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A. M. Sonnet[a]; E. G. Virga[b]
[a] Department of Mathematics and Statistics, University of Strathclyde, Glasgow, Scotland, UK [b] Dipartimento di Matematica and CNISM, Università di Pavia, Pavia, Italy

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INVITED ARTICLE

Reorientational dynamics of conjugated nematic point defects

A.M. Sonnet[a] and E.G. Virga[b]*

[a]*Department of Mathematics and Statistics, University of Strathclyde, Livingstone Tower, 26 Richmond Street, Glasgow G1 1XH, Scotland, UK;* [b]*Dipartimento di Matematica and CNISM, Università di Pavia, Via Ferrata 1, 27100 Pavia, Italy*

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To appreciate the universal qualitative features of defect annihilation in nematic liquid crystals, we study how the viscous force of reorientational dynamics behaves under a transformation that reverses the sign of the defect's topological charge. As an illustration of our general results, we consider a class of point defects that were first studied by A. Saupe. The reorientational viscous forces acting on them differ dramatically from those acting on line defects.

Keywords: liquid crystals; defect dynamics; parity

1. Introduction

Most nematic liquid crystals are optically uniaxial, that is, their Fresnel ellipsoid is symmetric about an axis, the nematic *director* $\boldsymbol{n}$. However, the director may change within the fluid, responding to both flow and external influences, such as electric or magnetic fields. The high susceptibility of the nematic director to such influences makes nematic liquid crystals fascinating fluids with impressive optical properties and a still unexhausted potential for applications.

Perhaps the most striking and colourful optical manifestations of nematic liquid crystals are their *defects*, which are singularities in the optic axis texture, where the nematic director field $\boldsymbol{n}$ is discontinuous. All possible types of defects are classified by their *topological charge*, according to the general ideas first put forward by Poincaré [1] in a purely mathematical context, and then applied to ordered media by Nabarro [2]. In nematic liquid crystals, the topological charge is either a half-integer or an integer, connected with either a line or point discontinuity in the director field. It can be computed from this field in a neighbourhood of the discontinuity, where $\boldsymbol{n}$ has regained smoothness. The topological charge is invariant under smooth deformations of the director field, and so it captures the characteristic qualitative features of a defect. Because of the absence of any positional order, all line defects found in nematic liquid crystals are of the *disclination*-type [3].

Technically, the topological charge of a line or point defect can be computed from the field $\boldsymbol{n}$ restricted along a path or upon a surface enclosing the defect (see, for example, [4] and [5], to the latter of which we also refer the reader for the general aspects of defect dynamics). Like the electric charge, the topological charge is additive: when, depending on the defect dimension, it is computed either along a path or upon a surface that encloses more than a single defect, the topological charge associated with such a collection of defects is the algebraic sum of the topological charges attributed to every single defect. In particular, when the director is prescribed on the boundary $\partial\mathscr{B}$ of a region $\mathscr{B}$ containing a liquid crystal, the boundary data prescribes the total topological charge of all defects present at any time within $\mathscr{B}$, either at equilibrium or out of it. Thus, whenever the director field on $\partial\mathscr{B}$ carries a topological charge different from zero, at least one defect is present in the interior of $\mathscr{B}$. Clearly, there may be more: only their total topological charge is determined by the boundary conditions.

Defects do not occur only in equilibrium director fields. Out of equilibrium, they tend to move within the fluid so as to reduce the elastic energy connected with director distortions. In the absence of boundary frustrations, the director field of an ordinary, non-chiral nematic would be uniform in space; distortions arise in response to non-uniform boundary conditions. For the nematic to attain the minimum of the elastic free energy, defects may move and annihilate, involving no or little hydrodynamic flow. Often, the relaxation dynamics of the director field is assumed to be purely *reorientational*: defects then move due to a change in director orientation at all points, without any material flow.

Phenomenologically, defect dynamics result from balancing gains in the elastic free energy and viscous losses, both associated with defect displacements. Even in the absence of flow, a viscous damping is

*Corresponding author. Email: eg.virga@unipv.it

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present; it has its physical origin in the microscopic reorientational dynamics. For clarity, we shall refer to the corresponding damping force acting on a defect as a *reorientational viscous force*, and to the extra damping force, associated with a possible flow, as a *viscous drag force*. The simple idea of balancing elastic gains and viscous losses was first applied by Brochard [6] to the motion of a domain wall and then extended to defect motion by numerous works, of which [7] is perhaps the earliest.

A phenomenological model for both elastic and reorientational viscous forces, although originally conceived for smectic C liquid crystals, was first proposed by Pleiner [8]. In [9], Ryskin and Kremenetsky phrased the problem of computing the reorientational viscous force acting on a moving disclination within the general dynamical Ericksen–Leslie theory (an extensive account of which can be found, for example, in [10]). In the approach of [9], the effective viscosity associated with the reorientational viscous force is computed for a drifting director configuration that solves the balance equation of torques, including the reorientational viscous torque resulting from the drift. This approach essentially relies on a dissipation identity stating that in the absence of flow the rate of change of the total elastic free energy stored in the domain occupied by the liquid crystal is counterbalanced by the total energy dissipated in the same domain by viscous losses. The method of [9] substantially improves upon the approximation of Imura and Okano [11], also followed by de Gennes [12], according to which the effective viscosity is computed on a drifting equilibrium configuration that solves the balance equation of torques, neglecting any viscous contribution to this balance. For this approximation to deliver a finite effective viscosity, the total dissipation must, however, be confined within a bounded region enclosing the disclination, with the disadvantage of making the effective viscosity depend on the size of such an arbitrary cut-off region. Notwithstanding this limitation, the *drifting equilibrium* approximation is capable of capturing the essence of defect dynamics even when an explicit solution to the complete balance equation of torques is not available. In the notable case of the motion of a straight disclination of arbitrary topological charge, the general analytic solution to the complete balance equation of torques was obtained by Denniston [13].

One of the most fascinating phenomena in defect dynamics is the annihilation of two defects with opposite topological charges. Many contributions have been made in the past decades to the modelling of this phenomenon. While most are mainly concerned with the annihilation of disclinations [7, 13–21], a few also consider the annihilation of point defects [22–25], among which [22] and [25], in particular, resort to a scaling argument to justify an evolution equation for annihilation dynamics.

Perhaps the most striking feature of annihilation dynamics, for both disclinations and point defects, is the asymmetry in the velocity under sign reversal of the topological charge. Such an asymmetry, also confirmed by the experiments of [20, 21, 24] and the numerical simulations of [15, 17, 18], is generally ascribed to backflow, that is, to flow induced by the defect motion. This flow can be different in the vicinity of defects with different topological charges, and so it can produce different viscous drag forces.

We have also contributed to this view, proposing in [26] a phenomenological model for the annihilation of disclination pairs of any topological charge, based on the balance of the three types of forces acting on defects, properly derived within the paradigm of the Ericksen–Leslie theory. These forces are the elastic force, the reorientational viscous force and the viscous drag force (see also [27]). We showed in [26] that the asymmetry in the disclination annihilation, as measured by an appropriate scalar parameter evolving in time, depends on both the viscous drag force and the reorientational viscous force, and depends significantly on the latter only for moderate inter-disclination distances. This result followed from the dependence of the asymmetry parameter on the relative reorientation velocity, which was assumed to be symmetric.

In this paper, we take a different, although complementary avenue to explain the asymmetry in defect annihilation, concentrating attention on point defects. Applying general concepts of continuum mechanics, we derive a supplementary balance law for the forces on a defect, be it a line or a point. For the sake of argument, we neglect backflow, so that the balance of forces includes only the elastic force and the reorientational viscous force. We explore how both these forces change under the *parity* transformation that reverses the sign of the defect's topological charge. Our general conclusion is that, even when backflow is neglected, an asymmetry in defect annihilation results from an asymmetry in the reorientational viscous force under sign reversal of the topological charge. There are, however, important differences in the behaviour of point and line disclinations. While for line disclinations the reorientational viscous force is simply proportional to the topological charge, only point defects with topological charge $s = 1$ feel any reorientational viscous force at all. Even in the case when $s = 1$, the magnitude and sign of the force still depend on the fine structure of the defect. Free defects can indeed continuously deform such that they would not feel any force. It can thus be expected that reorientational viscous forces lead to an asymmetric annihilation only if boundary conditions fix the defect structure, as is the case in [24], where the director is subject to homeotropic anchoring in a capillary.

The paper is organised as follows. In Section 2 we recall the basic balance laws of the Ericksen–Leslie theory and we deduce from them the balance of both elastic and viscous forces acting on a defect, making the very definition of these defect forces precise. In Section 3, we illustrate the analytic definition of topological charge for point defects that we adopt in this paper. In Section 4, we show how the topological charge is reversed in sign by the action of a reflection that thus constitutes a parity transformation, which also affects both the elastic force and the reorientational viscous force. The latter is computed in Section 5 for the *combed* defects [23] first studied by Saupe [28] in a special case. Finally, in Section 6 we summarise the main conclusions of our work. A technical appendix with an auxiliary result closes the paper.

2. Defect forces

The dynamics of nematic liquid crystals is commonly described by the Ericksen–Leslie equations, a system of coupled partial differential equations for flow and orientation. Finding solutions to the full set of these equations usually requires one to resort to numerical methods. Here, we do not aim to construct solutions but rather to assess the driving forces that govern defect motion. We choose to neglect material flow altogether, which leads to a significant simplification of the stress tensor. It consists of an *elastic stress* that depends on the director gradient $\nabla \boldsymbol{n}$ and a *reorientational viscous stress* that depends on the rate of change of the director $\boldsymbol{n}$. Furthermore, we take the elastic free-energy density, W, in the one-constant approximation,

$$W = \frac{1}{2} K (\nabla \boldsymbol{n})^2, \tag{1}$$

with a single elastic modulus K.

The elastic stress, sometimes called the Ericksen stress, can then be written in the form [29]

$$\mathbf{T}^{(\mathrm{e})} = \frac{1}{2} K (\nabla \boldsymbol{n})^2 \mathbf{I} - K (\nabla \boldsymbol{n})^T (\nabla \boldsymbol{n}), \tag{2}$$

where $\mathbf{I}$ is the identity tensor. In the absence of flow, the entire viscous stress is due to director reorientations,

$$\mathbf{T}^{(\mathrm{r})} = \frac{1}{2} \gamma_1 (\boldsymbol{n} \otimes \mathring{\boldsymbol{n}} - \mathring{\boldsymbol{n}} \otimes \boldsymbol{n}), \tag{3}$$

where γ_1 is a rotational viscosity coefficient and $\mathring{\boldsymbol{n}}$ is the director's co-rotational time derivative, which in the absence of material flow equals its partial time derivative, $\mathring{\boldsymbol{n}} = \partial \boldsymbol{n} / \partial t$.

We now consider a small region of liquid crystal $\mathscr{B}$ with boundary $\partial \mathscr{B}$. The stresses in Equations (2) and (3) result in tractions on the boundary and thereby, once integrated over the boundary, in contact forces on the region. With the two components of the stress as identified previously, we accordingly define an *elastic force* $\boldsymbol{f}^{(\mathrm{e})}$ and a *reorientational viscous force* $\boldsymbol{f}^{(\mathrm{r})}$ via

$$\boldsymbol{f}^{(\mathrm{e})} := \int_{\partial \mathscr{B}} \mathbf{T}^{(\mathrm{e})} \boldsymbol{\nu} \, \mathrm{d}a \tag{4}$$

and

$$\boldsymbol{f}^{(\mathrm{r})} := \int_{\partial \mathscr{B}} \mathbf{T}^{(\mathrm{r})} \boldsymbol{\nu} \, \mathrm{d}a, \tag{5}$$

where $\boldsymbol{\nu}$ is the outer unit normal to $\partial \mathscr{B}$ and a is the area measure. It is worth noting for later use that, by Equations (2) and (3), reversing $\boldsymbol{n}$ into $-\boldsymbol{n}$ changes neither $\mathbf{T}^{(\mathrm{e})}$ nor $\mathbf{T}^{(\mathrm{r})}$, thus also leaving $\boldsymbol{f}^{(\mathrm{e})}$ and $\boldsymbol{f}^{(\mathrm{r})}$ unchanged.

Let $\mathscr{B}$ contain a single defect. At equilibrium, $\mathbf{T} = \mathbf{T}^{(\mathrm{e})}$ and $\operatorname{div} \mathbf{T} = \boldsymbol{0}$. Even in this case the force $\boldsymbol{f}^{(\mathrm{e})}$ in Equation (4) may not vanish because $\mathbf{T}^{(\mathrm{e})}$ fails to be smooth in $\partial \mathscr{B}$ and so the divergence theorem cannot be applied in the whole of $\mathscr{B}$. This is certainly the case for defects *pinned* in space by some external agents. In fact, the elastic force will only be independent of $\mathscr{B}$, which makes it meaningful to speak of a *force on the defect*. In general, when $\operatorname{div} \mathbf{T} \neq \boldsymbol{0}$, it is still possible to define a force on the defect by considering the limit as $\mathscr{B}$ shrinks to the defect; see [29].

3. Topological charge

Defects are singularities in the director field, where the nematic order is effectively lost. Nematic point defects can be organised in distinct *topological classes* [4]; the members of each class are director fields that can be transformed into one another through continuous mappings, whereas members of different classes cannot be continuously connected. All topological classes are classified in terms of a topological invariant, which characterises the members in one and the same class. Here we show how this invariant is related to the topological charge of a nematic point defect. We explore in some detail this classical notion, reviewing the equally classical means to compute the topological charge, with the objective of learning later how it behaves under the parity transformation introduced in the following section.

An effective way to illuminate the topological charge of a point defect is to imagine the point singularity of the director field surrounded by a closed, regular, orientable surface $\mathscr{S}$. Restricting $\boldsymbol{n}$ onto $\mathscr{S}$, we may picture the restricted field $\boldsymbol{n}_{\mathscr{S}}$ as a mapping from $\mathscr{S}$ into the unit sphere $\mathbb{S}^2$ in three-dimensional space. Intuitively, the topological charge $N(\boldsymbol{n})$ of the defect enclosed by $\mathscr{S}$ is the number of times $\mathscr{S}$ is wrapped around $\mathbb{S}^2$ by $\boldsymbol{n}_{\mathscr{S}}$, counted algebraically, that is, with a positive or negative sign, according to whether the orientation of $\mathscr{S}$ is preserved or not by $\boldsymbol{n}_{\mathscr{S}}$ at each individual wrapping. By its very notion, $N(\boldsymbol{n})$ is an integer independent of $\mathscr{S}$. As pointed out in [30], the topological charge of a point defect in the director field $\boldsymbol{n}$ coincides with the *Brouwer degree* of $\boldsymbol{n}$ around that point; an abstract definition of this concept, central to non-linear functional analysis, can be found, for example, in [31].

Here we are interested in computing $N(\boldsymbol{n})$. Let the surface $\mathscr{S}$ be such that it is endowed with a system of orthogonal coordinates with integral lines having unit tangent vectors $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$, oriented so that $\boldsymbol{\nu} \cdot \boldsymbol{e}_1 \times \boldsymbol{e}_2 = 1$, where $\boldsymbol{\nu}$ is the outer unit normal to $\mathscr{S}$. Let p be a point on $\mathscr{S}$ mapped by $\boldsymbol{n}$ to the vector $\boldsymbol{n}(p)$ on $\mathbb{S}^2$. For $\varepsilon > 0$ sufficiently small, the points $p_i = p + \varepsilon \boldsymbol{e}_i$, $i \in \{1, 2\}$, are mapped to $\boldsymbol{n}_i = \boldsymbol{n}(p) + \varepsilon\nabla\, \boldsymbol{n}(p)\boldsymbol{e}_i$. Thus the triangle on the tangent plane to $\mathscr{S}$ at p with vertices p, p_1 and p_2 is mapped to the triangle on the tangent plane to $\mathbb{S}^2$ at $\boldsymbol{n}(p)$ with vertices $\boldsymbol{n}(p)$, $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$. The area of the former triangle is

$$A_p = \frac{1}{2}\boldsymbol{\nu} \cdot \varepsilon\boldsymbol{e}_1 \times \varepsilon\boldsymbol{e}_2 = \frac{1}{2}\varepsilon^2. \tag{6}$$

Similarly, since

$$\boldsymbol{n} \cdot (\nabla\boldsymbol{n})\boldsymbol{e}_i = 0 \quad \text{for} \quad i = 1, 2,$$

as $(\nabla\boldsymbol{n})^{\mathrm{T}}\, \boldsymbol{n} = \boldsymbol{0}$, the signed area of the latter triangle is

$$A_{\boldsymbol{n}(p)} = \frac{1}{2}\varepsilon^2 \boldsymbol{n} \cdot (\nabla\boldsymbol{n})\boldsymbol{e}_1 \times (\nabla\boldsymbol{n})\boldsymbol{e}_2 + o(\varepsilon^2), \tag{7}$$

where $A_{\boldsymbol{n}(p)}$ is positive or negative, depending on whether the vectors $(\nabla\boldsymbol{n})\, \boldsymbol{e}_1$, $(\nabla\boldsymbol{n})\, \boldsymbol{e}_2$ and $\boldsymbol{n}$ have the same orientation as $\boldsymbol{e}_1$, $\boldsymbol{e}_2$ and $\boldsymbol{\nu}$ or not. We conclude from Equations (6) and (7) that the Jacobian determinant $\boldsymbol{J}$ of $\boldsymbol{n}_{\mathscr{S}}$, seen as a transformation that maps $\mathscr{S}$ into $\mathbb{S}^2$, possibly more than once, is

$$J = \boldsymbol{n} \cdot (\nabla\boldsymbol{n})\boldsymbol{e}_1 \times (\nabla\boldsymbol{n})\boldsymbol{e}_2,$$

and so the *topological charge* of $\boldsymbol{n}$ is given by

$$\begin{aligned} N(\boldsymbol{n}) &= \frac{\int_{\mathscr{S}} \boldsymbol{n} \cdot (\nabla\boldsymbol{n})\boldsymbol{e}_1 \times (\nabla\boldsymbol{n})\boldsymbol{e}_2 \mathrm{d}a}{a(\mathbb{S}^2)} \\ &= \frac{1}{4\pi}\int_{\mathscr{S}} \boldsymbol{n} \cdot (\nabla\boldsymbol{n})\boldsymbol{e}_1 \times (\nabla\boldsymbol{n})\boldsymbol{e}_2 \mathrm{d}a. \end{aligned} \tag{8}$$

Apparently, this formula was first given in [32]. Strictly speaking, since both $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ are tangential unit vectors, $\nabla\boldsymbol{n}$ should be replaced in Equation (8) by the surface gradient $\nabla_{\mathrm{s}}\boldsymbol{n}$, thus making Equation (8) a formula defined solely in terms of the field $\boldsymbol{n}_{\mathscr{S}}$.

Equation (8) for $N(\boldsymbol{n})$ seems to require the existence on $\mathscr{S}$ of a system of global orthogonal coordinates. Actually, Equation (8) can be given an equivalent, intrinsic form that does not require this property of $\mathscr{S}$. For any second-rank tensor $\mathbf{L}$, there exists another second-rank tensor $\mathbf{L}^*$, which we call the *adjugate* of $\mathbf{L}$, characterised by the following property,

$$\mathbf{L}\boldsymbol{a} \times \mathbf{L}\boldsymbol{b} = \mathbf{L}^*(\boldsymbol{a} \times \boldsymbol{b}), \tag{9}$$

for all vectors $\boldsymbol{a}$ and $\boldsymbol{b}$. Whenever $\mathbf{L}$ is invertible, its adjugate $\mathbf{L}^*$ can be given the following explicit representation:

$$\mathbf{L}^* = \det\mathbf{L}(\mathbf{L}^{-1})^{\mathrm{T}}. \tag{10}$$

In general, the entries L^*_{ij} of the matrix representing $\mathbf{L}^*$ in any given basis are the cofactors of the matrix representing $\mathbf{L}$ in the same basis. In particular,

$$L^*_{ij} = \frac{1}{2}\varepsilon_{ihk}\varepsilon_{jlm}L_{hl}L_{km}, \tag{11}$$

where ε_{ihk} are the components of Ricci's alternator and summation is understood on repeated indices (see, for example, Chapter 2 of [33]). Since $\boldsymbol{\nu} = \boldsymbol{e}_1 \times \boldsymbol{e}_2$, by Equation (9) we can also rewrite Equation (8) as

$$N(\boldsymbol{n}) = \frac{1}{4\pi}\int_{\mathscr{S}} \boldsymbol{n} \cdot (\nabla\boldsymbol{n})^*\boldsymbol{\nu}\, \mathrm{d}a. \tag{12}$$

According to [5], this formula was first obtained in [34]. Here again $(\nabla\boldsymbol{n})^*$ could be replaced by $(\nabla_{s}\boldsymbol{n})^*$ to make it clear that also in Equation (12) $N(\boldsymbol{n})$ depends only on $\boldsymbol{n}_{\mathscr{S}}$. This conclusion could also be reached directly from Equation (12), ignoring that it derives from Equation (8), as

$$\boldsymbol{\nu} = (\boldsymbol{\nu} \otimes \boldsymbol{\nu})\boldsymbol{\nu} = (\mathbf{I} - \boldsymbol{\nu} \otimes \boldsymbol{\nu})^*\boldsymbol{\nu}$$

and then

$$(\nabla\boldsymbol{n})^*\boldsymbol{\nu} = (\nabla\boldsymbol{n})^*(\mathbf{I} - \boldsymbol{\nu}\otimes\boldsymbol{\nu})^*\boldsymbol{\nu} = (\nabla_{\mathrm{s}}\boldsymbol{n})^*\boldsymbol{\nu},$$

since by a classical result (see, for example, p 261 of [35]),

$$(\mathbf{AB})^* = \mathbf{A}^*\mathbf{B}^*, \tag{13}$$

for any two second-rank tensors **A** and **B**. Note that when both **A** and **B** are invertible Equation (13) follows directly from Equation (10).

In the following we shall indifferently employ either Equation (8) or (12) to compute the topological charge of a nematic point defect. A remarkable property of $N(\boldsymbol{n})$ is its additivity: if the surface $\mathscr{S}$ encloses more than one point defect, the topological charge of the director field is the sum of the individual topological charges that Equations (8) and (12) deliver when applied to surfaces that enclose a single point defect. For a pair of defects, this easily follows from computing the integral in Equation (12) on a dumb-bell surface $\mathscr{S}$ that encloses both defects within spheres connected through a slender cylinder: in the limit as the cylinder's radius shrinks to nothing, the integral in Equation (12) tends to the sum of the charges entrapped by the spheres.

As pointed out in Section VII.E.3 of [4], the topological charge $N(\boldsymbol{n})$ does *not* identify uniquely the topological class to which a point defect belongs: point defects with opposite topological charges are indeed topologically equivalent, as the director field describing the one can continuously be transformed into the director field describing the other. Thus, strictly speaking, the topological classes of non-trivial nematic point defects can be classified in terms of $|N(\boldsymbol{n})|$, and the positive integers would suffice to describe all of them. Perhaps, the easiest illustration of such a redundancy of $N(\boldsymbol{n})$ in classifying point defects is obtained by reversing the sign of $\boldsymbol{n}$, which does not effectively change the nematic director field, but reverses the sign of $N(\boldsymbol{n})$. This follows immediately from Equation (8) and also from Equation (12) upon noting that $(-\mathbf{I})^* = \mathbf{I}$.

Although it may not serve the purpose of classifying nematic point defects, still the topological charge $N(\boldsymbol{n})$ is a powerful tool; actually, our development will be built on its additivity. When defects with opposite topological charges occur in pairs, the overall director field has zero total charge and so it belongs to the same topological class as a continuous, defect-free director field. Thus, pairs of defects with opposite topological charges can be annihilated as a result of a continuous transformation, leaving behind no trace of their existence. In the following section, we shall introduce a transformation that reverses the sign of the topological charge of a point defect by acting on the director field $\boldsymbol{n}$ in a less trivial way than just reversing it into $-\boldsymbol{n}$; our major objective will be to see how this transformation affects the forces $\boldsymbol{f}^{(\mathrm{e})}$ and $\boldsymbol{f}^{(\mathrm{r})}$ introduced in the preceding section. The sign of the topological charge will play a role in these forces, despite the fact that defects with opposite topological charges belong to one and the same topological class.

4. Parity conjugation

Any defect is related to another defect, conjugated to it, by means of a *parity transformation*. For any fixed unit vector $\boldsymbol{e}$, such a parity transformation is given by

$$\mathbf{R} = \mathbf{I} - 2\boldsymbol{e} \otimes \boldsymbol{e} \tag{14}$$

and it defines for any director field $\boldsymbol{n}$ a conjugated field $\bar{\boldsymbol{n}}$ via

$$\bar{\boldsymbol{n}} := \mathbf{R}\boldsymbol{n}. \tag{15}$$

We note that $\mathbf{R}$ is an orthogonal transformation with $\det \mathbf{R} = -1$, and since it is also symmetric, it yields indeed a parity transformation, $\mathbf{R}^2 = \mathbf{I}$, so that

$$\boldsymbol{n} = \mathbf{R}\bar{\boldsymbol{n}}.$$

Let the topological charge $N(\bar{\boldsymbol{n}})$ of the parity-conjugated defect be computed as in either Equation (8) or (12). It follows from Equation (15) that

$$(\nabla\bar{\boldsymbol{n}})^* = (\mathbf{R}\nabla\boldsymbol{n})^* = \mathbf{R}^*(\nabla\boldsymbol{n})^*,$$

since $\mathbf{R}$ is constant. Moreover, by Equation (10), $\mathbf{R}^* = (\det \mathbf{R})\ \mathbf{R} = -\mathbf{R}$, and we easily obtain from Equation (12) that

$$\begin{aligned} N(\bar{\boldsymbol{n}}) &= \frac{1}{4\pi}\int_{\mathscr{S}} \bar{\boldsymbol{n}} \cdot (\nabla\bar{\boldsymbol{n}})^* \boldsymbol{\nu}\, \mathrm{d}a \\ &= -\frac{1}{4\pi}\int_{\mathscr{S}} \mathbf{R}\boldsymbol{n} \cdot \mathbf{R}(\nabla\boldsymbol{n})^* \boldsymbol{\nu}\, \mathrm{d}a = -N(\boldsymbol{n}). \end{aligned} \tag{16}$$

This shows that $N(\bar{\boldsymbol{n}}) = -N(\boldsymbol{n})$, independent of the choice of unit vector $\boldsymbol{e}$.

The classical example of a pair of parity-conjugated defects is that of the *radial* and *hyperbolic* hedgehogs. The radial hedgehog is represented by the director field $\boldsymbol{n}_{\mathrm{R}} := \boldsymbol{e}_r$, where $\boldsymbol{e}_r$ is the radial unit vector of spherical coordinates; the hyperbolic hedgehog is thus represented by $\boldsymbol{n}_{\mathrm{H}} := \bar{\boldsymbol{n}}_{\mathrm{R}} = \boldsymbol{R}\boldsymbol{e}_r$, where $\mathbf{R}$ is as in Equation (14). It is easily seen that $N(\boldsymbol{n}_{\mathrm{R}}) = 1$ and $N(\boldsymbol{n}_{\mathrm{H}}) = -1$.

We now examine how the elastic and reorientational viscous forces behave under the parity transformation. This will allow us to make qualitative predictions on the dynamics of the annihilation of a pair of parity-conjugated defects. To this end, we consider defects with director configurations $\boldsymbol{n}$ that exhibit an axis of symmetry $\boldsymbol{e}$, we use the parity transformation in Equation (14) defined by that axis $\boldsymbol{e}$ and we assume that the defects move along that same axis $\boldsymbol{e}$. By symmetry, the forces in Equations (4) and (5) then lie along $\boldsymbol{e}$, and so they take the forms

$$\boldsymbol{f}^{(\mathrm{e})} = f^{(\mathrm{e})}\boldsymbol{e} \quad \text{and} \quad \boldsymbol{f}^{(\mathrm{r})} = f^{(\mathrm{r})}\boldsymbol{e}. \tag{17}$$

Recalling that $\nabla\bar{\boldsymbol{n}} = \mathbf{R}\nabla\boldsymbol{n}$, the elastic stress $\bar{\mathbf{T}}^{(\mathrm{e})}$ in the configuration $\bar{\boldsymbol{n}}$ is found to be

$$\begin{aligned}\bar{\mathbf{T}}^{(\mathrm{e})} &= \frac{1}{2}K(\nabla\bar{\boldsymbol{n}})^2\mathbf{I} - K(\nabla\bar{\boldsymbol{n}})^T(\nabla\bar{\boldsymbol{n}}) \\ &= \frac{1}{2}K(\mathbf{R}\nabla\boldsymbol{n})^2\mathbf{I} - K(\nabla\boldsymbol{n})^T\mathbf{R}\mathbf{R}(\nabla\boldsymbol{n}) \\ &= \frac{1}{2}K(\nabla\boldsymbol{n})^2\mathbf{I} - K(\nabla\boldsymbol{n})^T(\nabla\boldsymbol{n}) = \mathbf{T}^{(\mathrm{e})}.\end{aligned} \tag{18}$$

It follows that $\bar{\boldsymbol{f}}^{(\mathrm{e})} = \boldsymbol{f}^{(\mathrm{e})}$. This is a special property of the one-constant approximation in Equation (1) and does not hold for more general elastic energy densities.

To evaluate the reorientational viscous force, notice that $\partial\bar{\boldsymbol{n}}/\partial t = \mathbf{R}\partial\boldsymbol{n}/\partial t$ so that $\bar{\mathbf{T}}^{(\mathrm{r})} = \mathbf{R}\mathbf{T}^{(\mathrm{r})}\mathbf{R}$. The scalar force $\bar{f}^{(\mathrm{r})}$ is then found to be

$$\begin{aligned}\bar{f}^{(\mathrm{r})} &= \bar{\boldsymbol{f}}^{(\mathrm{r})} \cdot \boldsymbol{e} = \int_{\partial\mathscr{B}} (\mathbf{R}\mathbf{T}^{(\mathrm{r})}\mathbf{R}\boldsymbol{\nu}) \cdot \boldsymbol{e}\,\mathrm{d}a \\ &= -\int_{\partial\mathscr{B}} (\mathbf{T}^{(\mathrm{r})}\mathbf{R}\boldsymbol{\nu}) \cdot \boldsymbol{e}\,\mathrm{d}a \\ &= -\boldsymbol{f}^{(r)} \cdot \boldsymbol{e} + 2\int_{\partial\mathscr{B}} (\boldsymbol{e}\cdot\boldsymbol{\nu})(\mathbf{T}^{(\mathrm{r})}\boldsymbol{e}) \cdot \boldsymbol{e}\,\mathrm{d}a = -f^{(\mathrm{r})},\end{aligned} \tag{19}$$

where we have used $\mathbf{R}\boldsymbol{e} = -\boldsymbol{e}$, the definition of $\mathbf{R}$ and the fact that $\mathbf{T}^{(\mathrm{r})}$ is skew symmetric. In [15, 17], the authors made the conjecture that $\mathbf{T}^{(\mathrm{r})} = -\bar{\mathbf{T}}^{(\mathrm{r})}$. However, it is evident from Equation (19) that the anti-symmetry is a property of the reorientational viscous *force* and in general not of the stress.

In defect annihilation, a defect and its parity-conjugated companion approach each other and eventually a defect free state ensues. The elastic and reorientational viscous forces on the defects would induce backflow, which in view of Equations (18) and (19) would be clearly non-symmetric. For a pair of annihilating defects, the situation is as sketched in Figure 1. The defect on the left, $\boldsymbol{n}_2$, is obtained from the one on the right, $\boldsymbol{n}_1$, by applying both the parity transformation $\mathbf{R}$ in $\mathbb{S}^2$, as shown in Equation (15), and the mirror reflection in space through the mid-plane $\Pi_{\boldsymbol{e}}$ between the defects, represented by

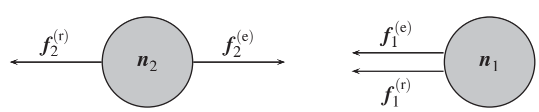

Figure 1. Elastic and viscous forces acting on a defect pair. The elastic forces set both defects in motion towards one another, and the reorientational viscous forces speed up one defect and slow down the other.

$$(p - o) \mapsto \mathbf{R}(p - o),$$

for all points p in space and $o \in \Pi_{\boldsymbol{e}}$. Thus, in view of Equations (17), (18) and (19), the elastic and viscous forces $\boldsymbol{f}_2^{(\mathrm{e})}$ and $\boldsymbol{f}_2^{(\mathrm{r})}$ acting on $\boldsymbol{n}_2$ are related to the corresponding forces $\boldsymbol{f}_1^{(\mathrm{e})}$ and $\boldsymbol{f}_1^{(\mathrm{r})}$ acting on $\boldsymbol{n}_1$ through the relations

$$\boldsymbol{f}_2^{(\mathrm{e})} = -\boldsymbol{f}_1^{(\mathrm{e})} \text{ and } \boldsymbol{f}_2^{(\mathrm{r})} = \boldsymbol{f}_1^{(\mathrm{r})}. \tag{20}$$

The elastic forces drive the annihilation process by dragging the defects towards each other, and in this process the resulting reorientational viscous forces accelerate one defect and slow down the other. We examine in the following section the way in which the reorientational viscous force and its sign depend on the topological charge of the defect.

5. Combed point defects

To obtain an analytical estimate of the reorientational viscous force that acts on a moving defect, we consider equilibrium defect configurations, that is, configurations that are minimisers of the elastic free energy in Equation (1). This entails two seemingly severe limitations. First, for equilibrium configurations with free, unpinned defects, the elastic force vanishes identically [29], and so there would be nothing to set the defect in motion in the first place. Secondly, a moving defect can be expected to experience a dynamical deformation. However, since a moving defect and its stationary equilibrium counterpart are in the same topological defect class, it stands to reason that the reorientational viscous force in our somehow artificial scenario is a good approximation to that experienced by a real moving defect. In particular, our simplified model should predict correctly the dependence of the force on the topological nature of the defect.

5.1 *Director field*

We now consider point defects with a director field that minimises the free energy. A class of defects of this type was first described by Saupe [28]. Here, we consider the larger class of solutions studied in [23].

We start by introducing spherical coordinates both in space and for the director orientation. Following the notation of [28], we write the director $\boldsymbol{n}$ in terms of its azimuthal angle ϑ and its polar angle φ according to

$$\boldsymbol{n} = \sin\vartheta\cos\varphi\boldsymbol{e}_x + \sin\vartheta\sin\varphi\boldsymbol{e}_y + \cos\vartheta\boldsymbol{e}_z \tag{21}$$

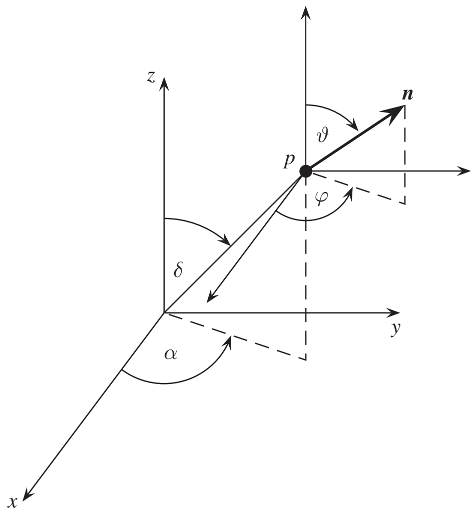

Figure 2. Spherical coordinates for space and orientation: at any point with coordinates (r, α, δ) the director orientation is given in terms of the polar and azimuthal angles ϑ and φ.

and we express any point p in space in terms of its polar angle δ, its azimuthal angle α and its distance from the origin r (see Figure 2).

Then the Cartesian unit vectors $(\boldsymbol{e}_x, \boldsymbol{e}_y, \boldsymbol{e}_z)$ and the local frame $(\boldsymbol{e}_r, \boldsymbol{e}_\delta, \boldsymbol{e}_\alpha)$ are connected by the following relations:

$$\boldsymbol{e}_r = \sin\delta\cos\alpha\boldsymbol{e}_x + \sin\delta\sin\alpha\boldsymbol{e}_y + \cos\delta\boldsymbol{e}_z, \tag{22a}$$

$$\boldsymbol{e}_\delta = \cos\delta\cos\alpha\boldsymbol{e}_x + \cos\delta\sin\alpha\boldsymbol{e}_y - \sin\delta\boldsymbol{e}_z, \tag{22b}$$

$$\boldsymbol{e}_\alpha = -\sin\alpha\boldsymbol{e}_x + \cos\alpha\boldsymbol{e}_y \tag{22c}$$

and

$$\boldsymbol{e}_x = \sin\delta\cos\alpha\boldsymbol{e}_r + \cos\delta\cos\alpha\boldsymbol{e}_\delta - \sin\alpha\boldsymbol{e}_\alpha, \tag{23a}$$

$$\boldsymbol{e}_y = \sin\delta\sin\alpha\boldsymbol{e}_r + \cos\delta\sin\alpha\boldsymbol{e}_\delta + \cos\alpha\boldsymbol{e}_\alpha, \tag{23b}$$

$$\boldsymbol{e}_z = \cos\delta\boldsymbol{e}_r - \sin\delta\boldsymbol{e}_\delta. \tag{23c}$$

We look for director fields that are both independent of r and cylindrically symmetric around the z-axis. For such a director field, the z-component of Equation (21) cannot depend on α and so ϑ is a function of δ only, $\vartheta = \vartheta(\delta)$. We make the additional assumption that the defect structure is not twisted along the z-axis, that is, we assume that $\varphi = \varphi(\alpha)$ so that the normalised projection $\mathbf{n}_\perp \in \mathbb{S}^2$ of the director field $\boldsymbol{n}$ on the xy-plane is the same for all z. The gradients of ϑ and φ then take the simple forms

$$\nabla\vartheta = \frac{\vartheta'}{r}\boldsymbol{e}_\delta \quad \text{and} \quad \nabla\varphi = \frac{\varphi'}{r\sin\delta}\boldsymbol{e}_\alpha. \tag{24}$$

With this, the gradient of $\boldsymbol{n}$ becomes

$$\begin{aligned}\nabla\boldsymbol{n} = {}& \boldsymbol{e}_x \otimes \left(\cos\vartheta\cos\varphi\frac{\vartheta'}{r}\boldsymbol{e}_\delta - \sin\vartheta\sin\varphi\frac{\varphi'}{r\sin\delta}\boldsymbol{e}_\alpha\right) \\ & + \boldsymbol{e}_y \otimes \left(\cos\vartheta\sin\varphi\frac{\vartheta'}{r}\boldsymbol{e}_\delta + \sin\vartheta\cos\varphi\frac{\varphi'}{r\sin\delta}\boldsymbol{e}_\alpha\right) \\ & - \sin\vartheta\frac{\vartheta'}{r}\boldsymbol{e}_z \otimes \boldsymbol{e}_\delta.\end{aligned} \tag{25}$$

With the aid of Equation (8), we can now compute the topological charge of a defect represented as in Equation (21). We take $\mathscr{S}$ as a sphere of radius a centred at the origin, and we choose $\boldsymbol{e}_\delta$ and $\boldsymbol{e}_\alpha$ as the two vectors in the tangent plane to $\mathscr{S}$ corresponding to $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ in Equation (8). We then obtain from Equations (25), (22c) and (22b) that

$$\begin{aligned}(\nabla\boldsymbol{n})\boldsymbol{e}_\delta &= \frac{1}{r}\vartheta'(\cos\vartheta\cos\varphi\boldsymbol{e}_x + \cos\vartheta\sin\varphi\boldsymbol{e}_y - \sin\vartheta\boldsymbol{e}_z), \\ (\nabla\boldsymbol{n})\boldsymbol{e}_\alpha &= \frac{1}{r\sin\delta}\varphi'\sin\vartheta(-\sin\varphi\boldsymbol{e}_x + \cos\varphi\boldsymbol{e}_y),\end{aligned}$$

whence, by Equation (21), it follows that

$$\boldsymbol{n}\cdot(\nabla\boldsymbol{n})\boldsymbol{e}_\delta \times (\nabla\boldsymbol{n})\boldsymbol{e}_\alpha = \frac{1}{r^2\sin\delta}\vartheta'\varphi'\sin\vartheta.$$

We then readily arrive at

$$\begin{aligned}N(\boldsymbol{n}) &= \frac{1}{4\pi}\int_0^\pi a\sin\delta\,\mathrm{d}\delta\int_0^{2\pi} a\frac{\sin\vartheta}{a^2\sin\delta}\frac{\mathrm{d}\vartheta}{\mathrm{d}\delta}\frac{\mathrm{d}\varphi}{\mathrm{d}\alpha}\mathrm{d}\alpha \\ &= \frac{1}{4\pi}[\varphi(2\pi) - \varphi(0)][\cos\vartheta(0) - \cos\vartheta(\pi)].\end{aligned} \tag{26}$$

At equilibrium, $\Delta\boldsymbol{n}$ has to be parallel to $\boldsymbol{n}$, where Δ is the Laplace operator, that is, the equilibrium equation is $(\mathbf{I} - \boldsymbol{n}\otimes\boldsymbol{n})\,\Delta\boldsymbol{n} = \boldsymbol{0}$. An explicit computation shows that

$$\begin{aligned}& r^2(\Delta\boldsymbol{n} - (\Delta\boldsymbol{n}\cdot\boldsymbol{n})\boldsymbol{n}) \\ &\quad = \cos\vartheta\cos\varphi\left(\vartheta'' - \frac{\tan\vartheta\tan\varphi}{\sin^2\delta}\varphi'' \right. \\ &\qquad\qquad \left. + \cot\delta\vartheta' - \frac{\sin\vartheta\cos\vartheta}{\sin^2\delta}\varphi'^2\right)\boldsymbol{e}_x \\ &\qquad + \cos\vartheta\sin\varphi\left(\vartheta'' - \frac{\tan\vartheta\cot\varphi}{\sin^2\delta}\varphi'' \right. \\ &\qquad\qquad \left. + \cot\delta\vartheta' - \frac{\sin\vartheta\cos\vartheta}{\sin^2\delta}\varphi'^2\right)\boldsymbol{e}_y \\ &\qquad - \sin\vartheta\left(\vartheta'' + \cot\delta\vartheta' - \frac{\sin\vartheta\cos\vartheta}{\sin^2\delta}\varphi'^2\right)\boldsymbol{e}_z.\end{aligned} \tag{27}$$

This can be identically zero only when $\varphi'' = 0$ so that

$$\varphi = s\alpha + \varphi_0 \quad \text{with} \quad s \in \mathbb{Z}, \quad \varphi_0 \in [0, 2\pi], \tag{28}$$

where $s \in \mathbb{Z}$ follows from the requirement that $\boldsymbol{n}_\perp|_{\alpha=0} = \boldsymbol{n}_\perp|_{\alpha=2\pi}$ [1]. With φ given by Equation (28), $\varphi'^2 = s^2$, and from all three components of Equation (27) we arrive at the same differential equation for ϑ:

$$\sin^2\delta\vartheta'' + \sin\delta\cos\delta\vartheta' - s^2\sin\vartheta\cos\vartheta = 0. \tag{29}$$

Equation (29) can be solved by using the substitutions

$$t := \tan\frac{\vartheta}{2} \quad \text{and} \quad \tau := \tan\frac{\delta}{2}. \tag{30}$$

These lead to

$$\left(1+t^2\right)\tau^2\ddot{t} - 2t\tau^2\dot{t}^2 + \left(1+t^2\right)\tau\dot{t} - s^2\left(1-t^2\right)t = 0, \tag{31}$$

where the dot denotes differentiation with respect to τ. This equation has a solution of the form $t = A\tau^\beta$ with $\beta^2 = s^2$, so that

$$\tan\frac{\vartheta}{2} = A_\pm\left(\tan\frac{\delta}{2}\right)^{\pm|s|}. \tag{32}$$

By computing Equation (26) on a solution given by Equations (28) and (32), we easily find that the topological charge of the defect is

$$N(\boldsymbol{n}) = \pm s, \tag{33}$$

where the choice of either sign is the same as in the exponent of the right-hand side of Equation (32).

In [28], Saupe chose $A_\pm = 1$ to obtain defects with mirror symmetry with respect to the xy-plane. However, it proves very interesting to consider also the case with general A, which leads to *combed defects* [23]. First, notice that changing $-|s|$ into $+|s|$ leaves the director field unchanged when A is changed into $-1/A$ at the same time:

$$A\left(\tan\frac{\delta}{2}\right)^{-|s|} = \tan\frac{\vartheta}{2}$$
$$\Rightarrow -A^{-1}\left(\tan\frac{\delta}{2}\right)^{|s|} = -\cot\frac{\vartheta}{2} = \tan\frac{\vartheta-\pi}{2},$$

and changing ϑ by π merely sends $\boldsymbol{n}$ into $-\boldsymbol{n}$ in Equation (21). If $\boldsymbol{n}$ is identified with $-\boldsymbol{n}$, it is therefore sufficient to consider only the solutions with $+|s|$, which we will henceforth do.

The parity transformation in Equation (14) with $\boldsymbol{e} = \boldsymbol{e}_z$ can now simply be realised by replacing A by $-A$, which by Equation (32) maps ϑ to $-\vartheta$, and so, by Equation (21), maps $\boldsymbol{n}$ to $-\bar{\boldsymbol{n}}$. In this case, the transformation $A \mapsto -A$ does not affect the topological charge of $\boldsymbol{n}$ because it also entails a director inversion. This clearly agrees with Equation (26), according to which $N(\boldsymbol{n})$ is independent of A.

Since both the elastic and viscous forces $\boldsymbol{f}^{(e)}$ and $\boldsymbol{f}^{(r)}$ on a defect are invariant under inversion of $\boldsymbol{n}$, the transformation $A \mapsto -A$ has exactly the same effect on them as the parity transformation in Equation (14) with $\boldsymbol{e} = \boldsymbol{e}_z$.

It is worth noting that for combed point defects the parity transformation may be trivial. For example, this is the case for $s = -1$, as shown in Appendix A. As a consequence of Equation (19), the reorientational viscous force $\boldsymbol{f}^{(r)}$ acting on this defect must vanish.

As mentioned before, when $A = \pm 1$, a defect given by Equation (32) is mirror-symmetric with respect to the xy-plane. The mapping $A \mapsto 1/A$ sends a defect into its mirror image with respect to the xy-plane, $\boldsymbol{n} \mapsto \tilde{\boldsymbol{n}}$, and so it reverses the direction of the combing. If $\tan\frac{\vartheta}{2} = A\left(\tan\frac{\delta}{2}\right)^{|s|}$, then

$$\tan\frac{\tilde{\vartheta}}{2} = A^{-1}\left(\tan\frac{\delta}{2}\right)^{|s|} \Leftrightarrow \cot\frac{\tilde{\vartheta}}{2} = A\cot\left(\frac{\delta}{2}\right)^{|s|}$$
$$\Leftrightarrow \tan\frac{\pi-\tilde{\vartheta}}{2} = A\left(\tan\frac{\pi-\delta}{2}\right)^{|s|},$$

which implies that $\tilde{\vartheta}(\delta) = \pi - \vartheta(\pi - \delta)$, that is, $\tilde{n}_z(x, y, z) = -n_z(x, y, -z)$.

Figure 3 shows the integral lines on the zx-plane of the field $\boldsymbol{n}$ in Equation (21) when $s = 1$ and $\varphi_0 = 0$ in Equation (28); the parameter A takes the values $-\frac{1}{2}$, -2, $\frac{1}{2}$ and 2 to illustrate the effects of the transformations $A \mapsto 1/A$ and $A \mapsto -A$ discussed previously. These graphs show why these defects are said to be *combed*.

5.2 Free energy

We now compute the free energy of the equilibrium director fields in Equations (21). For functions ϑ (δ) and φ (α), from Equations (21) and (24) we find that

$$|\nabla\boldsymbol{n}|^2 = \frac{1}{r^2}\left(\vartheta'^2 + \frac{\sin^2\vartheta}{\sin^2\delta}\varphi'^2\right). \tag{34}$$

An expression for ϑ' can be obtained by implicit differentiation of Equation (32) with respect to δ:

$$\vartheta' = A|s|\frac{\left(1+\tan^2\frac{\delta}{2}\right)\tan^{|s|-1}\frac{\delta}{2}}{1 + A^2\tan^{2|s|}\frac{\delta}{2}}. \tag{35}$$

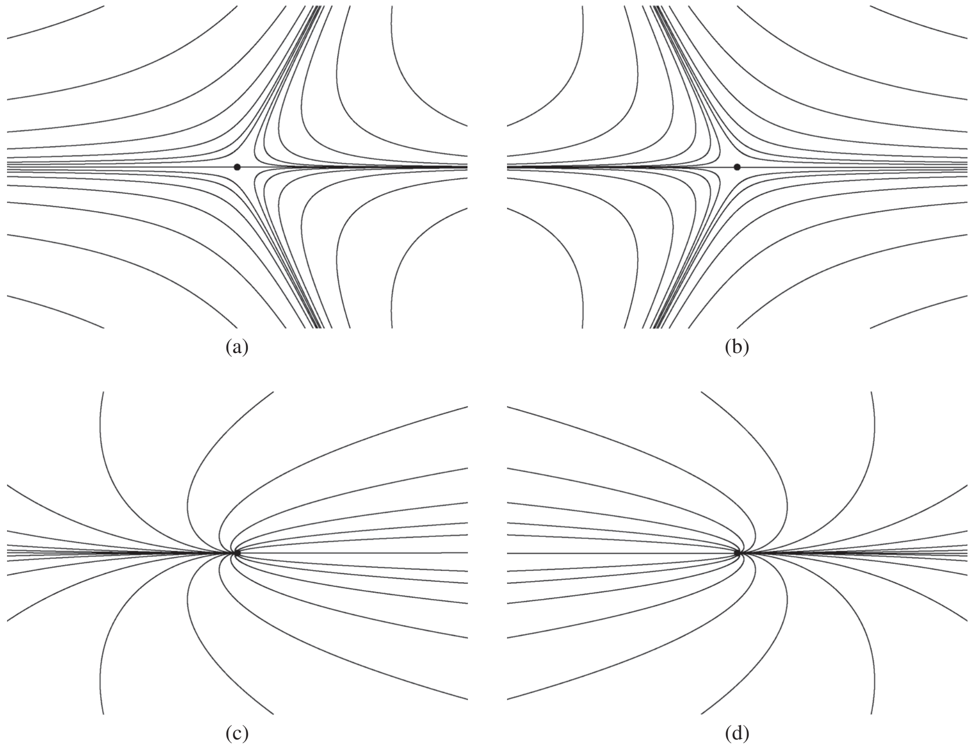

Figure 3. Integral lines on the zx-plane of the director field $\boldsymbol{n}$ in Equation (21), for $s = 1$, $\varphi_0 = 0$ in Equation (28), and (a) $A = -2$, (b) $A = -\frac{1}{2}$, (c) $A = \frac{1}{2}$ and (d) $A = 2$. A dot marks the point where the director field is discontinuous.

While φ' is simply s, making use of the identity $\sin\vartheta = 2\tan\frac{\vartheta}{2}/\left(1+\tan^2\frac{\vartheta}{2}\right)$ and the equivalent one for $\sin\delta$ shows that

$$\frac{\sin\vartheta}{\sin\delta} = A\frac{\left(1+\tan^2\frac{\delta}{2}\right)\tan^{|s|-1}\frac{\delta}{2}}{1+A^2\tan^{2|s|}\frac{\delta}{2}} \tag{36}$$

and so both terms on the right-hand side of Equation (34) yield the same contribution, independent of α. Hence, the free energy density of Equation (1) takes the form

$$\frac{1}{2}K|\nabla\boldsymbol{n}|^2 = \frac{K}{r^2}\vartheta'^2. \tag{37}$$

In particular, it follows from Equations (37) and (35) that for $|s| = 1$, along the z-axis,

$$\frac{1}{2}K|\nabla\boldsymbol{n}|^2 = \frac{K}{z^2}\begin{cases} A^2 & z > 0 \\ \frac{1}{A^2} & z < 0. \end{cases}$$

Thus, when $|A| > 1$, the distortion caused by the defect is concentrated in the region where $z > 0$, and when $|A| < 1$, the distortion caused by the defect is concentrated in the region where $z < 0$.

Moreover, the free energy stored in a ball of radius R with the defect at its centre is found as

$$\begin{aligned} F &= K\int_0^R\int_0^{2\pi}\int_0^{\pi}\frac{\vartheta'^2}{r^2}r^2\sin\delta\,\mathrm{d}\delta\,\mathrm{d}\alpha\,\mathrm{d}r \\ &= 4\pi KRA^2s^2\int_0^{\pi}\frac{\tan^{2|s|-1}\frac{\delta}{2}+\tan^{2|s|+1}\frac{\delta}{2}}{\left(1+A^2\tan^{2|s|}\frac{\delta}{2}\right)^2}\,\mathrm{d}\delta. \end{aligned} \tag{38}$$

The last integral can be evaluated using the substitution $\tau = \tan\frac{\delta}{2}$, and we find

$$F = 4\pi KR|s|. \tag{39}$$

The result in Equation (39) shows that the free energy is proportional to the defect strength $|s|$ and that it is *independent of A*. First, this shows that any defect has the same free energy as its conjugated counterpart. Furthermore, at least in the one-constant approximation, an ideally symmetric defect with $|A| = 1$ has the same elastic free energy as a deformed one with $|A| \neq 1$.

In particular, in the limiting cases as $|A| \to 0$ and $|A| \to \infty$ the director field becomes homogeneous everywhere except for an infinitesimal tubular region around the positive (or negative) z-axis; see Figure 4.

This explains the frequent occurrence in Schlieren textures of $s = 1$ disclination lines joining two point defects: this configuration indeed minimises the overall free energy. This same limit can also be reached by

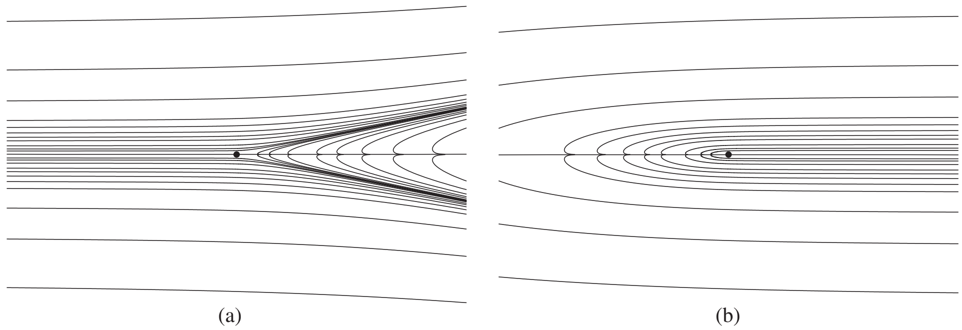

Figure 4. Integral lines as in Figure 3, for (a) $A = -50$ and (b) $A = 1/50$, illustrating how the director distortion is concentrated along a narrow tubular region on one side of the z-axis, the other side being covered when A is transformed into $1/A$.

scaling another family of equilibrium director fields, which in some recent literature (see, for example, [36]), have been called *skyrmions*, from the Skyrme model for concentrated structures in nuclear physics [37], while they are formally equivalent to the *escaped* director fields of Cladis and Kléman [38]. In [36], these equilibrium fields have been studied for the general energy density with three unequal elastic constants, K_1, K_2 and K_3, that reduces to Equation (1) for $K_1 = K_2 = K_3 = K$. A remarkable result of [36] is that when all K are not equal only skyrmions with $s = 1$ are equilibrium solutions. The occurrence of one and the same limit for both skyrmions and combed defects suggests that for unequal elastic constants the latter might also exist at equilibrium only for $s = 1$, a conjecture that deserves further consideration.

While by Equation (39) a single defect has, in principle, infinite energy (in practice only limited by the container size), if a second defect is present the two can pair up without any expenditure of elastic energy. If the distance between the two defects is $L = 2R$, the total free energy then becomes $F = 4\pi KL|s|$ with the director field away from the defects being homogeneous, a conclusion anticipated in [39] with an intuitive argument. This mechanism realises the absolute minimiser of the free energy: it was shown that for equal elastic constants the minimum energy of a set of point defects with topological charge $\pm s$ is $4\pi KL|s|$, where L is the minimal total length of dipoles formed by pairing the point defects [40–42]. This conclusion was further extended in [43] to the general case of unequal elastic constants, arriving at a formula for the minimum elastic energy that was later rediscovered in [36].

It should, finally, be noted that for any finite $A \neq 0$ two matched director fields described by Equations (28) and (32) would not be true minimisers of the free energy for a pair of point defects. Unlike for disclinations in the two-dimensional case, for point defects in three dimensions there is no superposition principle that would allow the solutions for two individual defects to be added.

5.3 Reorientational viscous force

To assess the reorientational viscous force, we assume that a defect is *drifting* with instantaneous velocity $\boldsymbol{u}$ in a given direction so that the director field at a point p at time $t + \varepsilon$ is given by

$$\boldsymbol{n}(p, t + \varepsilon) = \boldsymbol{n}(p - \varepsilon \boldsymbol{u}, t). \tag{40}$$

By no means is $\boldsymbol{u}$ to be thought of as being constant in time. It follows that

$$\frac{\partial \boldsymbol{n}}{\partial t} = -(\nabla \boldsymbol{n})\boldsymbol{u}, \tag{41}$$

so that $\frac{\partial \boldsymbol{n}}{\partial t} = \overset{\circ}{\boldsymbol{n}}$ is, in this case, completely determined by the director field, $\boldsymbol{n}$, and the drift velocity, $\boldsymbol{u}$. The reorientational viscous force, $\boldsymbol{f}^{(\mathrm{r})}$, can then in principle be found explicitly by computing the integral in Equation (5). We want to compute it for a combed point defect. If the defect drifts along its symmetry axis in the z-direction with velocity $\boldsymbol{u} = u\boldsymbol{e}_z$ and the force is computed on a ball with radius r_c centred on the defect, by symmetry it must be in the z-direction, $\boldsymbol{f}^{(\mathrm{r})} = f^{(\mathrm{r})}\boldsymbol{e}_z$. From Equation (5) with Equations (3) and (41),

$$f^{(\mathrm{r})} = \boldsymbol{e}_z \cdot \boldsymbol{f}^{(\mathrm{r})} = \frac{1}{2}\gamma_1 u \int_0^{2\pi} \int_0^{\pi} [(\boldsymbol{n} \cdot \boldsymbol{e}_r)(\boldsymbol{e}_z \cdot (\nabla \boldsymbol{n})\boldsymbol{e}_z) - (\boldsymbol{n} \cdot \boldsymbol{e}_z)(\boldsymbol{e}_r \cdot (\nabla \boldsymbol{n})\boldsymbol{e}_z)] r_c^2 \sin\delta \, \mathrm{d}\delta \, \mathrm{d}\alpha, \tag{42}$$

which turns out to be

$$f^{(\mathrm{r})} = \frac{1}{2}\gamma_1 u r_c \int_0^{2\pi} \int_0^{\pi} \vartheta' \cos(\varphi - \alpha) \sin^3 \delta \, \mathrm{d}\delta \, \mathrm{d}\alpha. \tag{43}$$

With φ as in Equation (28), $\cos(\varphi - \alpha) = \cos((s-1)\alpha + \varphi_0)$, and carrying out the integration in α yields

$$f^{(r)} = \begin{cases} 0 & s \neq 1 \\ \pi\gamma_1 u r_c \cos\varphi_0 \int_0^\pi \vartheta' \sin^3 \delta \mathrm{d}\delta & s = 1. \end{cases} \tag{44}$$

This shows that the situation for point defects is strikingly different from that for disclinations studied in [26, 27]. Not only is the force not proportional to the topological charge s, it is different from zero only for $s = 1$. Furthermore, the magnitude and sign of $f^{(r)}$ depend on $\cos\varphi_0$ and so can be changed by a continuous local transformation of the director field. In particular, for $\varphi_0 = \pi/2$, the force vanishes.

Our last task is to assess the effect of A in Equation (32) on the force. Since only $s = 1$ is of interest, from Equation (35)

$$\vartheta' = A\frac{1 + \tan^2\frac{\delta}{2}}{1 + A^2\tan^2\frac{\delta}{2}} \tag{45}$$

and then

$$\int_0^\pi \vartheta' \sin^3\delta \, \mathrm{d}\delta = \frac{4A}{(A^2-1)^3}\left(A^4 - 1 - 2A^2\ln A^2\right). \tag{46}$$

Thus, for $s = 1$,

$$f^{(r)} = \pi\gamma_1 u r_c \cos\varphi_0 g(A) \tag{47}$$

with

$$g(A) := \frac{4A}{(A^2-1)^3}(A^4 - 1 - 2A^2\ln A^2). \tag{48}$$

The function g has the symmetry properties

$$g(A) = -g(-A) \quad \text{and} \quad g(A) = g(A^{-1}). \tag{49}$$

This means that the parity transformation of changing A into $-A$ in Equation (32) merely changes the sign of g. Hence the reorientational viscous force on a defect is equal and opposite to the force on its parity-conjugated defect. Reversing the combing direction, $A \mapsto 1/A$, leaves the force unchanged.

The graph of g illustrated in Figure 5 clearly exhibits these properties. The function $g(A)$ approaches zero for $A \to 0$ and $A \to \pm\infty$. Its extrema are attained as $\lim_{A\to\pm1} g(A) = \pm\frac{4}{3}$. This means that the symmetric defects will feel the highest viscous force, while the deformed tubular defects that join two dipoles would see zero viscous force. This means that no symmetric defects should occur in any dynamical situation.

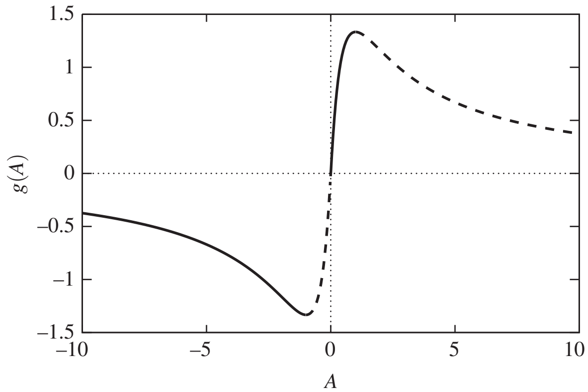

Figure 5. Graph of g against A. Dashed and solid lines correspond to one another through the transformation $A \to -1/A$, while they are exchanged under the transformation $A \to -A$.

6. Conclusions

The dynamics of defect annihilation in nematic liquid crystals is a fascinating problem which challenges the mathematical modeller. Proper numerical solutions of the general governing equations are difficult to obtain and to interpret correctly. One important conclusion of our work is that numerical results obtained in two-dimensional computations for disclinations *cannot* be used to explain the behaviour of point defect dynamics, as an important player such as the reorientational viscous force computed here for combed point defects is completely different from its counterpart computed for disclinations in [26, 27], to the point of vanishing for most values of the topological charge.

In our search for distinctive qualitative features of defect dynamics, we have also reached a conclusion that helps to explain experimental results. Specifically, in the Cladis–Brand experiment [24], the boundary conditions at the capillary wall fix the defect structure so that $s = 1$ and $\varphi_0 = 0$ on the boundary and $\varphi_0 \neq \frac{\pi}{2}$ in the bulk. Since g is odd in A and by Equation (47) $f^{(r)}$ is odd in u, when a defect and its parity-conjugated companion move one towards the other, they suffer the *same* reorientational viscous force; see also Equation (20). In particular, orienting the z-axis opposite to the direction of motion of the radial hedgehog, in the annihilation we have $\boldsymbol{u} = u\boldsymbol{e}_z$ with $u < 0$, and so by Equation (47) the radial hedgehog will be accelerated by the reorientational viscous force and the hyperbolic hedgehog will be slowed down, as was indeed observed in [24].

In general, it would be interesting to see how moving point defects that are free to choose their fine structure will deform dynamically: will they minimise, maximise or try to eliminate the viscous force? This question can, in principle, be answered by numerical computations.

Point defects with $s \neq 1$ are extremely rare animals: because of their high elastic energy, they are not observed in practice. For them we found a vanishing reorientational viscous force. We also conjectured that they may fail to be at equilibrium as soon as the elastic constants fail to be equal to one another.

Note

1. Half-integer values of s are allowed in Equation (28), but they do not lead to point defects. Indeed, changing φ by π leaves $\boldsymbol{n}$ invariant in Equation (21) for the defect-free homogeneous director field $\vartheta \equiv 0$, and it leads to $-\boldsymbol{n}$ when $\vartheta \equiv \frac{\pi}{2}$, which gives line defects.

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Appendix A. Point defects with $s = -1$

It was remarked in [44] that for $s = -1$ the symmetric defect (in our notation, $A = 1$) and its parity-conjugated defect coincide. We show here a slightly more general result.

For point defects of the type considered in Section 5 with $\vartheta = \vartheta(\delta)$ and $s = -1$, $\varphi = -\alpha + \varphi_0$, the conjugated defect $\bar{\boldsymbol{n}}$ can be obtained by rotating the defect $\boldsymbol{n}$ by an angle of $\pi/2$ around the z-axis, i.e.

$$\mathbf{Q}\boldsymbol{n}(r) = -\bar{\boldsymbol{n}}(\mathbf{Q}r), \tag{A1}$$

where $\mathbf{Q} = \boldsymbol{e}_y \otimes \boldsymbol{e}_x - \boldsymbol{e}_x \otimes \boldsymbol{e}_y + \boldsymbol{e}_z \otimes \boldsymbol{e}_z$. To see this, call $\tilde{\alpha} := \alpha - \varphi_0$. Then $\varphi = -\tilde{\alpha}$ and Equation (21) becomes

$$\boldsymbol{n} = \sin\vartheta\cos\tilde{\alpha}\boldsymbol{e}_x - \sin\vartheta\sin\tilde{\alpha}\boldsymbol{e}_y + \cos\vartheta\boldsymbol{e}_z \tag{A2}$$

and correspondingly

$$-\bar{\boldsymbol{n}} = -\sin\vartheta\cos\tilde{\alpha}\boldsymbol{e}_x + \sin\vartheta\sin\tilde{\alpha}\boldsymbol{e}_y + \cos\vartheta\boldsymbol{e}_z. \tag{A3}$$

Since the rotation simply adds $\pi/2$ to α and hence to $\tilde{\alpha}$,

$$\begin{aligned} -\bar{\boldsymbol{n}}(\mathbf{Q}\boldsymbol{r}) = &-\sin\vartheta\cos(\tilde{\alpha}+\frac{\pi}{2})\boldsymbol{e}_x \\ &+ \sin\vartheta\sin(\tilde{\alpha}+\frac{\pi}{2})\boldsymbol{e}_y + \cos\vartheta\boldsymbol{e}_z. \end{aligned} \tag{A4}$$

At the same time,

$$\mathbf{Q}\boldsymbol{n} = \sin\vartheta\sin\tilde{\alpha}\boldsymbol{e}_x + \sin\vartheta\cos\tilde{\alpha}\boldsymbol{e}_y + \cos\vartheta\boldsymbol{e}_z, \tag{A5}$$

and Equations (A4) and (A5) indeed coincide.

This means that as long as symmetry around the z-axis is maintained, all forces in the z-direction on $\boldsymbol{n}$ and $\bar{\boldsymbol{n}}$ must be equal. Since the reorientational viscous forces are equal and opposite it follows that they are zero. This holds for any function $\vartheta(\delta)$.