\boldsymbol{x}).$$

Let

$$H(\boldsymbol{x}, \boldsymbol{p}) = \boldsymbol{p} \cdot \boldsymbol{A}_\alpha(\boldsymbol{x}) \boldsymbol{p},$$

be the Hamiltonian, and notice that it is non-convex in $\boldsymbol{p}$. Recall that, according to the geometric theory of the Hamilton-Jacobi equation, local solutions of (3) may be obtained by the method of characteristics, which are the solutions of the canonical system

$$\begin{cases} \dot{\boldsymbol{x}} = \dfrac{\partial H}{\partial \boldsymbol{p}} = 2(\cos^2 \alpha \boldsymbol{p} - (\boldsymbol{m} \cdot \boldsymbol{p})\boldsymbol{m}), \\[2mm] \dot{\boldsymbol{p}} = -\dfrac{\partial H}{\partial \boldsymbol{x}} = 2(\boldsymbol{m} \cdot \boldsymbol{p})(\nabla \boldsymbol{m})^\top \boldsymbol{p}, \end{cases} \tag{4}$$

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When $\alpha = 0$ the method of characteristics fails, since the equation $H(\boldsymbol{x}, \boldsymbol{p}) = 0$ does not define a hypersurface of the 1-jet space (see Arnold [1]). Indeed, when $\alpha = 0$, $\boldsymbol{A}_\alpha$ is positive semidefinite, and the equation $H(\boldsymbol{x}, \boldsymbol{p}) = 0$ gives an overdetermined system that can be studied by Frobenius theory. Thus, solutions of (1) for $\alpha = 0$ exist if and only if $\boldsymbol{m} \cdot \operatorname{curl} \boldsymbol{m} = 0$ in Ω. We restrict to $\alpha \in (0, \pi)$ in this paper, with the exception of Section 3.1.

We study here (3) for some special choices of the direction field $\boldsymbol{m}$. Namely, we characterize (i) cylindrical and conical surfaces arising when $\boldsymbol{m}$ is singular along a straight line and orthogonal to that line (line defects in nematics) and (ii) conical surfaces corresponding to a constant orientation field $\boldsymbol{m} = \boldsymbol{m}_0$ (layered structures in smectics C).

We now discuss briefly two physical examples which lead to equations of the form (1).

1.1 Applications to nematics

A nematic liquid crystal is an ordered fluid whose constituents are macromolecules which locally tend to align parallel to each other (cf., e.g., De Gennes and Prost [3]). At equilibrium a nematic liquid crystal may be described in terms of a direction field $\boldsymbol{m}$ that measures the average local orientation of the macromolecules. In the simplest approximation, a smooth direction field $\boldsymbol{m}$ at equilibrium is a stationary point of the (one-constant) Frank energy functional

$$\int_\Omega \frac{k}{2} |\nabla \boldsymbol{m}|^2 \, dv, \tag{5}$$

whose Euler equation is (see Eells and Sampson [4] where such kind of mapping - called harmonic map - is introduced and studied in a very general setting)

$$\triangle \boldsymbol{m} + |\nabla \boldsymbol{m}|^2 \boldsymbol{m} = 0. \tag{6}$$

Actually, the direction field describing the orientational order in a nematic is often not defined on the whole Ω: the most common singularities being straight disclinations and hedgehogs. Specifically, disclinations are line defects such that $\boldsymbol{m}$ is smooth in $\Omega \setminus \{\ell\}$, with ℓ a straight line in $\mathbb{R}^3$, $\boldsymbol{m}$ is orthogonal to ℓ and the degree of the mapping $\boldsymbol{m} : \Omega \setminus \{\ell\} \to \mathbb{P}^1(\mathbb{R})$ is an integer k. Hedgehogs are point defects such that $\boldsymbol{m}$ is smooth in $\Omega \setminus \{\boldsymbol{x}_0\}$, with $\boldsymbol{x}_0$ a point in Ω, but the degree of the mapping $\boldsymbol{m} : \Omega \setminus \{\boldsymbol{x}_0\} \to \mathbb{P}^2(\mathbb{R})$ is 2.

We assume that in both cases $\boldsymbol{m}$ satisfies (6) away from the singularity.

Equations of the form (1) arise in the study of free surfaces of nematic liquid crystal drops. In fact, denoting by $\boldsymbol{n} : \partial\Omega \to S^2$ the outward unit normal to $\partial\Omega$, which we view as the free surface of a drop, it is often assumed that the *strong anchoring* boundary condition holds at $\partial\Omega$:

$$|\boldsymbol{n} \cdot \boldsymbol{m}| = \cos\alpha, \tag{7}$$

with $\alpha \in (0, 2\pi)$, which is an equation of the form (1).

It is important to notice, however, that the surface tension φ_0 which plays an important role in regularizing the shape of the drop. Since our main interest is in (7), we neglect surface tension effects in what follows, and our results may be applicable only when surface tension is negligible.

In Sections 2 and 3 we restrict to two special cases: first, assuming that $\boldsymbol{m}$ is a constant solution of (6), we show that surfaces satisfying (7) are ruled surfaces, that can be described explicitly. Second, assuming that $\boldsymbol{m}$ has a line singularity with arbitrary integer topological charge, we study cylindrical surfaces which satisfy (7), and discuss how their topology depends on the charge.

1.2 Applications to smectics C

Smectic C liquid crystals are ordered fluids characterized by a layered structure (De Gennes and Prost [3]). When density fluctuations are neglected, the description of equilibrium configurations of smectics requires, in addition to the orientation field $\boldsymbol{m}$, a scalar order parameter $f : \Omega \subset \mathbb{R}^3 \to \mathbb{R}$ whose level sets define the layers. In smectics C, the director field $\boldsymbol{m}$ is constrained to a constant angle α with the layer normal $\boldsymbol{n} = \nabla f / |\nabla f|$, i.e.,

$$|\boldsymbol{m} \cdot \boldsymbol{n}| = \cos\alpha, \tag{8}$$

with $\alpha \in (0, 2\pi)$.

The energy of a smectic C liquid crystals may be written as the sum of a nematic energy term, which in the simplest approximation is the Frank energy (5), and a smectic term of the form (cf. [2], [3])

$$\int_\Omega \left(A|\nabla f - q\boldsymbol{m}|^2 + B|\boldsymbol{m} \cdot \nabla f - q|^2 \right) \, dv. \tag{9}$$

We restrict to special configurations such that:

- the orientation field $\boldsymbol{m}$ is assigned in Ω;

- the smectic order parameter is an absolute minimizer of the smectic energy density (9) subject to the constraint (8).

Some algebra shows that the above requirements reduce to

$$\begin{cases} |\boldsymbol{P}\nabla f| = \gamma \tan \alpha, \\ \boldsymbol{m} \cdot \nabla f = \gamma, \end{cases} \tag{10}$$

with

$$\gamma = \frac{(A+B)q}{(A+B) + Aq\tan^2\alpha}, \qquad \boldsymbol{P} = \mathbf{1} - \boldsymbol{m} \otimes \boldsymbol{m}.$$

We will show that, contrary to (3), (10) has no solution for a large class of orientation fields, and discuss two cases when the solution does exist, i.e., for a uniform orientation field, and line disclination with topological charge 2.

2 Conical surfaces for a constant orientation field

For a constant orientation field $\boldsymbol{m} = \boldsymbol{m}_0$ on $\mathbb{R}^3$ (1) reduces to

$$|\boldsymbol{n} \cdot \boldsymbol{m}_0| = \cos \alpha, \tag{11}$$

with $\alpha \in (0, \pi/2)$.

Let S be a solution of (11): as a first remark we notice that smooth portions of S are flat, since the Gaussian curvature K identically vanishes on these portions. By consequence, S' is also ruled.

To see this, let $S' \subset S$ be smooth, and notice that (11) implies that the image of S' by the Gauss map $\boldsymbol{n} : S' \to S^2$ is a circle. By consequence, the Gaussian curvature vanishes, since

$$K = \lim_{\text{area}(S') \to 0} \frac{\text{area}(\boldsymbol{n}(S'))}{\text{area}(S')} = 0,$$

and S' is flat.

To solve (11), choose Cartesian coordinates (x, y, z), with associated basis $(\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k})$ such that $\boldsymbol{k} = \boldsymbol{m}_0$. Assume that S is smooth and is locally the graph of a function $g := D \subset \mathbb{R}^2 \to \mathbb{R}$, i.e.,

$$S = \{(x, y, z) \,/\, z = g(x, y)\}.$$

Since $\boldsymbol{n} = (-\nabla g + \boldsymbol{k})/\sqrt{1 + |\nabla g|^2}$, with $\nabla g = (\partial_x g)\boldsymbol{i} + (\partial_y g)\boldsymbol{j}$, (11) reduces to the eikonal equation

$$|\nabla g| = \tan \alpha. \tag{12}$$

Let $\ell_0 = S \cap \{z = 0\}$ be the trace of S on the (x, y)-plane. Then S may be explicitly represented as a conical surface generated by ℓ_0. To see this, let $\boldsymbol{x}_0(s)$ be a parametrization of ℓ_0 with arc parameter s, and let $\boldsymbol{\tau} = \boldsymbol{\tau}(s)$ and $\boldsymbol{\nu} = \boldsymbol{\nu}(s)$ be the unit tangent and normal vectors to ℓ_0. Writing $\boldsymbol{x} = x\boldsymbol{i} + y\boldsymbol{j}$, let also $t = t(\boldsymbol{x}) := \mathrm{dist}(\boldsymbol{x}, \ell_0)$ be the distance of a point $\boldsymbol{x}$ from ℓ_0, and notice that the solution of (12) with boundary condition $g(x, y) = 0$ on ℓ_0 is

$$g(x, y) = t(x, y) \tan \alpha. \tag{13}$$

In fact, consider the local change of coordinates $((s, t)$ are known as Fermi coordinates)

$$\boldsymbol{x}(s, t) = \boldsymbol{x}_0(s) + t\boldsymbol{\nu}(s),$$

and let

$$\hat{g}(s, t) := g(\boldsymbol{x}(s, t)).$$

Since $\nabla g \cdot \boldsymbol{\nu} = \partial_t \hat{g}$, and $\nabla g \cdot \boldsymbol{\tau} = \partial_s \hat{g}/(1 - ct)$, with c the curvature of ℓ_0, it follows, upon taking $\hat{g}(s, t) = t \tan \alpha$, that $\nabla g = \tan \alpha \, \boldsymbol{\nu}$, so that (12) is satisfied.

The above argument implies that S can be given a parametrization in terms of the Fermi coordinates (s, t) as follows:

$$\boldsymbol{x}_0(s) + t\boldsymbol{\nu}(s) + (t \tan \alpha) \, \boldsymbol{m}_0, \tag{14}$$

which only requires the knowledge of ℓ_0.

As t varies in $\mathbb{R}$, (14) is a global parametrization of the solution of (11): the corresponding surface may have self-intersections, for instance at points (s, t) corresponding to caustics of (12) (Figure 4).

The above construction may be generalized to Riemannian manifolds as follows. Consider the eikonal equation

$$\|\nabla g\|^2 = 1, \tag{15}$$

for functions $g : M \to \mathbb{R}$, where M is a Riemannian manifold. If X is a vector field on a manifold M then by F_t^X we mean the associated flow, i.e. $\frac{\partial F_t^X}{\partial t} = X$.

We start with the following observation.

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Lemma 2.1. *Let $(M, \langle, \rangle)$ be a Riemannian manifold and $g : M \to \mathbb{R}$ be a solution of the eikonal equation (15). Then,*

$$F_t^{\nabla g}(p) = \exp_p(t.(\nabla g)(p))$$

where $\exp$ *is the exponential map of M, i.e. the geodesic flow.*

Proof. Just note that $\|\nabla g\|^2 = 1$ implies

$$0 = D_V \langle \nabla g, \nabla g \rangle = 2 \langle D_V \nabla g, \nabla g \rangle = 2 \langle D_{\nabla g} \nabla g, V \rangle$$

for any vector field V, where D is the Levi-Civita connection of $(M, \langle, \rangle)$. So

$$D_{\nabla g} \nabla g = 0$$

which means that the integral curves of ∇g are geodesics. $\qquad \square$

The next proposition indicates how to construct all solutions of (15).

Proposition 2.2. *Let g be a solution of (15) and let $p \in M$. Then*

$$g(\exp_p(t.(\nabla g)(p))) = t + g(p)$$

Proof. Observe that

$$\frac{\partial g(\exp_p(t.(\nabla g)(p)))}{\partial t} = \langle \nabla g(F_t^{\nabla g}(p)), \nabla g(F_t^{\nabla g}(p)) \rangle = 1$$

as a consequence of the previous lemma and the fact that g is a solution of the eikonal equation. $\qquad \square$

Theorem 2.3. *Let H be an oriented hypersurface of M and let $\phi : H \to \mathbb{R}$ a smooth function. Then there exists a unique local solution g of the eikonal equation defined in a neighborhood of H such that $g|_H = \phi$ and ∇g gives the orientation of H.*

3 Cylindrical surfaces in the presence of a disclination

Let $\Omega = D \times \mathbb{R}$ be a cylindrical domain, with $D \subset \mathbb{R}^2$, and consider an orientation field $\boldsymbol{m} : \Omega \to \mathbb{P}^2(\mathbb{R})$. Assume that $\boldsymbol{m}$ is planar and independent of the vertical coordinate, so that

$$\boldsymbol{m} = \boldsymbol{m}(\boldsymbol{x}), \qquad \boldsymbol{m} \cdot \boldsymbol{k} = 0, \tag{16}$$

with $\boldsymbol{x} \in D$, and $(\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k})$ an orthonormal basis with $\boldsymbol{k}$ orthogonal to the plane containing D. Under the above assumptions the problem is 2-dimensional and we may view $\boldsymbol{m} : D \to \mathbb{P}^1(\mathbb{R})$.

For nematic orientation fields, $\boldsymbol{m}$ is a solution of (6) away from the singularities: in that case, writing

$$\boldsymbol{m}(\boldsymbol{x}) = \cos \varphi(\boldsymbol{x}) \, \boldsymbol{i} + \sin \varphi(\boldsymbol{x}) \, \boldsymbol{j},$$

it is easy to see that $\boldsymbol{m}$ satisfies (6) if and only if φ is harmonic in D

$$\Delta \varphi = 0, \tag{17}$$

with Δ the laplacian in $\mathbb{R}^2$.

3.1 Surfaces orthogonal to $\boldsymbol{m}$: $\alpha = 0$

We first look for surfaces $S \subset \Omega$ such that

$$|\boldsymbol{n} \cdot \boldsymbol{m}| = 1, \tag{18}$$

holds at S, with $\boldsymbol{n}$ a choice of unit normal for S. Notice that $\boldsymbol{m} \cdot \operatorname{curl} \boldsymbol{m} = 0$, and Frobenius theorem is trivially satisfied. Hence, local solutions to (18) exist, and by the same argument as in Section 2 the corresponding surfaces are flat and ruled.

More precisely, solutions of (18) are cylinders $S = C \times \mathbb{R}$ with vertical axis, with $C \subset D$ a planar curve.

By construction, C is still defined by (18), since $\boldsymbol{n}$ represents a choice of unit normal for C in the plane orthogonal to $\boldsymbol{k}$.

Equation (18) defines the family of (orthogonal) integral curves of the direction field $\boldsymbol{m}$. Describing C as a level set of a function $f : D \subset \mathbb{R}^2 \to \mathbb{R}$:

$$C = \{\boldsymbol{x} \ : \ f(\boldsymbol{x}) = c\},$$

with $c \in \mathbb{R}$, (18) is equivalent to

$$\nabla f \times \boldsymbol{m} = 0. \tag{19}$$

Assume first that D is simply connected and $\boldsymbol{m}$ is regular, and no defect is present: then there exists a single-valued representative of $\boldsymbol{m}$ in D, and

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$\varphi : D \to S^1$ is also single-valued. Denote by w the harmonic conjugate of φ, solution of the Cauchy–Riemann equations

$$\frac{\partial \varphi}{\partial x} + \frac{\partial w}{\partial y} = 0, \qquad \frac{\partial \varphi}{\partial y} - \frac{\partial w}{\partial x} = 0,$$

and define

$$\boldsymbol{u} = e^{-w}\boldsymbol{m} = e^{-w}(\cos \varphi \boldsymbol{i} + \sin \varphi \boldsymbol{j}), \tag{20}$$

so that $\boldsymbol{u}$ is a non-zero vector field on D. The function e^{-w} is an integrating factor for $\boldsymbol{m}$, and it is easy to see that $\operatorname{Div} \boldsymbol{u} = 0$ and $\operatorname{Curl} \boldsymbol{u} = 0$, with $\operatorname{Curl} \boldsymbol{u} = u_x^2 - u_y^1$ for $\boldsymbol{u} = u^1(x,y)\boldsymbol{i} + u^2(x,y)\boldsymbol{j}$. By consequence, $\Delta \boldsymbol{u} = 0$ in D. In particular, there exists $f : D \to \mathbb{R}$ such that

$$\nabla f = \boldsymbol{u}, \tag{21}$$

so that $\boldsymbol{n} = \nabla f/|\nabla f| = \boldsymbol{m}$ and $\{f(\boldsymbol{x}) = c\}$ is an orthogonal integral curve of the direction field $\boldsymbol{m}$, i.e., is a solution of (18).

Equivalently, identify $\mathbb{R}^2$ to $\mathbb{C}$ and, for $z = x + iy$, define

$$m(z) = e^{-i\varphi(z)} \qquad \text{and} \qquad u(z) = e^{-(w(z)+i\varphi(z))}, \tag{22}$$

where $w(z)$ and $\varphi(z)$ are $w(x,y)$ and $\varphi(x,y)$ expressed in terms of the complex variable z. By construction u is holomorphic in D.

Consider now a holomorphic function on D

$$F = f + ig, \tag{23}$$

with f and g real valued. Since F is holomorphic,

$$F' = 2\frac{\partial f}{\partial z} = \frac{\partial f}{\partial x} - i\frac{\partial f}{\partial y}.$$

Comparing (21) and (22) we conclude that f, as a function on $D \subset \mathbb{R}$, satisfies (18) and (19) if and only if F as defined by (23) satisfies

$$F'(z) = \lambda(z)u(z),$$

for some real function $\lambda(z)$ on D. However, since F' and u are holomorphic, λ is a real constant, so that (18) and (19) reduce (modulo a multiplicative real constant) to

$$F'(z) = u(z). \tag{24}$$

Therefore, the solutions of (18) are the level sets of the real part f of any primitive F of u, i.e.,

$$C = \{z \in \mathbb{C} : \mathrm{Re}(F(z)) = c\}. \tag{25}$$

Assume now that $\mathbf{0} \in D$, let $D_0 = D \setminus \{\mathbf{0}\}$ and $\mathbf{m} : D_0 \to \mathbb{P}^1(\mathbb{R})$ is singular at $\mathbf{0}$, i.e., the nematic director field $\mathbf{m}$ has a point defect at $\mathbf{0}$. The topological charge $k \in \mathbb{Z}$ of the defect at $\mathbf{0}$ is defined as the net number of rotations of $\mathbf{m}$ by π along any simple closed loop encircling $\mathbf{0}$, given by the relation

$$\frac{k}{2} = \frac{1}{2\pi} \int_\gamma (-m^2 \nabla m^1 + m^1 \nabla m^2) \cdot d\boldsymbol{x} = \frac{1}{2\pi} \int_\gamma d\varphi.$$

Equivalently, k is the topological degree of $\varphi : D \setminus \{\mathbf{0}\} \to \mathbb{P}^{\mathbf{1}}(\mathbb{R})$.

Fix now $k \in \mathbb{Z}$: any solution of (17) with given degree k may be written in the form

$$\varphi(\varrho, \vartheta) = \frac{k}{2} \vartheta + g(\varrho, \vartheta), \tag{26}$$

with $g : D \setminus \{\mathbf{0}\} \to \mathbb{R}$ harmonic (and single-valued) and (ϱ, ϑ) polar coordinates centered at $\{\mathbf{0}\}$. Therefore, by means of a conformal transformation[1], we may focus on director fields that have the form

$$\boldsymbol{m} = \cos\left(\frac{k\vartheta}{2}\right) \boldsymbol{i} + \sin\left(\frac{k\vartheta}{2}\right) \boldsymbol{j}. \tag{27}$$

Switching to complex-variables, and letting $\varphi = k\vartheta/2$ in (22) we obtain

$$u(z) = z^{-\frac{k}{2}}. \tag{28}$$

Now recall that the orthogonal integral curves of $\boldsymbol{m}$ are given by (25), where F is a primitive of u:

$$F'(z) = z^{-\frac{k}{2}}. \tag{29}$$

The solution of this equation is immediate:

$$F(z) = \begin{cases} \frac{2}{2-k} z^{\frac{2-k}{2}}, & k \neq 2, \\ \log z, & k = 2. \end{cases} \tag{30}$$

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[1] In complex coordinates the conformal (holomorphic) transformation is $z \mapsto z \exp(\frac{2}{k}(w_g + ig))$, with w_g the harmonic conjugate of g.

and it follows that the curve C has the form $f(z) = c$, with

$$f(z) = \begin{cases} \operatorname{Re}\left(z^{\frac{2-k}{2}}\right) = \frac{1}{2}\left(z^{\frac{2-k}{2}} + \bar{z}^{\frac{2-k}{2}}\right), & k \neq 2, \\ \log|z|, & k = 2. \end{cases} \tag{31}$$

To avoid discussing the sign of c, consider the curves C' defined by $|f(z)| = c \geq 0$. The topology of C' depends on k as follows:

- For $k \leq 1$, $k \neq 0$, the curve $|f(z)| = c$ is not bounded, does not contain the defect $z = 0$ and has $2 - k$ connected components with $2 - k$ asymptotic directions. In polar coordinates C has the explicit representation

$$\varrho = \frac{c}{\left|\cos\left(\frac{2-k}{2}\vartheta\right)\right|^{\frac{2}{2-k}}}. \tag{32}$$

- For $k = 2$, the field $\boldsymbol{m}$ is radial and the curves $|f(z)| = c$ are circles centered at 0.

- For $k \geq 3$ the curve C' contains the defect at $z = 0$. C' is bounded, and has a clover-like shape with $k - 2$ leafs. In polar coordinates C' has the explicit representation

$$\varrho = c\left|\cos\left(\frac{k-2}{2}\vartheta\right)\right|^{\frac{2}{k-2}}. \tag{33}$$

3.2 Surfaces with α arbitrary

The above results may easily be extended to surfaces such that

$$|\boldsymbol{m} \cdot \boldsymbol{n}| = \cos\alpha, \tag{34}$$

with $\alpha \in (0, \pi/2)$. Again, solutions of (34) are cylinders $S = C \times \mathbb{R}$ with vertical axis, with $C \subset D$ a plane curve solution of (34) in D.

Since (34) is equivalent to

$$\varphi - \psi = \pm\alpha,$$

all considerations in Section 3.1 hold, with

$$u(z) = e^{-(w(z) + i(\varphi(z) \pm \alpha))}. \tag{35}$$

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For the class of singular fields considered above, (28) becomes

$$u(z) = e^{\pm i\alpha} \, z^{-\frac{k}{2}}, \tag{36}$$

and

$$F(z) = \left\{ \begin{array}{ll} \frac{2}{2-k} \, e^{\pm i\alpha} \, z^{\frac{2-k}{2}}, & k \neq 2, \\ e^{\pm i\alpha} \, \log z, & k = 2. \end{array} \right. \tag{37}$$

and it follows that the curve C has the form $f(z) = c$, with

$$f(z) = \left\{ \begin{array}{ll} \varrho^{\frac{2-k}{2}} \cos\left(\frac{2-k}{2}\theta \pm \alpha\right), & k \neq 2, \\ \log \varrho \pm \theta \tan \alpha, & k = 2. \end{array} \right. \tag{38}$$

Consider as in Section 3.1 the curves C' defined by $|f(z)| = c \geq 0$. Then

- For $k \neq 2$, the curve C' is a rigid rotation (of angle $\frac{2}{2-k}\alpha$) of the curves defined by (32) and (33).

- For $k = 2$, the curves $|f(z)| = c$ are logarithmic spirals of the form

$$\varrho = ce^{\pm \theta \tan \alpha}.$$

3.3   Applications to nematics

The shape of a nematic drop, or an isotropic inclusion in nematic sea, is strongly influenced by surface tension. Hence, cylindrical interfaces such as those described above are unlikely to be observed. However, it may be of interest to discuss the shape of a domain with boundary a constant angle-surface S, since it may give some clue on the shape of defect cores. Indeed, a defect core can be viewed, in a crude approximation, as an isotropic inclusion in a nematic environment.

Therefore, consider a singular orientation field $\boldsymbol{m}$ as in (27), and consider a cylindrical domain $K = D' \times \mathbb{R} \subset D \times \mathbb{R}$, with $C' = \partial D' \subset C$. From the above discussion it follows that

- For $k \leq 1$ K is unbounded, and either contains the disclination in its interior or does not contain it at all. This class of domains corresponds to curved bounding surfaces of domains without defects, or to a meniscus connecting films containing a disclination (Figure 1). When $k = 0$ we obtain a film in which the orientation field is aligned.
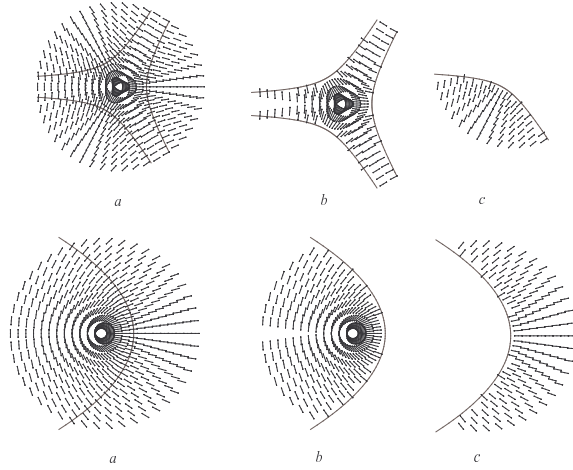
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Figure 1: Sections of cylindrical domains $D' \times \mathbb{R}$ with boundary a constant-angle surface for $\alpha = 0$. The upper row corresponds to $k = -1$, and the lower to $k = 1$. (a) constant angle surfaces; (b) domains containing the disclination; (c) domains not containing the disclination.

- For $k = 2$, K is either a circular cylindrical filament centered at the disclination, or its complement, which corresponds to a cylindrical isotropic core about a straight disclination (Figure 2).

- For $k \geq 3$, K necessarily contains the defect at its boundary. Again, when K is unbounded its complement may give some information about the shape of the disclination core. (Figure 3)

3.4   Applications to smectics C

For layered structures such as smectics C, the constraint $(10)_2$ poses serious restrictions to the existence of solutions of the Hamilton-Jacobi equation $(10)_1$. Also, while for nematics the basic unknown is the surface S and f is just an auxiliary function of which S is a level set, in smectics the function f is an ordered parameter which should be uniquely determined by (10) and suitable boundary conditions.

To see this, fix the direction field $\boldsymbol{m}$ as before and consider the local coordinate system $(s, \boldsymbol{\xi})$ on $\mathbb{R}^3$, with $\boldsymbol{\xi}$ a coordinate system on a surface S_0 transversal to $\boldsymbol{m}$, and s the arc parameter along the integral curves of $\boldsymbol{m}$,
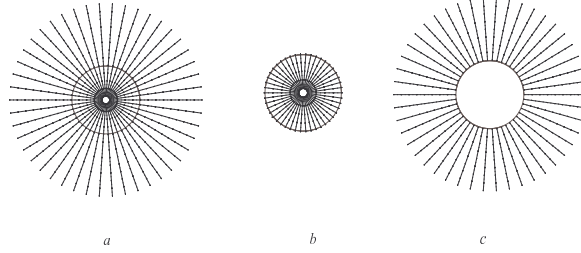
Figure 2: Sections of cylindrical domains $D' \times \mathbb{R}$ with boundary a constant-angle surface for $\alpha = 0$ and $k = 2$. (a) constant angle surface; (b) section of a filament containing the disclination; (c) isotropic core of the disclination.

measured from the intersection of the corresponding integral curve and the initial surface S_0. In other words, $s = s(\boldsymbol{x})$ and $\boldsymbol{\xi} = \boldsymbol{\xi}(\boldsymbol{x})$ are defined so that $\boldsymbol{\xi}(\boldsymbol{x})$ is the point of intersection of the integral curve of $\boldsymbol{m}$ passing through $\boldsymbol{x}$ and the surface S_0, and s is the length of the arc of this curve between $\boldsymbol{\xi}$ and $\boldsymbol{x}$.

It follows that $(10)_2$ is equivalent to

$$\frac{\partial f}{\partial s} = \gamma,$$

so that

$$f(\boldsymbol{\xi}, s) = \gamma s + g(\boldsymbol{\xi}). \tag{39}$$

Using the fact that $\boldsymbol{m} \cdot \nabla s = 1$, $(10)_1$ can be rewritten as

$$|\nabla_{\boldsymbol{\xi}} g|^2 + \gamma(\nabla s \cdot \nabla_{\boldsymbol{\xi}} g) + \gamma^2(|\nabla s|^2 - 1) = \gamma^2 \tan^2 \alpha. \tag{40}$$

We discuss here a few special cases of (40).

Consider first a constant orientation field $\boldsymbol{m} = \boldsymbol{m}_0$ in a cylindrical domain $D \times \mathbb{R}$, with coordinates (x, y, z) with z along the axis of the cylinder. Then by the above argument we may write the solution of (10) in the form

$$f(x, y, z) = \gamma(z - g(x, y)). \tag{41}$$

Also, (40) reduces to the two-dimensional eikonal equation (12) for g.

Assume that the boundary condition

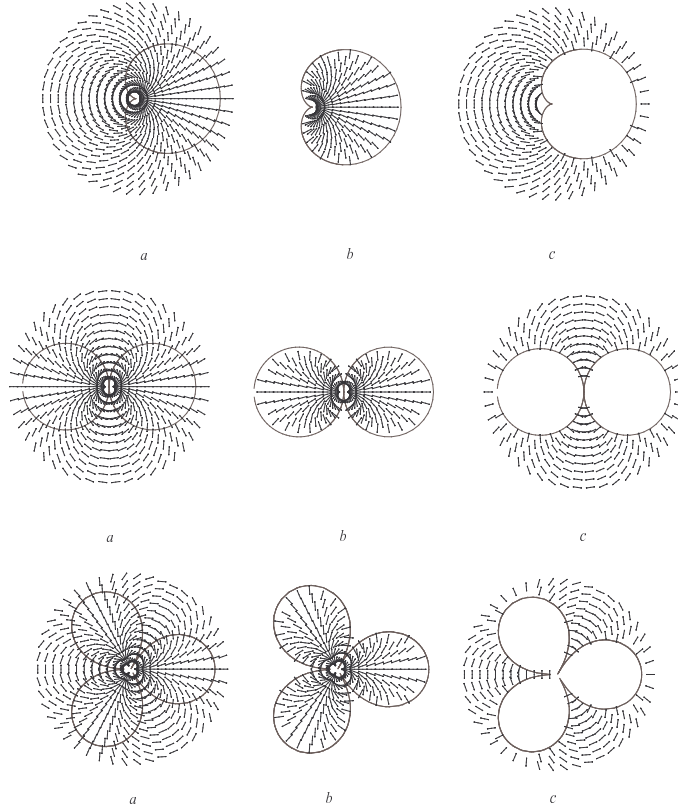$$g(x, y) = 0 \qquad \text{on } \partial D \tag{42}$$

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Figure 3: Sections of cylindrical domains $D' \times \mathbb{R}$ with boundary a constant-angle surface for $\alpha = 0$. The upper row corresponds to $k = 3$, the middle to $k = 4$ and the lower to $k = 5$. (a) constant angle surfaces; (b) sections of filaments containing the disclination; (c) isotropic inclusions (possible core shapes).

holds: then the arguments of Section 2 apply here also, and this yields the local solution (13) $f(x, y, z) = \gamma(z - t(x, y) \tan \alpha)$.

As discussed in section 2, the distance function $t(x, y)$ is in general multivalued, with branching at the caustics, and a selection rule is necessary, for instance by requiring that g be a viscosity solution of the two-dimensional eikonal equation (12) (cf. e.g., Lions [8] and Lions, Rouy and Tourin [9]). Figure 4 shows the viscosity solution corresponding to a smectic layer in a cylindrical tube with elliptic cross- section. The smectic layers are equidistant portions of conical surfaces.

As a second example, consider a singular direction field $\boldsymbol{m}$ corresponding

to a disclination line with charge $k = 2$, as in Section 3. Specifically, let $\boldsymbol{m} = \boldsymbol{e}_r$, with (r, ϑ, z) cylindrical coordinates with z along the disclination. Then $s = r$, $\boldsymbol{\xi} = (\vartheta, z)$ and $\nabla_{\boldsymbol{\xi}} g = \partial_z g \boldsymbol{e}_z + \frac{1}{r} \partial_\vartheta g \boldsymbol{e}_\vartheta$, so that (40) yields the eikonal equation on the cylinder

$$(\partial_z g)^2 + \frac{1}{r^2} (\partial_\vartheta g)^2 = \gamma^2 \tan^2 \alpha. \tag{43}$$

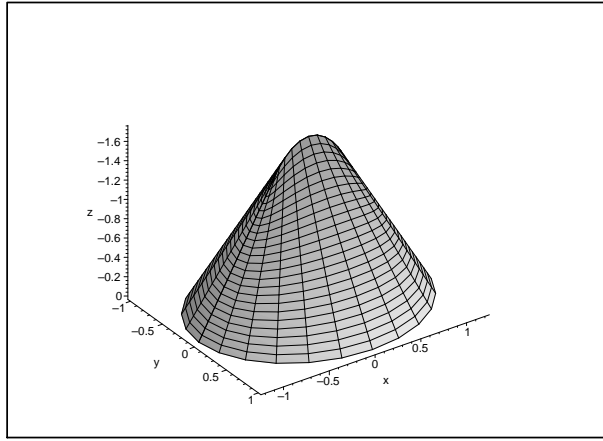Since g is independent of r, $\partial_\vartheta g = 0$ and

Figure 4: A conical constant angle surface with vertical uniform orientation field $\boldsymbol{m} = \boldsymbol{m}_0$. The plane curve generating the cone is an ellipse.

$$g = \gamma s + z \gamma \tan \alpha + \text{const.} \tag{44}$$

Hence, the layers are families of equidistant half-cones with axis the disclination line.

Consider finally a hedgehog defect described by the orientation field $\boldsymbol{m} = \boldsymbol{e}_R$, with (R, ϑ, ψ) spherical coordinates in $\mathbb{R}^3$. Here $s = R$, $\boldsymbol{\xi} = (\vartheta, \psi)$ and $\nabla_{\boldsymbol{\xi}} g = \frac{1}{R} \partial_\vartheta g \boldsymbol{e}_\vartheta + \frac{1}{R \sin \vartheta} \partial_\psi g \boldsymbol{e}_\psi$, so that (40) yields the eikonal equation on the sphere

$$\frac{1}{R^2} (\partial_\vartheta g)^2 + \frac{1}{R^2 \sin^2 \vartheta} (\partial_\psi g)^2 = \gamma^2 \tan^2 \alpha. \tag{45}$$

As before, g is independent of R, but now this implies that the above equation has no solutions for $\alpha \neq 0$. Therefore, there is no smectic C configuration for which the orientation field has a hedgehog defect.

Acknowledgments

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