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Orientable and Non-Orientable Line Field Models for Uniaxial Nematic Liquid Crystals

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Uniaxial nematic liquid crystals are often modeled using the Oseen-Frank theory, in which the mean orientation of the rod-like molecules is described through a unit vector field n. *This theory has the apparent drawback that it does not respect the head-to-tail symmetry in which* n *should be equivalent to* −n*; that is, instead of* n *taking values in the unit sphere* S^2, *it should take values in the sphere with opposite points identified, i.e., in the real projective plane* $R\mathrm{P}^2$. *The Landau-de Gennes theory respects this symmetry by working with the tensor* $\mathrm{Q} = \mathrm{s}\,(\mathrm{n}\otimes\mathrm{n} - 1/3\,Id)$. *In the case of a non-zero constant scalar order parameter s the Landau-de Gennes theory is equivalent to that of Oseen-Frank when the director field is orientable.*

We report on a general study of when the director fields can be oriented, described in terms of the topology of the domain filled by the liquid crystal, the boundary data and the rate of blow-up of possible singularities. We also analyze the circumstances in which the non-orientable configurations are energetically favoured over the orientable ones.

Keywords: nematic; orientable; projective plane; Q-tensor; simply-connected; uniaxial

1. INTRODUCTION

The most common way of modelling uniaxial nematic liquid crystals is to associate to each point in the macroscopic physical space a *director* describing the preferred direction of the molecules at that point. One of the most popular models, the Oseen-Frank model [1], takes this director to be a unit-length vector $n = (n_1, n_2, n_3)$. This has the effect of automatically assigning an orientation to the locally preferred direction of the molecules. On the other hand, in practice, the material

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is seen to be locally invariant with respect to reflection in the plane perpendicular to the director. Thus it is physically more appropriate to take the director to be a line, that determined by the pair of antipodal unit vectors $\{n, -n\}$. This is one of the advantages of the Landau-de Gennes theory [2], that in the uniaxial case uses for the director a symmetric, traceless matrix with two equal eigenvalues. Such a 3×3 matrix Q can be written as

$$Q = s\left(n \otimes n - \frac{1}{3}Id\right), \tag{1}$$

where the scalar order parameter s is a real number, $n = (n_1, n_2, n_3)$ is a unit vector, $(n \otimes n)_{ij} = n_i n_j$, and Id denotes the identity matrix. One notices that for fixed nonzero s one can associate uniquely to Q a pair of unit vectors $\{n, -n\}$, that is a point in the real projective plane $\mathbb{R}P^2$. In the rest of the paper we adopt the terminology *Q-tensors* for position-dependent matrices of the form (1). In addition we assume that s is a nonzero constant. For experimental determinations of s see for instance [3].

The main purpose of this work is to compare the two theories, Oseen-Frank and constant s Landau-de Gennes, and to determine what they have in common and how they differ.

The Oseen-Frank theory has been successful in predicting the equilibrium states as local or global minimizers of an energy functional:

$$E_{OF} = \int_\Omega W(n, \nabla n)dx, \tag{2}$$

where

$$\begin{aligned} W(n, \nabla n) = {} & K_1(\text{div } n)^2 + K_2(n \cdot \text{curl } n)^2 + K_3|n \wedge \text{curl } n|^2 \\ & + (K_2 + K_4)(\text{tr}(\nabla n)^2 - (\text{div } n)^2) \end{aligned} \tag{3}$$

and the K_i are elastic constants.

We consider a special case of the Landau-de Gennes theory, in which the elastic energy density is defined by

$$\psi(Q, \nabla Q) = L_1 I_1 + L_2 I_2 + L_3 I_3 + L_4 I_4,$$

where the L_i are constants and the four elastic invariants $I_1, \ldots, I_4$ are given by

$$I_1 = Q_{ij,j}Q_{ik,k}, \quad I_2 = Q_{ik,j}Q_{ij,k}, \quad I_3 = Q_{ij,k}Q_{ij,k}, \quad I_4 = Q_{lk}Q_{ij,l}Q_{ij,k},$$

where we have used the summation convention with $i, j, k \in \{1, 2, 3\}$.

It can be checked that the Oseen-Frank energy is expressible in terms of the constant s Landau-de Gennes Q-tensors (see [4]). We have that

$$I_1 = s^2(|\text{div } n|^2 + |n \wedge \text{curl } n|^2), \quad I_2 = s^2(|n \wedge \text{curl } n|^2 + \text{tr } (\nabla n)^2),$$

$$I_3 = 2s^2(\text{tr } (\nabla n)^2 + |n \cdot \text{curl } n|^2 + |n \wedge \text{curl } n|^2),$$

$$I_4 = 2s^3\left(\frac{2}{3}|n \wedge \text{curl } n|^2 - \frac{1}{3}\text{tr}(\nabla n)^2 - \frac{1}{3}|n \cdot \text{curl } n|^2\right)$$

Letting

$$K_1 = L_1 s^2 + L_2 s^2 + 2L_3 s^2 - \frac{2}{3}L_4 s^3, \quad K_2 = 2L_3 s^2 - \frac{2}{3}L_4 s^3,$$

$$K_3 = L_1 s^2 + L_2 s^2 + 2L_3 s^2 + \frac{4}{3}L_4 s^3, \quad K_4 = L_2 s^2,$$

we have that

$$W(n, \nabla n) = \psi(Q, \nabla Q),$$

and thus the Oseen-Frank elastic energy is the same as the Landau-de Gennes elastic energy, but with different notation.

For more information concerning the form of the Landau-de Gennes energy ψ and its relationship to the Oseen-Frank energy see [5,6].

On the other hand, although the energy density can be regarded as being the same in the two theories, in the constant s Landau-de Gennes theory there are more possibilities for energy minimization than in the Oseen-Frank theory. Indeed, there are more line fields than vector fields. Consider a vector field $n(x) : \Omega \to \mathbb{S}^2$ (where the bounded domain Ω denotes the container to which the liquid crystal is confined and where $\mathbb{S}^2$ is the unit sphere). To such a vector field one can associate a line field $\{n(x), -n(x)\} \sim Q(x) = s(n(x) \otimes n(x) -1/3(Id))$. Apparently one can do the opposite as well, that is to replace a line field $\{n(x), -n(x)\}$ by a vector field just by choosing at each point either $n(x)$ or $-n(x)$. But in making the changes from the line field to a vector field one needs to create as few jumps in the director as possible, in order not to create a vector field having infinite energy.

In fact it turns out that there are continuous, even smooth, line fields for which it is impossible to 'assign arrows to the lines'; that is, one cannot make a choice of a vector out of each line in such a

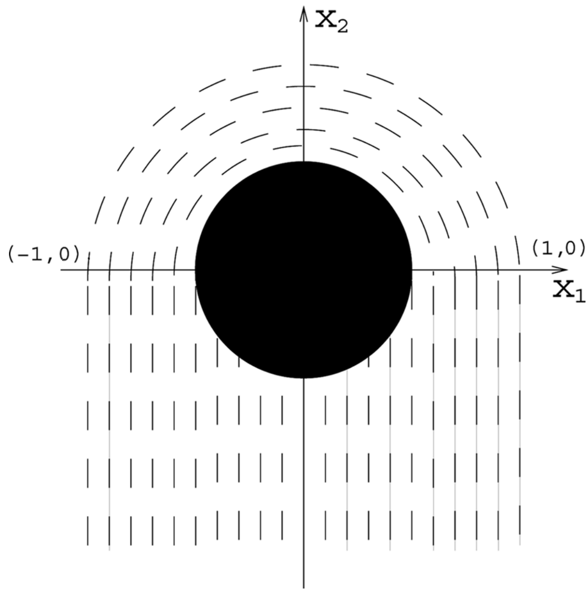


FIGURE 1 A non-orientable director field.

way that no discontinuity is created. To see this, consider the line field illustrated in Figure 1, which is defined in the exterior of a circular cylinder with generators parallel to the x_3-axis. The line field is in the (x_1, x_2)–plane, i.e., the vectors $\{n(x), -n(x)\}$ have x_3-component zero. Thus we can consider it as a two-dimensional line field defined in the exterior of the circle shown, with centre the origin and radius 1/2. For $x_2 > 0$ the line field at the points (x_1, x_2) is parallel to the vector $(x_2, -x_1)$, while for $x_2 \leq 0$ all lines are parallel to the x_2-axis. Let us try to 'orient' this line field, that is to assign arrows to all the lines, those tangent to the upper semicircles, and those parallel to the x_2-axis. We want to do this without creating any discontinuity, so that in particular this leaves us with just two choices for choosing the vectors at $(-1, 0)$ and $(0, 1)$: if you pick the arrow to point up at $(-1, 0)$ you will have to take it pointing down at $(1, 0)$, and vice versa. On the other hand if one looks at the line field below (and including) the x_1-axis one sees that the only possibility of assigning arrows without creating jumps is by putting them all in the same direction, in particular in the same direction at $(-1, 0)$ and $(1, 0)$. This shows that we must necessarily create a jump by trying to make this line field into a vector field.

This example also shows that in order to orient a line field that has no jumps one needs to look at what happens along curves, because along each curve the orientation 'propagates' by continuity along the curve. Also, the example shows that the only issue that might appear is when these curves have self-intersections, so that they form a loop (in our example the loops that cause the problem are those that go around the shaded disk). Thus in order to decide whether a line field is orientable or not we need to check its orientability along all possible loops. As some thought will show, if a line field is orientable on a loop A, it is also orientable on any other loop B that can be obtained from A through a continuous deformation that keeps the loop within the domain.

In particular we have orientability along any loop that can be continuously deformed to a single point while staying in the domain. Hence, in so-called *simply-connected domains* (in which any loop can be continuously deformed into a point while staying in the domain), we have that continuous line fields can be replaced by continuous vector fields.

However, in practice director fields often do have discontinuities corresponding to defects. In order to understand whether it is possible to orient a line field in the case when defects are present we first need to introduce a framework for measuring how bad such defects can be.

2. SOBOLEV SPACES AS A MEASUREMENT SCALE FOR DEFECTS

In defining the functions that describe the orientation of the director, be it a line or a vector, we make the convention of considering two functions to be the same if they differ only on a set of *measure zero*, i.e., of zero volume. We say that a set has measure zero if it can be completely covered with balls the sum of whose volumes can be made as small as desired. Thus our convention amounts to saying that the functions we consider only see those features that are on large enough scales. This is particularly useful in our case as we do not know what happens on very small sets, the locations of defects, where we do not know whether the director is defined or not.

We need to reinterpret the definition of the derivative so that it makes sense in the new framework. Denoting by $\mathbb{R}^d$ d-dimensional real Euclidean space, for a function $f:\Omega\subset\mathbb{R}^d\to\mathbb{R}$ we define the *generalized partial derivative in direction* x_k to be a function $g_k:\Omega\subset\mathbb{R}^d\to\mathbb{R}$ such that

$$\int_\Omega f(x)\frac{\partial\varphi(x)}{\partial x_k}dx = -\int_\Omega g_k(x)\varphi(x)dx \tag{4}$$

where the equality holds for *any function* φ that is differentiable on Ω, in the usual sense, with continuous derivative, and that is zero outside a bounded set. An example of such a function φ is

$$\varphi_0(x) = \begin{cases} \exp\left(\frac{1}{|x|^2-1}\right) & \text{if } |x| < 1 \\ 0 & \text{if } |x| \geq 1 \end{cases} \tag{5}$$

that is differentiable in $\mathbb{R}^d$ in the usual sense, with continuous derivative, and zero outside the bounded set $\{x \in \mathbb{R}^d; |x| < 1\}$.

When the function f is differentiable in the usual sense g_k is precisely the partial derivative $\partial f/\partial x_k$. However the relation above makes sense even if f is not differentiable. To see this take $d = 1, \Omega = (-1, 1)$ and $f(x) = |x|$. This function is not differentiable at $x = 0$ but nevertheless it has a generalized derivative

$$g(x) = \begin{cases} -1, & \text{for } x < 0 \\ 1, & \text{for } x > 0 \end{cases}$$

(note that g is not defined at $x = 0$ in agreement with our convention, as one point has measure zero).

To see that g satisfies relation (4) it suffices to break the interval $[-1, 1]$ into two parts $[-1, 0]$ and $[0, 1]$, on which f is smooth, and integrate by parts on each of the intervals.

Another example of generalized derivative is that of the hedgehog, given by the vector-valued function $n(x) = (x_1/|x|, x_2/|x|, \ldots, x_d/|x|)$ with $x \in \mathbb{R}^d$, $|x| = \sqrt{\Sigma_{i=1}^d x_i^2}$. In this case the function is not even defined at $x = 0$ but one can check that it has a generalized gradient $\nabla n(x) = \frac{1}{|x|}(1 - n(x) \otimes n(x))$. As before, the generalized gradient coincides with the usual one at all points where n is differentiable in the usual sense. The hedgehog is a significant example that is often encountered as a prototypical defect. The usual treatment of such a defect is to consider a small hole around the singularity and analyze everything outside that hole. However this kind of treatment requires a knowledge of the location of the defect. The generalized derivative as we have defined it has the advantage that it does not require such *a priori* knowledge of defect locations.

It is desirable to be able to classify the functions that have generalized derivatives on a scale that measures "how bad the *possible* defects could be." A possible way of doing this is by considering the average of powers of the derivatives. We define the Sobolev space $W^{1,p}(\Omega)$ as the space of all vector functions f that have a generalized gradient ∇f such that both $\int_\Omega |f(x)|^p dx < \infty$ and $\int_\Omega |\nabla f(x)|^p dx < \infty$. In this framework the functions of finite energy are those in $W^{1,2}$, since the Oseen-Frank and Landau-de Gennes energy densities are quadratic in the gradient, but there are nevertheless examples of index one-half singularities that can only be in the larger space $W^{1,p}$, $p<2$ (see Fig. 2 and the next section). In the case of the hedgehog we have $n(x) \in W^{1,p}(\Omega)$ if and only if $p<d$, so that when $d=3$ it has finite energy. On the other hand the function $f(x)=|x|$ in our first example is in $W^{1,p}$ for any p. In general, for Ω a bounded set, we have that $W^{1,p}(\Omega) \subset W^{1,q}(\Omega)$ if $q<p$; thus the smaller the index the larger the space and the more general the type of defects allowed. Functions that have *too strong a discontinuity* will not be in any Sobolev space of the type considered so far. For instance consider the function $f:(0,1)^2 \to \mathbb{R}$ defined by

$$f(x,y) = \begin{cases} 1, & \text{for } x \geq 0,\ y \in (-1,1) \\ -1 & \text{for } x < 0,\ y \in (-1,1) \end{cases}$$

Then $f \notin W^{1,p}$ for any p. In fact f does not have generalized partial derivatives. One might be tempted to state that the generalized partial derivatives f are 0 almost everywhere. This is not the case. If one takes $g_1 = 0$ to be the generalized derivative in the x direction and φ to be the φ_0, as in (5), one obtains a contradiction when replacing f, g_1, φ

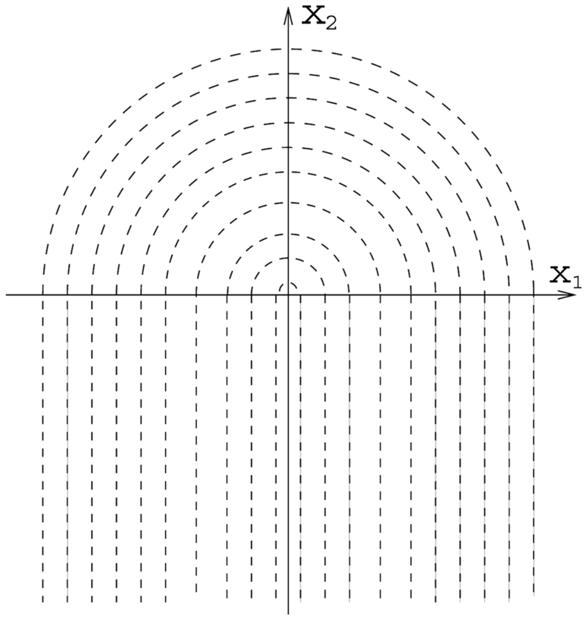


FIGURE 2 A non-orientable director field on a simply-connected domain, for $p<2$.

in relation (4). This kind of discontinuity arises in attempting to orient the director field in Figure 1, which can be shown to be impossible even in Sobolev spaces.

Generalized derivatives and the framework exposed in this section have proved their usefulness in other kinds of problems involving discontinuities. For example, a study was made in [7] in which it was theoretically predicted that, under suitable conditions, a spherical cavity will form at the centre of a ball of isotropic, homogeneous non-linearly elastic material subjected to hydrostatic tension or outward radial displacement. In that study it was shown that the energy minimizers depend on the particular Sobolev space considered, so that the function space *is part of the mathematical model*. This raises the question as to how to decide which function space is appropriate. For liquid crystals this question might be answerable by means of an analysis of the passage from a molecular model to a continuum one, but this has not been done. For further examples and discussion see [8].

For more details about Sobolev spaces the reader is referred to [9,10].

3. THE OVERLAPPING OF THE TWO THEORIES

In the framework developed in the previous section we call a line field $Q \in W^{1,p}(\Omega)$ orientable if and only there exists a vector field *in the same functional space*, that is an $n \in W^{1,p}(\Omega)$ such that $n(x) \in \mathbb{S}^2$ and $Q(x) = s(n(x) \otimes n(x) - 1/3(Id))$ for all $x \in \Omega$, except for possibly a set of measure zero. This amounts to saying that Q is orientable if and only if we can find a corresponding vector field whose singularities are no worse than those of the line field. In fact it can be shown (see [11]) that if we can find a unit vector field m in the largest Sobolev space $W^{1,1}(\Omega)$ such that $Q(x) = s(m(x) \otimes m(x) - 1/3(Id))$ then in fact $m \in W^{1,p}(\Omega)$ and thus Q is orientable in $W^{1,p}(\Omega)$.

One might wonder whether there could be several distinct ways of orienting a line field into a vector field. The intuition of the continuous case seems to indicate that there can be only two possible orientations, one being obtained from the other by a change of sign. This can be shown to be the case in the Sobolev space framework as well (see [11]), namely if you have a unit vector field $n \in W^{1,p}(\Omega)$ corresponding to a line field $Q \in W^{1,p}(\Omega)$ there can be only one other vector field corresponding to the same Q, namely the vector field $-n$.

Recall that in the first section we showed that the natural way to check the orientability is to do it along all possible loops. We also saw that in simply-connected domains, that is domains where any loops can be continuously deformed into a point, line fields without jumps, that is continuous line fields, can be oriented into vector fields.

In the framework of Sobolev spaces the idea of checking the orientability along all possible loops cannot work any longer in the same manner because loops are sets of measure zero. However the intuition provided by the continuous case is still valid, as long as the spaces $W^{1,p}$ are not 'too far' from the continuous case. In fact the following result is proved in [11] (see also [12]).

Theorem. *For simply-connected domains, line fields belonging to $W^{1,p}$ for some $p \geq 2$ are orientable.*

However for $p < 2$ this is no longer true and there are line fields on simply connected domains that are not orientable. An example is provided in Figure 2. This is a line field $Q(x) = s(n(x) \otimes n(x) - 1/3(Id))$ on $\Omega = (-1,1)^3 \subset \mathbb{R}^3$ corresponding to an index one-half singularity, where

$$n(x_1,x_2,x_3) = \begin{cases} (x_2,-x_1,0) & \text{for } (x_1,x_2,x_3) \in (-1,1) \times (0,1) \times (-1,1) \\ (0,1,0) & \text{for } (x_1,x_2,x_3) \in (-1,1) \times (-1,0) \times (-1,1) \end{cases}$$

One can check that the generalized gradient of Q is equal to the classical gradient everywhere in $\Omega \backslash \{x_1 = x_2 = 0\}$, and that $|\nabla Q|^2 = Q_{ij,k}Q_{ij,k} = 2/|x|^2$. Thus $Q \in W^{1,p}(\Omega)$ only for $p < 2$. An interesting consequence of the theorem is that this line field cannot be modified in a cylindrical core $x_1^2 + x_2^2 \leq \varepsilon^2$ so that it has finite (constant s) Landau-de Gennes energy. For if this were possible the line field would be orientable, and our earlier reasoning applied to the domain $x_1^2 + x_2^2 > \varepsilon^2$ shows that this is not the case. This can be contrasted with the case of a line disclination given by the orientable director field $n(x) = (x_1/r, x_2/r, 0)$, $r = \sqrt{x_1^2 + x_2^2}$, which has infinite Oseen-Frank energy, but for which the analysis in [13] shows that n may be modified in a core $x_1^2 + x_2^2 \leq \varepsilon^2$ by 'escape into the third dimension' so that it has finite energy.

4. DIFFERENCES BETWEEN THE TWO THEORIES

In this last section we restrict ourselves to two-dimensional planar domains and consequently we take the line fields to lie in the plane. This is a physically relevant geometry, for instance for thin films.

We are interested in studying situations when both orientable and non-orientable line fields can exist, and thus we consider domains with holes, as in Figure 3, that is domains that are of the form $G = \Omega \setminus \cup_{i=1}^N U_i$ where Ω is a simply connected domain out of which one cuts n holes, each hole U_i again being simply connected. The boundary ∂G of this domain consists of $N + 1$ parts, namely the outer boundary, the boundary $\partial\Omega$ of Ω, and the boundaries of the N holes, denoted ∂U_i.

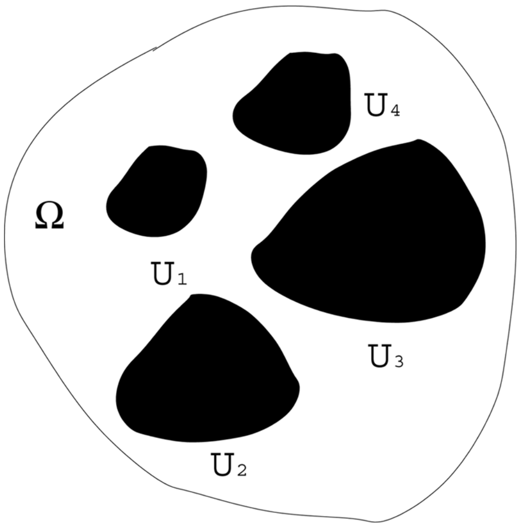


FIGURE 3 A domain with holes.

Each of the $N+1$ components of the boundary of G is a loop, on which non-orientable boundary conditions can thus be imposed. It can be shown (see [11]) that imposing non-orientable boundary conditions, on any part of the boundary, has the effect of excluding any orientable line field from matching them. Thus there is no finite energy (in $W^{1,2}$) line field that is orientable in G but matches the non-orientable line boundary conditions.

On the other hand, if one puts orientable boundary conditions *on all* $N+1$ *components of the boundary* then one cannot find a finite-energy line field that is non-orientable and matches the orientable boundary conditions. In this sense one can recognize the orientability just by checking it at the boundary.

Nevertheless, if one puts boundary conditions just on one part of the boundary, say on $\partial\Omega$, one could have on the remaining components, $\partial U_i, i = 1, \dots, N$, either orientable or non-orientable boundary conditions. In fact it can be shown that if one imposes orientable boundary conditions just on a component of the boundary then in general one can match those boundary conditions both with orientable and non-orientable line fields. In order to see this we need to introduce a device that allows us to think of line fields in terms of auxiliary vector fields.

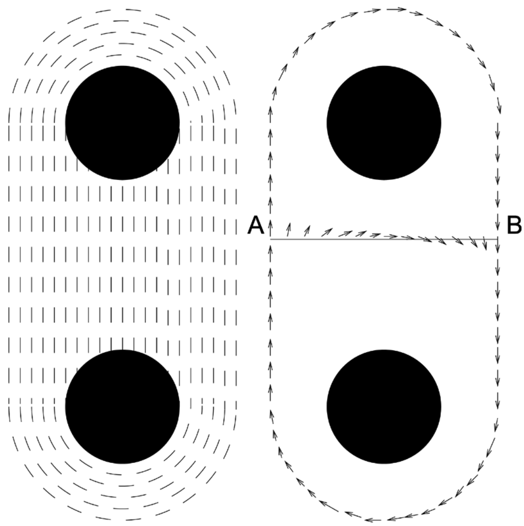
We can think of any line in the plane as determined by two vectors of length one having opposite signs. In complex notation a line is determined by the pair $\{z, -z\}$ with $z = x_1 + ix_2, x_1^2 + x_2^2 = 1$. We associate to such a line the unit length vector $A(z) = z^2 = x_1^2 - x_2^2 + 2ix_1x_2$. One can check that for each such unit vector there exists a unique line and also that the line field and the auxiliary vector field are in the same $W^{1,p}$ space. Moreover it can be checked that if we have a line field Q on a loop, then to it corresponds a vector field *A(Q)* that has even degree if and only if Q is orientable (for the definition of degree see [14,15]).

As an application of the auxiliary line field, we show how it can be used for extending a continuous line field on the outer boundary to a continuous line field on the whole domain. To this end it is useful to recall a well known theorem from topology (see [13,14]) which says that one can extend a *unit vector field* from the boundary to a *unit vector field* on the whole domain, provided that the unit vector field on the boundary has degree zero.

Thus if we put a continuous line field q_Ω on the outer boundary, $\partial\Omega$, we can associate to it the auxiliary vector field $A(q_\Omega)$, which has a certain degree, let us call it w_0. In order to apply the above mentioned result we need to have a degree zero unit vector field on the whole boundary of G. Hence we take some arbitrary line fields m_{U_i} on the boundary ∂U_i for $i = 1, 2, \ldots, N$. If we denote by w_i the degree of m_{U_i} the condition that the unit length vector field on the whole boundary, ∂G, has degree zero becomes, in terms of degrees, $w_0 + w_1 + \cdots + w_N = 0$ (note that one can always find vector fields m_{U_i}, $i = 1, 2, \ldots, N$ so that this last condition is satisfied). Using the above mentioned topological result we extend the continuous unit length vector field on the boundary ∂G to a continuous unit length vector field m_G on G. Then $A^{-1}(m_G)$ is a continuous line field on G that matches the boundary condition q_Ω on $\partial\Omega$. In order to know whether the line field is orientable or not it suffices to observe that this can be determined at the level of the auxiliary vector field. Namely the line field $A^{-1}(m_G)$ is non-orientable if and only if at least one of the numbers w_i, $i = 0, 1, \ldots, N$, is odd.

In the first section we hinted that although the elastic energies can be taken to be the same in the Oseen-Frank and Landau-de Gennes theories, the result of the energy minimization might be different because there are ‘more line fields than vector fields’. Thus the Oseen-Frank theory would miss those minimizers that are non-orientable line fields.

In Figure 4 we present a geometry in which the global minimizer is necessarily non-orientable, even though the configuration admits both orientable and non-orientable line fields. We consider a stadium out of which two disks are removed. We impose tangential boundary conditions on the outer boundary of the stadium. However no restrictions are imposed on the boundaries of the two disks. The line field on the



(a) (b)

FIGURE 4 A situation in which the energy minimizer is non-orientable.

outer boundary can be oriented in two ways (that differ only by change of sign) and one orientation is shown in the Figure 4b. A line field matching the boundary conditions is shown in Figure 4a. We *do not claim* that the line field shown in Figure 4a is the global energy minimizer. What we can say is that if the distance between the two disks is large enough the line field configuration in Figure 4a will have lower energy than any possible vector field configuration in Figure 4b. This can be seen by observing that along a line AB the directional derivative will be zero in the case of the line field in Figure 4a, while for the situation in Figure 4b, along almost any such line AB there will be a non-zero gradient, a configuration of minimum energy (just along AB) being shown.

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