Continuum Mechanics of Line Defects in Liquid Crystals and Liquid Crystal Elastomers

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Abstract

This paper generalizes the Ericksen-Leslie continuum model of liquid crystals to allow for dynamically evolving line defect distributions. In analogy with recent mesoscale models of dislocations, we introduce fields that represent defects in orientational and positional order through the incompatibility of the director and deformation 'gradient' fields. These fields have several practical implications: first, they enable a clear separation between energetics and kinetics; second, they bypass the need to explicitly track defect motion; third, they allow easy prescription of complex defect kinetics in contrast to usual regularization approaches; and finally, the conservation form of the dynamics of the defect fields has advantages for numerical schemes.

We present a dynamics of the defect fields, motivating the choice physically and geometrically. This dynamics is shown to satisfy the constraints, in this case quite restrictive, imposed by material-frame indifference. The phenomenon of permeation appears as a natural consequence of our kinematic approach. We outline the specialization of the theory to specific material classes such as nematics, cholesterics, smectics and liquid crystal elastomers. We use our aproach to derive new, non-singular, finite-energy planar solutions for a family of axial wedge disclinations.

Keywords: liquid crystals; disclinations; Ericksen-Leslie theory

1 Introduction

Liquid crystals are composed of rod-like molecules. Depending on temperature, chemical composition and other factors, assemblies of the molecules display varying degrees of orientational and positional order. Applied loads such as stress fields cause deformation but also changes in orientation and both these changes cost energy. Hence, the orientation of the molecule is important to elasticity and deformation. Therefore, coarse-grained continuum theories retain orientation information through the director field

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that provides a unit-vector aligned along the long axis of the molecule. The deformations of liquid crystals can then be described through internal energies that include the director field and its gradient as argument [e.g., Ste04]. When the liquid crystal molecules are linked to polymer molecule backbones, director elasticity is strongly coupled to conventional positional elasticity and the internal energy density involves both contributions [e.g., WT07].

Defect-free liquid crystals have been studied for many decades through continuum approaches, most notably the Ericksen-Leslie (EL) [Eri61; Les68] model. The EL model is widely accepted and experimentally well-characterized through the measurement of the various parameters in the model. However, certain types of observed defects such as *disclinations*, where the orientation of the director is ambiguous along curves in the body, cannot be predicted by the EL model, in particular disclinations of strength $\frac{1}{2}$. Such defects, and others such as dislocations and focal conics, have been observed in both static and dynamic situations [e.g., dGP95; Fra58; KF08; SZA06]. In addition, defects in both orientational and positional order (e.g. disclinations and dislocations) are observed in certain types of liquid crystals, e.g. smectics [dGP95].

This paper generalizes the EL dynamical theory of liquid crystals to allow for solid-like behavior as in the liquid crystal elastomer [WT07] phase and deal with defects in the director $(\boldsymbol{n})$ and position $(\boldsymbol{x})$ configurations, including disclinations and dislocations. The defects are viewed as non-singular localizations in physically appropriate fields representing densities of lines carrying vectorial attributes. Being spatial densities, they satisfy balance laws, thus providing a direct geometric route to specify defect dynamics.

The main idea is to allow for smooth incompatibilities in the director and deformation 'gradient' fields, henceforth referred to as the corresponding distortion tensors since they are not globally irrotational (curl-free). We do this by introducing defect fields that represent these incompatibilities. This is an expedient device to deal with topological defects without having to deal with discontinuities in the basic fields $(\boldsymbol{n}, \boldsymbol{x})$ whose generalized gradients could be strongly singular. We emphasize that allowing for smooth, incompatible distortion fields is not the same as smoothing the director/position fields in any sense since no continuous global vector field can be defined whose generalized gradient may be equated to the smooth incompatible distortion field. Rather, roughly speaking, if $\boldsymbol{E}$ is a sufficiently smooth director distortion field on the body, it can be written as

$$\boldsymbol{E} = \operatorname{grad} \boldsymbol{n} + \operatorname{curl} \hat{\boldsymbol{Q}}$$

through a Stokes-Helmholtz decomposition. $\boldsymbol{n}$ is a vector field and $\hat{\boldsymbol{Q}}$ is a solenoidal (divergence-free) second-order tensor field that is directly related to the away-from-gradient defect content of $\boldsymbol{E}$.

Thus, our model works with a director field and an incompatible director distortion field. Therefore, our model has more state variables that the 5-parameter DeGennes $\boldsymbol{Q}$-tensor formalism [dGP95]. However, the director field approach does not immediately allow a kinematic accommodation of the head-to-tail symmetry of liquid crystal molecules, as is readily possible in the $\boldsymbol{Q}$-tensor approach. This generality of the $\boldsymbol{Q}$-tensor approach gives it ability to easily represent defect fields through its spectral decomposition. On the other hand, this makes it difficult to physically motivate an evolution law for $\boldsymbol{Q}$ beyond gradient flows [SKH95] or Rayleigh dissipation principles [SMV04]. There is a formalism for producing an evolution equation for $\boldsymbol{Q}$ based on ideas from kinetic theory [e.g., KLGCC08; YFMW09], originally developed for the flow of dumb-bell shaped polymer molecules [Pra57]. However, this formalism leaves significant unanswered questions of constitutive closure – precisely, the closure law for the fourth moment of the angular orientation distribution function. In contrast, our approach provides a mesoscale model that is based on the dynamics of the director unit vector field and allows precisely defined constitutive

input from either experiment or theory. This physically motivated basis in the director field provides a straightforward route to connect to molecular dynamics or analogous experiments to obtain constitutive input for defect dynamics.

Our point of view relies on the definition of geometrically precise order parameters for posing conservation laws with physically unambiguous ingredients amenable to constitutive input from finer length scales. A defect tensor field is rationalized that has the natural interpretation of a 'vector-valued' two-form[1] that naturally lends itself to integration over surface patches allowing recourse to the standard kinematic tautology "rate of change = flux in + source," to specify dynamics through balance laws. These are made material-specific by the addition of constitutive equations. Admittedly, a great deal rests on accurate modeling of the flux and source terms, but the basic format of such equations of evolution, for a rigorously defined and physically natural spatial density, is a useful kinematic fact. In addition, merely from the kinematical fact that these two-forms can be physically interpreted as a field density of lines, a natural consequence is that their flux admits a velocity that moves the lines, thus allowing defect kinetics to be specified independently from model energetics. By recourse to Coleman-Noll-Gurtin [CN63; CG67] thermodynamic reasoning in spirit, we set up a multiscale, dynamical, PDE model with favorable dissipative properties while allowing for energetic and kinetic input from molecular scales. Also, tying the identity of defects to values of a field has the practical advantage that individual defects do not need to be tracked as discontinuities or singularities in numerical computations.

The model also allows for accommodating the standard Oseen-Zocher-Frank (OZF) [Ose33; Zoc33; Fra58] energy by replacing $\operatorname{grad} \boldsymbol{n} =: \boldsymbol{G}$ by $\boldsymbol{E}$ in that energy density. Since defects can be represented here as non-singular localizations of the director incompatibility field, the OZF energy of the body containing defects can be bounded in the model. As in the crystal elasticity case [e.g., Pei40], it is possible that nonconvexity in the OZF energy is required to obtain localized defect cores. This may be justified for large director distortions (as no elasticity can persist indefinitely), and a physical regularization for avoiding singularities, attributed to extra core energy, is also accommodated. We find it particularly satisfying that our model incorporates defects within OZF orientational elasticity without any additional elasticity related to the 'degree of orientation' variable, a feature in contrast with Ericksen [Eri91] and discussed at some length therein.

The nematic, cholesteric, and smectic (A and C) liquid crystal phases, the nematic and smectic liquid crystal elastomer phases can all be modeled in our formulation by appropriately restricting the kinematics and using standard generalizations of the OZF energy. In the smectic phase, a permeation velocity field appears on purely kinematic grounds. We note that its spatial gradient is conceptually similar to compatible plastic strain rate (e.g. lattice- invariant shears) in crystal plasticity [DP91; Ach04].

A special case of our model is a dissipative, dynamic, nonlinear theory of elasticity with dislocations refining the work in [Ach04; Ach10]. Interestingly, within our setting a unifying mathematical structure emerges for treatment of director incompatibility and dislocation defect evolution. It is characterized in the most simple of circumstances by a scalar equation of the form

$$\phi_t = \frac{|\phi_x|}{B}\left[\epsilon\phi_{xx} + \tau\left(\phi\right)\right]$$

where $0 < \epsilon \ll 1$, $0 < B$ are material parameters and τ is a nonconvex function [Ach10; AMZ10].

We do not provide a comprehensive review of the vast literature relevant to a dynamic model of liquid crystalline materials. Our understanding of liquid crystal materials has greatly benefited from the books

[1] A rigorously defined areal density on a manifold in Euclidean space.

of DeGennes and Prost [dGP95], Stewart [Ste04], Warner and Terentjev [WT07], and [KL03]; the papers of Friedel and Kleman [KF08], Leslie [Les92], Ericksen [Eri91], and Stephen and Straley [SS74]. Beyond practical computation, it is clear that the nonlinear PDE structure that emerges here will benefit from rigorous mathematical analysis to understand the finer points of defect dynamics and microstructure [Tar10]. The mathematics of static defect configurations within a director- based theory has been studied, e.g. [Kin91; LP94; CLV01; GHL$^+$10], and continues to be studied within the $\boldsymbol{Q}$-tensor formalism, e.g. [DGJ98; BZ08; BM09; MZ09]. Dynamics [LL00] and numerical analysis of the EL theory has been studied by [LW00; LW02] and possibly such analyses can be extended to a theory that deals with moving line defects. There is an emerging body of work due to Fried and co-workers [e.g., SSF09] that uses a configurational-force approach to defect dynamics in liquid crystalline materials, and understanding the connections with our approach would be useful.

The paper is organized as follows:

- Section 2 provides notation and some definitions
- Section 3 outlines the balance laws
- Section 4 deals with the geometry and evolution of director line defects
- Section 5 deals with the geometry and evolution of dislocations
- Section 6 summarizes the field equations including those of the defects
- Sections 7 and 8 examine the restrictions imposed by frame-indifference and thermodynamics
- Section 9 outlines the constitutive choices to model various classes of liquid crystal materials
- Section 10 concludes with a discussion
- Appendix A provides a geometric interpretation of the director line defect balance of Section 4
- Appendix B constructs a solution to a family of wedge disclinations for the 1-constant OZF energy

2 Definitions and Notation

A superposed dot on a symbol represents a material time derivative. The statement $a := b$ indicates that a is defined to be equal to b. The summation convention is implied unless otherwise mentioned. We denote by $\boldsymbol{A}\boldsymbol{b}$ the action of the second-order (third-order, fourth-order) tensor $\boldsymbol{A}$ on the vector (second-order tensor, second-order tensor) $\boldsymbol{b}$, producing a vector (vector, second-order tensor). A $\cdot$ represents the inner product of two vectors, a : represents the trace inner product of two second-order tensors (in rectangular Cartesian components, $\boldsymbol{A} : \boldsymbol{B} = A_{ij}B_{ij}$) and matrices and the contraction of the last two indices of a third-order tensor with a second order tensor. The symbol $\boldsymbol{A}\boldsymbol{B}$ represents tensor multiplication of the second-order tensors $\boldsymbol{A}$ and $\boldsymbol{B}$. The notation $(\cdot)_{\text{sym}}$ and $(\cdot)_{\text{skw}}$ represent the symmetric and skew symmetric parts, respectively, of the second order tensor $(\cdot)$. The symbol div represents the divergence, grad the gradient, and $\operatorname{div}\operatorname{grad}$ the Laplacian. The curl operation and the cross product of a second-order tensor

and a vector are defined in analogy with the vectorial case and the divergence of a second-order tensor: for a second-order tensor $\boldsymbol{A}$, a vector $\boldsymbol{v}$, and a spatially constant vector field $\boldsymbol{c}$,

$$\begin{aligned}(\boldsymbol{A}\times\boldsymbol{v})^T\boldsymbol{c}&=\left(\boldsymbol{A}^T\boldsymbol{c}\right)\times\boldsymbol{v}\quad\forall\boldsymbol{c}\\(\operatorname{div}\boldsymbol{A})\cdot\boldsymbol{c}&=\operatorname{div}\left(\boldsymbol{A}^T\boldsymbol{c}\right)\quad\forall\boldsymbol{c}\\(\operatorname{curl}\boldsymbol{A})^T\cdot\boldsymbol{c}&=\operatorname{curl}\left(\boldsymbol{A}^T\boldsymbol{c}\right)\quad\forall\boldsymbol{c}.\end{aligned}$$

In rectangular Cartesian components,

$$\begin{aligned}(\boldsymbol{A}\times\boldsymbol{v})_{im}&=e_{mjk}A_{ij}v_k\\(\operatorname{div}\boldsymbol{A})_i&=A_{ij,j}\\(\operatorname{curl}\boldsymbol{A})_{im}&=e_{mjk}A_{ik,j}.\end{aligned}$$

where e_{mjk} is a component of the third-order alternating tensor $\boldsymbol{X}$. Also, the vector $\boldsymbol{XAB}$ is defined as

$$(\boldsymbol{XAB})_i=e_{ijk}A_{jr}B_{rk}.$$

The spatial derivative for the component representation is with respect to rectangular Cartesian coordinates on the current configuration of the body. For manipulations with components, we shall always use such rectangular Cartesian coordinates. Positions of particles are measured from the origin of this arbitrarily fixed Cartesian coordinate system. We use the identity $\operatorname{curl}\operatorname{curl}(\cdot)=\operatorname{grad}\operatorname{div}(\cdot)-\operatorname{div}\operatorname{grad}(\cdot)$, often for an argument for which $\operatorname{div}(\cdot)=0$.

The following list describes some of the mathematical symbols we use in this paper.

$\boldsymbol{n}$: director
$\boldsymbol{x}$: current position
$\boldsymbol{E}$: director distortion tensor
$\boldsymbol{F}^e$: elastic distortion tensor
$\boldsymbol{W}=(\boldsymbol{F}^e)^{-1}$: inverse of elastic distortion tensor
$\boldsymbol{\beta}$: director incompatibility tensor
$\boldsymbol{\alpha}$: dislocation density tensor
$\boldsymbol{v}$: material velocity
$\boldsymbol{\omega}$: director angular velocity; $\dot{\boldsymbol{n}}=\boldsymbol{\omega}\times\boldsymbol{n}$
$\boldsymbol{L}$: velocity gradient
$\boldsymbol{D}=\boldsymbol{L}_{\text{sym}}$: rate of deformation tensor
$\boldsymbol{\Omega}=\boldsymbol{L}_{\text{skw}}$: spin tensor
$\boldsymbol{G}=\operatorname{grad}\boldsymbol{n}$: director gradient tensor
$\boldsymbol{M}=\operatorname{grad}\boldsymbol{\omega}$: director angular velocity gradient
$\boldsymbol{T}$: Cauchy stress tensor
$\boldsymbol{\Lambda}$: couple stress tensor
$\boldsymbol{\Gamma}$: skew-symmetric tensor corresponding to $\boldsymbol{\omega}$; $\boldsymbol{\Gamma}:=\boldsymbol{X\omega}$
$\boldsymbol{R}$: rotation tensor defined from $\boldsymbol{\Gamma}$; $\dot{\boldsymbol{R}}\boldsymbol{R}^T=-\boldsymbol{\Gamma}$
$\boldsymbol{p}$: permeation velocity
$\boldsymbol{K}$: external body moment per unit mass
$\boldsymbol{b}$: external body force per unit mass
ρ: mass density
ψ: free energy per unit mass

${}^{\beta}\boldsymbol{V}$: director incompatibility velocity
${}^{\alpha}\boldsymbol{V}$: dislocation velocity

In contrast to standard EL theory, we relax the requirement that the director distortion be the gradient of a vector field. Due to incompatibility, the constraints on $\boldsymbol{G}$ arising from the fixed length of the director [ACF99; CF06] cannot be translated to a constraint on $\boldsymbol{E}$. Thus, we follow in spirit Leslie [Les68] and, more generally, liquid crystal theories with variable degree of orientation to adopt a compatible director field that is not necessarily of fixed length, but allow only small deviations from the fixed length by appropriate constitutive energetic penalty.

The symbol

$$\overset{\circ}{\overline{(\cdot)}} = \operatorname{div} \boldsymbol{v}\,(\cdot) + \dot{\overline{(\cdot)}} - (\cdot)\,\boldsymbol{L}^T \tag{2.1}$$

for a second-order tensor argument $(\cdot)$ is defined as the "back-leg, contravariant, convected derivative with respect to the time-dependent tensor function $J\boldsymbol{F}$" of that tensor, where $\boldsymbol{F}$ is the deformation gradient with respect to an arbitrarily chosen fixed reference configuration and $J = \det \boldsymbol{F}$. This convected derivative arises most naturally in connection with two-point tensor fields whose domain is a tangent bundle on a time-dependent manifold. For a succint introduction to convected derivatives, see [Hil78].

Finally, we use the notion of a 2-form in a 3-d Euclidean space interchangeably with the vector representation of its adjoint 1-form [Fle77].

3 Balance laws and mechanical dissipation

For any fixed set of material particles occupying the volume $V(t)$ at time t with boundary $\partial V(t)$ having outward unit normal field $\boldsymbol{\nu}$

$$\begin{aligned}
\dot{\overline{\int_{V(t)} \rho\, dv}} &= 0,\\
\dot{\overline{\int_{V(t)} \rho \boldsymbol{v}\, dv}} &= \int_{\partial V(t)} \boldsymbol{T}\boldsymbol{\nu}\, da + \int_{V(t)} \rho \boldsymbol{b}\, dv,\\
\dot{\overline{\int_{V(t)} \rho \left(\boldsymbol{x}\times\boldsymbol{v} + \boldsymbol{n}\times\dot{\boldsymbol{n}}\right)\, dv}} &= \int_{\partial V(t)} (\boldsymbol{x}\times\boldsymbol{T} + \boldsymbol{\Lambda})\,\boldsymbol{\nu}\, da + \int_{V(t)} \rho\,(\boldsymbol{x}\times\boldsymbol{b} + \boldsymbol{K})\, dv,
\end{aligned}$$

represent the statements of balance of mass, linear and angular momentum, respectively. In geometric language appropriate to Euclidean space, one can think of mass as a scalar-valued 3-form (i.e., a 'true' differential form that has meaning apart from the Euclidean structure), and linear momentum and angular momentum as vector-valued 3-forms. Here, we have followed [ACF99] in defining the director contribution to the angular momentum density[2]. Using Reynold's transport theorem, the corresponding local forms for these equations are:

$$\begin{aligned}
\dot{\rho} + \rho \operatorname{div} \boldsymbol{v} &= 0\\
\rho\dot{\boldsymbol{v}} &= \operatorname{div} \boldsymbol{T} + \rho\boldsymbol{b}\\
\rho\boldsymbol{n}\times\ddot{\boldsymbol{n}} &= \operatorname{div}\boldsymbol{\Lambda} - \boldsymbol{X} : \boldsymbol{T} + \rho\boldsymbol{K}.
\end{aligned} \tag{3.1}$$

[2]While allowing for the relaxation of the unit vector constraint on the director.

The external power supplied to the body at any given time is expressed as:

$$\begin{aligned} P(t) &= \int_{V(t)} \rho \boldsymbol{b} \cdot \boldsymbol{v} \, dv + \int_{\partial V(t)} (\boldsymbol{T}\boldsymbol{\nu}) \cdot \boldsymbol{v} \, da + \int_{\partial V(t)} (\boldsymbol{\Lambda}\boldsymbol{\nu}) \cdot \boldsymbol{\omega} \, da + \int_{V(t)} \rho \boldsymbol{K} \cdot \boldsymbol{\omega} \, dv \\ &= \int_{V(t)} \left(\rho \boldsymbol{v} \cdot \dot{\boldsymbol{v}} + \rho \dot{\boldsymbol{n}} \cdot \ddot{\boldsymbol{n}} \right) \, dv + \int_{V(t)} \left(\boldsymbol{T} \cdot \boldsymbol{L} + \boldsymbol{\Lambda} : \boldsymbol{M} + \boldsymbol{T} : \boldsymbol{\Gamma} \right) \, dv. \end{aligned}$$

On defining the generalized kinetic energy and the free energy of the body as

$$\begin{aligned} K &= \int_{V(t)} \frac{1}{2} \left(\rho \boldsymbol{v} \cdot \boldsymbol{v} + \rho \dot{\boldsymbol{n}} \cdot \dot{\boldsymbol{n}} \right) \, dv, \\ F &= \int_{V(t)} \rho \psi \, dv, \end{aligned}$$

respectively, and using Reynold's transport theorem, we obtain the mechanical dissipation

$$D := P - \dot{\overline{K + F}} = \int_{V(t)} \left(\boldsymbol{T} : \boldsymbol{L} + \boldsymbol{\Lambda} : \boldsymbol{M} + \boldsymbol{T} : \boldsymbol{\Gamma} - \rho \dot{\psi} \right) \, dv. \tag{3.2}$$

The first equality above shows the distribution of applied mechanical power into kinetic, stored and dissipated parts. The second equality, as we show subsequently, is used to identify driving forces for dissipative mechanisms.

4 Balance law for director incompatibility and consequent evolution equation for director distortion

We define the director incompatibility tensor as the departure of the director distortion from being the director gradient. So,

$$\operatorname{curl} \boldsymbol{E} = \operatorname{curl}(\boldsymbol{E} - \boldsymbol{G}) =: \boldsymbol{\beta}. \tag{4.1}$$

Both $\boldsymbol{E}$ and $\boldsymbol{\beta}$ are tensor fields on the current configuration, i.e., their values at any given point on the current configuration act on vectors from the tangent space at that point and produce vectors on the same tangent space. Therefore, if the current configuration is subjected to a rigid rotation characterized by a tensor $\tilde{\boldsymbol{R}}$, then $\boldsymbol{E}$ transforms to the fields $\tilde{\boldsymbol{R}}\boldsymbol{E}\tilde{\boldsymbol{R}}^T$ on the rotated configuration and similarly for $\boldsymbol{\beta}$.

The definition of $\boldsymbol{G}$ as a spatial gradient suggests that it is a vector-valued 1-form, i.e., an object that can be integrated on curves to produce a vector. In the absence of defects $\boldsymbol{E} = \boldsymbol{G}$, and hence $\boldsymbol{E}$ belongs to the same class of geometric objects. By (4.1), $\boldsymbol{\beta}$ is an areal density of defect lines, including disclinations, that represents director non-integrability. This is best appreciated at a spatial point where $\boldsymbol{\beta}$ can be written as a tensor product of two vectors, so that the defect density may be visualized as a line carrying a vectorial attribute (Figure 1). If a is any oriented area patch with unit normal field $\boldsymbol{\nu}$ and bounded by the closed curve c, and a has no defect lines intersecting it, then $\boldsymbol{E}$ can be written as a gradient on the patch. On the other hand, for an area patch intersected by the defect line, the integral

$$\int_a \boldsymbol{\beta}\boldsymbol{\nu} \, da$$

quantifies the failure of $\boldsymbol{E}$ to define a single-valued director field when integrated along the closed curve c. Thus

$$\boldsymbol{\beta}\boldsymbol{\nu}\, da$$

characterizes the director vector defect content in the oriented infinitesimal area element $\boldsymbol{\nu} da$. Hence, $\boldsymbol{\beta}$ is a vector-valued two-form. An immediate consequence of the definition (4.1) is that $\boldsymbol{\beta}$ is a solenoidal field and this implies that the defect lines either end at boundaries or are closed loops.

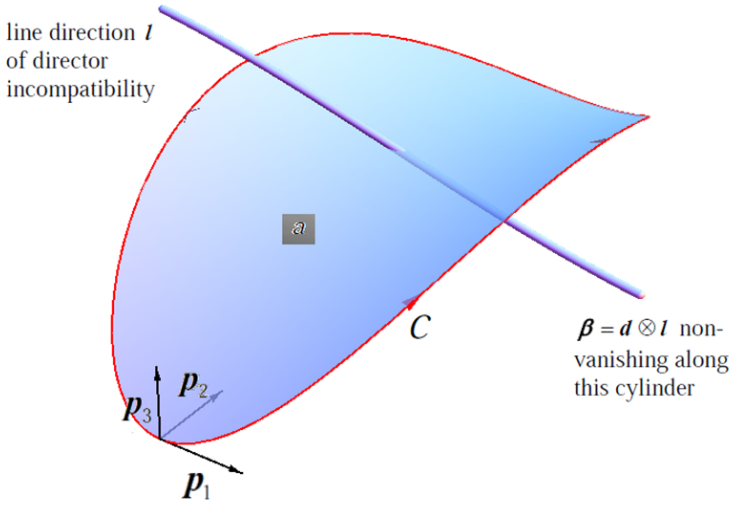

Figure 1: Director incompatibility defect lines.

It is natural to assume that these line-like objects move with a velocity and thus a velocity field ${}^{\beta}\boldsymbol{V}$, relative to the material, can be attributed to the director incompatibility field. The defect density field may also be integrated over an area and an accounting of the defect content of a particular area-patch of material particles over time can be carried out. This is the basis of the conservation laws that provide the dynamics of such fields. In posing this dynamical statement, a central goal is to stay as close as possible to the EL [Les92] theory. In particular, it is desirable that:

1. the EL dissipation is augmented only by the motion of director incompatibility defects (e.g. disclinations) and dislocations, and the occurrence of permeation,
2. the governing equations and constitutive equations are stated in terms of the current state of the material and information on the current configuration, without reference to prior states except for defining positional elastic response, and
3. the theory is consistent with material frame-indifference.

As we demonstrate, a conservation law that is consistent with these three requirements is of the form

$$\overline{\int_{a(t)} \boldsymbol{\beta}\boldsymbol{\nu}\, da}^{\cdot} = -\int_{c(t)} \boldsymbol{\beta} \times {}^{\beta}\boldsymbol{V}\, d\boldsymbol{x} - \int_{a(t)} \left(\operatorname{curl}\left(\boldsymbol{\Gamma}\left(\boldsymbol{E}-\boldsymbol{G}\right)\right)\right)\boldsymbol{\nu}\, da, \tag{4.2}$$

where $a(t)$ is the area patch occupied by an arbitrarily fixed set of material particles at time t and $c(t)$ is its closed bounding curve. The corresponding local form of (4.2) is

$$\overset{\circ}{\boldsymbol{\beta}} = -\operatorname{curl}\left(\boldsymbol{\beta} \times {}^{\beta}\boldsymbol{V}\right) - \operatorname{curl}\left(\boldsymbol{\Gamma}\left(\boldsymbol{E}-\boldsymbol{G}\right)\right).$$

The first term on the right side of (4.2) represents the flux of director incompatibility carried by defect lines entering the material area patch a. This is best understood by decomposing $\boldsymbol{\beta}$ and ${}^{\beta}\boldsymbol{V}$ on a special orthonormal basis oriented with respect to an infinitesimal segment of the bounding curve c as shown in Figure 2. Without loss of generality, we also assume that the basis chosen is such that $\boldsymbol{\nu}$ of the infinitesimal area element at the boundary is not parallel to $\boldsymbol{p}_1 \times \boldsymbol{p}_2$ or $\boldsymbol{p}_1 \times \boldsymbol{p}_3$.

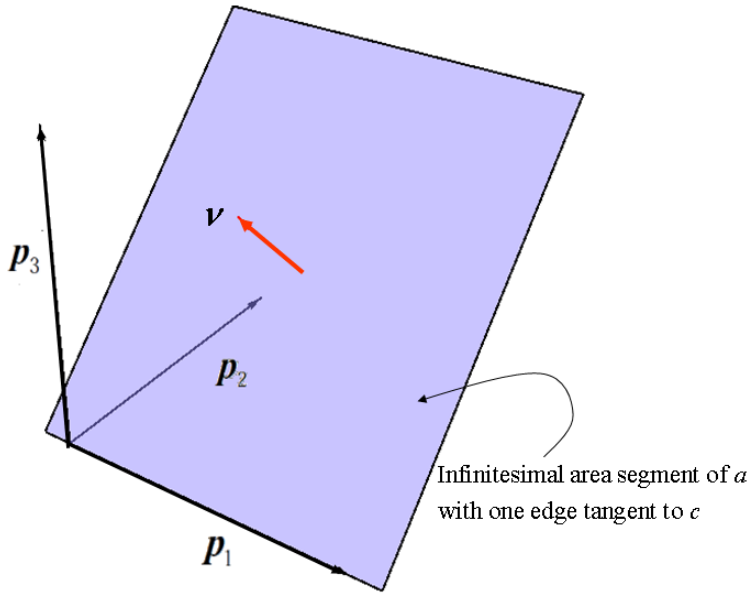

Figure 2: Orientation of local frame for understanding defect flux.

$$
\begin{aligned}
\left(\boldsymbol{\beta} \times {}^{\beta}\boldsymbol{V}\right) d\boldsymbol{x} &= -dx \left[\left(\boldsymbol{\beta}\boldsymbol{p}_i\right) \otimes \left(\boldsymbol{p}_i \times {}^{\beta}\boldsymbol{V}\right)\right] \boldsymbol{p}_1 \\
&= -\left(\boldsymbol{\beta}\boldsymbol{p}_1\right) dx \left[\boldsymbol{p}_1 \times \left({}^{\beta}V^1\boldsymbol{p}_1 + {}^{\beta}V^2\boldsymbol{p}_2 + {}^{\beta}V^3\boldsymbol{p}_3\right)\right] \cdot \boldsymbol{p}_1 \\
&\quad -\left(\boldsymbol{\beta}\boldsymbol{p}_2\right) dx \left[\boldsymbol{p}_2 \times \left({}^{\beta}V^1\boldsymbol{p}_1 + {}^{\beta}V^2\boldsymbol{p}_2 + {}^{\beta}V^3\boldsymbol{p}_3\right)\right] \cdot \boldsymbol{p}_1 \\
&\quad -\left(\boldsymbol{\beta}\boldsymbol{p}_3\right) dx \left[\boldsymbol{p}_3 \times \left({}^{\beta}V^1\boldsymbol{p}_1 + {}^{\beta}V^2\boldsymbol{p}_2 + {}^{\beta}V^3\boldsymbol{p}_3\right)\right] \cdot \boldsymbol{p}_1.
\end{aligned}
$$

Mathematically it is clear that there is no contribution to the flux from the first term on the right side above. Physically, this is because the motion of any defect line along itself clearly produces no flux into the area element. Furthermore the motions along directions $\boldsymbol{p}_2$ and $\boldsymbol{p}_3$, of the defect line component along $\boldsymbol{p}_1$, produce no intersection of this line component with the area element. Similar reasoning gives the physical meaning of

$$
\left(-\boldsymbol{\beta} \times {}^{\beta}\boldsymbol{V}\right) d\boldsymbol{x} = -\left(\boldsymbol{\beta}\boldsymbol{p}_2\right) dx {}^{\beta}V^3 + \left(\boldsymbol{\beta}\boldsymbol{p}_3\right) dx {}^{\beta}V^2.
$$

Note that the signs are consistent with the chosen orientation of a and c.

The second term on the right-hand-side of (4.2) represents a geometric source term that enables consistency of the conservation law with the first and third requirements above, as we show at the end of Section 8. Interestingly, it allows us to write the evolution equation for the director distortion implied by (4.2) as an adapted convected derivative as we now show.

Arbitrarily fix an instant of time, say s, in the motion of a body and let $\boldsymbol{F}$ denote the time-dependent deformation gradient field corresponding to this motion with respect to the configuration at the time s.

Denote positions on the configuration at time s as $\boldsymbol{x}_s$ and the image of the area patch $a(t)$ as $a(s)$. We similarly associate the closed curves $c(t)$ and $c(s)$. Then, using the definition (4.1) and Stokes theorem, (4.2) can be written as

$$\begin{aligned}
&\overset{\cdot}{\overline{\int_{a(t)} \left(\operatorname{curl}\left(\boldsymbol{E}-\boldsymbol{G}\right)\right)\boldsymbol{\nu}\, da}} = -\int_{a(t)} \operatorname{curl}\left(\boldsymbol{\beta}\times {}^{\beta}\boldsymbol{V}+\boldsymbol{\Gamma}\left(\boldsymbol{E}-\boldsymbol{G}\right)\right)\boldsymbol{\nu}\, da \\
&\Rightarrow \overset{\cdot}{\overline{\int_{c(s)} \left(\boldsymbol{E}-\boldsymbol{G}\right)\boldsymbol{F}\, d\boldsymbol{x}_s}} = -\int_{c(s)} \left(\boldsymbol{\beta}\times {}^{\beta}\boldsymbol{V}+\boldsymbol{\Gamma}\left(\boldsymbol{E}-\boldsymbol{G}\right)\right)\boldsymbol{F}\, d\boldsymbol{x}_s \\
&\Rightarrow \int_{a(s)} \operatorname{curl}\left(\overset{\cdot}{\overline{\left(\boldsymbol{E}-\boldsymbol{G}\right)\boldsymbol{F}}}+\left[\boldsymbol{\beta}\times {}^{\beta}\boldsymbol{V}+\boldsymbol{\Gamma}\left(\boldsymbol{E}-\boldsymbol{G}\right)\right]\boldsymbol{F}\right)\boldsymbol{\nu}\, da = \boldsymbol{0} \\
&\Rightarrow \overset{\cdot}{\overline{\left(\boldsymbol{E}-\boldsymbol{G}\right)\boldsymbol{F}}} = -\left[\boldsymbol{\beta}\times {}^{\beta}\boldsymbol{V}+\boldsymbol{\Gamma}\left(\boldsymbol{E}-\boldsymbol{G}\right)\right]\boldsymbol{F},
\end{aligned} \tag{4.3}$$

since the conservation law holds for all area patches. Without loss of generality, we have made the assumption that a possibly additive gradient vanishes. Consequently, we have

$$\overset{\cdot}{\overline{\left(\boldsymbol{E}-\boldsymbol{G}\right)}}\boldsymbol{F}+\left(\boldsymbol{E}-\boldsymbol{G}\right)\boldsymbol{L}\boldsymbol{F} = -\left[\boldsymbol{\beta}\times {}^{\beta}\boldsymbol{V}+\boldsymbol{\Gamma}\left(\boldsymbol{E}-\boldsymbol{G}\right)\right]\boldsymbol{F} \tag{4.4}$$

and choosing $s=t$, we obtain (4.2) in the form

$$\overset{\odot}{\overline{\left(\boldsymbol{E}-\boldsymbol{G}\right)}}:=\boldsymbol{\Gamma}\left(\boldsymbol{E}-\boldsymbol{G}\right)+\overset{\cdot}{\overline{\left(\boldsymbol{E}-\boldsymbol{G}\right)}}+\left(\boldsymbol{E}-\boldsymbol{G}\right)\boldsymbol{L} = -\boldsymbol{\beta}\times {}^{\beta}\boldsymbol{V}. \tag{4.5}$$

where $\overset{\odot}{\overline{\left(\boldsymbol{E}-\boldsymbol{G}\right)}}$ defines a convected derivative.

Eqn. (4.2) can be accepted as a natural balance law that satisfies frame-indifference and thermodynamics; however, in Appendix A we also the provide a geometric interpretation for the extremely specific convected time derivative and source term in (4.2).

5 Balance law for dislocation density and the evolution equation for the inverse elastic distortion

The physical idea behind the dislocation density tensor $\boldsymbol{\alpha}$ and the inverse elastic distortion $\boldsymbol{W}$ begins by considering the body in the current configuration and an additive decomposition[3] of the stress

$$\boldsymbol{T}=\boldsymbol{T}^{e}+\boldsymbol{T}^{d},$$

where $\boldsymbol{T}^{e}(t)$ is independent of the velocity field at time t.

The fundamental assumption of conventional plasticity [e.g., LL67] is as follows. Grid the current configuration, $\mathcal{C}$, into a union of small, non-intersecting, elements. Now assume that there is a collection of pieces composed of *identical*, unstressed, elastic material, one corresponding to each element of the grid. These pieces may be of different sizes, but always of same orientation when such orientation can be defined. The collection has the following properties:

[3] An additive decomposition into equilibrium and viscous parts is partially justified in [CM64].

1. each piece can be mapped to the corresponding element in the current configuration by a homogeneous deformation. That is, if e_x is the element around $\boldsymbol{x} \in \mathcal{C}$ and p_x its corresponding elastic reference (e_x, p_x are sets of points), then there exists an invertible second-order tensor field $\boldsymbol{F}^e(\boldsymbol{x})$, and a position field $\boldsymbol{f}_x$, such that
$$\begin{aligned}&\boldsymbol{f}_x(p_x) \mapsto e_x\\ &\boldsymbol{f}_x(\boldsymbol{X}) = \boldsymbol{F}^e(\boldsymbol{x})\,(\boldsymbol{X} - \boldsymbol{X}_0) + \boldsymbol{x} \quad \forall \boldsymbol{X} \in p_x, \boldsymbol{X}_0 \in p_x;\end{aligned}$$
2. there exists a function $\mathfrak{T}$ *independent* of $\boldsymbol{x}$, such that
$$\boldsymbol{T}^e(\boldsymbol{x}) = \mathfrak{T}\left(\boldsymbol{F}^e(\boldsymbol{x})\right) \quad \forall \boldsymbol{x} \in \mathcal{C}.$$

Noll [Nol67] uses the suggestive name 'materially uniform bodies' for materials displaying an elastic response as described above. In conventional plasticity, the collection $\{p_x\}$ has a one-to-one correspondence with $\boldsymbol{x} \in \mathcal{C}$ and is called the 'intermediate configuration'. These definitions naturally extend to time-varying fields with the field $\boldsymbol{F}^e$ defined for $(\boldsymbol{x}, t)$ and
$$\boldsymbol{T}^e(\boldsymbol{x}, t) = \mathfrak{T}\left(\boldsymbol{F}^e(\boldsymbol{x}, t)\right),$$
with $\mathfrak{T}$ independent of time.

Define the *inverse elastic distortion tensor*
$$\boldsymbol{W}(\boldsymbol{x}, t) := \left(\boldsymbol{F}^e(\boldsymbol{x}, t)\right)^{-1}. \tag{5.1}$$
It is often true that
$$\operatorname{curl} \boldsymbol{W} = \boldsymbol{0},$$
in which case it is possible that the pieces $\{p_x : \boldsymbol{x} \in \mathcal{C}\}$ fit together to form a coherent configuration and, under appropriate topological assumptions, $\boldsymbol{W}$ is the gradient of a position field on $\mathcal{C}$. An example is a deforming elastic material without any dislocations.

By unloading the body, then making small pieces such that there are no incompatibilities remaining in any of the unstressed pieces, and finally rotating all pieces to a common orientation, this procedure provides a route to define the field $\boldsymbol{W}$ from microscopic simulations or experiments.

Thus, we define the departure of $\boldsymbol{W}$ from being a gradient on $\mathcal{C}$ as a measure of dislocation density:
$$\operatorname{curl} \boldsymbol{W} = -\boldsymbol{\alpha}. \tag{5.2}$$
As in the case of the director incompatibility measure, the dislocation density may be physically visualized as an areal density of lines carrying the Burgers vector as a vectorial attribute.

The object $\boldsymbol{W}$ is a two-point tensor between the current configuration and the intermediate configuration. The intuition behind the conceptualization of the intermediate configuration implies that for two motions that differ only by a time-dependent rigid transformation, the intermediate configuration can be assumed to remain invariant without any loss of physical generality. Thus, under rigid rotations of the current configuration characterized by an orthogonal tensor $\tilde{\boldsymbol{R}}$, $\boldsymbol{W}$ transforms as $\boldsymbol{W}\tilde{\boldsymbol{R}}^T$.

We now pose a conservation law for the Burgers vector content of dislocation lines threading any arbitrary area patch in the body, using the same geometric justification as for any well-defined spatial density:
$$\begin{aligned}&\overset{\cdot}{\overline{\int_{a(t)} \boldsymbol{\alpha}\boldsymbol{\nu}\, da}} = -\int_{c(t)} \boldsymbol{\alpha} \times {}^{\alpha}\boldsymbol{V}\, d\boldsymbol{x}\\ &\Rightarrow \mathring{\boldsymbol{\alpha}} = -\operatorname{curl}\left(\boldsymbol{\alpha} \times {}^{\alpha}\boldsymbol{V}\right).\end{aligned} \tag{5.3}$$

Unlike the conservation law for the director incompatibility, there is no geometric source term since the target-space of $\boldsymbol{W}$ remains invariant under superposed rigid motions of the current configuration. Now, following similar reasoning as in (4.3), but *not ignoring the vector field gradient that can arise*, we have

$$\dot{\boldsymbol{W}} + \boldsymbol{W}\boldsymbol{L} = \boldsymbol{\alpha} \times {}^{\alpha}\boldsymbol{V} + \operatorname{grad} \boldsymbol{p}. \tag{5.4}$$

In smectic liquid crystals, we associate $\operatorname{grad} \boldsymbol{p}$ with the permeation velocity gradient, where permeation refers to the transverse flow of molecules relative to the smectic layers keeping the layers intact (up to identity of molecules) [Hel69; dGP95; E97; Ste07]. This is in analogy with crystal plasticity where such a gradient represents dissipative, compatible permanent deformation that, up to boundary constraints, produces no stress in the body [Ach04], e.g., lattice-invariant shears wherein the lattice remains unchanged but lattice sites are occupied by different atoms in the course of time. Since the permeation velocity is a field that affects the physics predicted by the model, it requires constitutive specification and may not be thought of in the spirit of a gauge field.

We note that all terms in (5.4) are well-defined in terms of information available from operations on the current configuration. Of course, the definition of $\boldsymbol{W}, \boldsymbol{\alpha}, \boldsymbol{p}$ depend upon a pre-multiplying orthogonal tensor (that is constant in time and space) characterizing the orientation of the undistorted reference which is also naturally involved in the definition of the materially uniform response function $\mathfrak{T}$. As in material symmetry arguments in standard nonlinear elasticity, the changes induced in $\boldsymbol{W}$ and $\mathfrak{T}$ cancel each other so that the stress predicted on the current configuration is invariant with respect to the choice of the undistorted reference. In addition, here we also require that if $(\boldsymbol{W}, \boldsymbol{\alpha}, \boldsymbol{p})$ is a set of time-dependent fields satisfying (5.4), then $(\tilde{\boldsymbol{R}}\boldsymbol{W}, \tilde{\boldsymbol{R}}\boldsymbol{\alpha}, \tilde{\boldsymbol{R}}\boldsymbol{p})$ also satisfy (5.4) for arbitrary orthogonal $\tilde{\boldsymbol{R}}$, as indeed they do.

6 Summary of field equations

For ease of reference, we collect the field equations of the theory:

$$\begin{aligned}
&\dot{\rho} + \rho \operatorname{div} \boldsymbol{v} = 0 \\
&\rho \dot{\boldsymbol{v}} = \operatorname{div} \boldsymbol{T} + \rho \boldsymbol{b} \\
&\rho \boldsymbol{n} \times \ddot{\boldsymbol{n}} = \operatorname{div} \boldsymbol{\Lambda} - \boldsymbol{X} : \boldsymbol{T} + \rho \boldsymbol{K} \\
&\boldsymbol{\Gamma}(\boldsymbol{E} - \boldsymbol{G}) + \dot{\overline{(\boldsymbol{E} - \boldsymbol{G})}} + (\boldsymbol{E} - \boldsymbol{G})\boldsymbol{L} = -(\operatorname{curl} \boldsymbol{E}) \times {}^{\beta}\boldsymbol{V} \\
&\dot{\boldsymbol{W}} + \boldsymbol{W}\boldsymbol{L} = -(\operatorname{curl} \boldsymbol{W}) \times {}^{\alpha}\boldsymbol{V} + \operatorname{grad} \boldsymbol{p}.
\end{aligned} \tag{6.1}$$

The equations $(6.1)_{4,5}$ are derived from integral balance laws and hence satisfy jump conditions on surfaces of discontinuity [Ach07]. On any arbitrary surface with unit normal field $\boldsymbol{N}$ and moving with normal velocity $u_{\boldsymbol{N}}$ with respect to the material,

$$\begin{aligned}
&[\![-\boldsymbol{\beta} \times {}^{\beta}\boldsymbol{V} - \boldsymbol{\Gamma}(\boldsymbol{E} - \boldsymbol{G})]\!] \times \boldsymbol{N} = [\![\boldsymbol{\beta}_{\text{tan}} (u_{\boldsymbol{N}} - \boldsymbol{v} \cdot \boldsymbol{N})]\!] + [\![\boldsymbol{\beta}\boldsymbol{N} \otimes \boldsymbol{v}_{\text{tan}}]\!] \\
&[\![-\boldsymbol{\alpha} \times {}^{\alpha}\boldsymbol{V}]\!] \times \boldsymbol{N} = [\![\boldsymbol{\alpha}_{\text{tan}} (u_{\boldsymbol{N}} - \boldsymbol{v} \cdot \boldsymbol{N})]\!] + [\![\boldsymbol{\alpha}\boldsymbol{N} \otimes \boldsymbol{v}_{\text{tan}}]\!],
\end{aligned} \tag{6.2}$$

where $[\![\cdot]\!]$ is the difference of the limiting values of its argument evaluated on either side of the surface of discontinuity, and $\boldsymbol{A}_{\text{tan}} := \boldsymbol{A} - (\boldsymbol{A}\boldsymbol{N}) \otimes \boldsymbol{N}$ and $\boldsymbol{g}_{\text{tan}} := \boldsymbol{g} - (\boldsymbol{g} \cdot \boldsymbol{N})\boldsymbol{N}$ are the tangential actions of, respectively, a second order tensor and a vector with respect to an orientation $\boldsymbol{N}$. Equation (6.2) is geometric in

nature and includes the situation when the surface is 'material' in the sense that its normal velocity (with respect to itself) coincides with that of the material surface it is coincident with instantaneously.

Using the fact that the fields $\boldsymbol{\beta}, \boldsymbol{\alpha}$ are solenoidal, the local forms of the integral balances for the director incompatibility and dislocation density,

$$\begin{aligned} \mathring{\boldsymbol{\beta}} &= -\operatorname{curl}\left(\boldsymbol{\beta} \times {}^{\beta}\boldsymbol{V}\right) - \operatorname{curl}\left(\boldsymbol{\Gamma}(\boldsymbol{E}-\boldsymbol{G})\right) \\ \mathring{\boldsymbol{\alpha}} &= -\operatorname{curl}\left(\boldsymbol{\alpha} \times {}^{\alpha}\boldsymbol{V}\right), \end{aligned} \tag{6.3}$$

can be expressed in Eulerian form [cf. Ach07]:

$$\begin{aligned} \frac{\partial \boldsymbol{\beta}}{\partial t} &= -\operatorname{curl}\left(\boldsymbol{\beta} \times \left[\boldsymbol{v} + {}^{\beta}\boldsymbol{V}\right]\right) - \operatorname{curl}\left(\boldsymbol{\Gamma}(\boldsymbol{E}-\boldsymbol{G})\right) \\ \frac{\partial \boldsymbol{\alpha}}{\partial t} &= -\operatorname{curl}\left(\boldsymbol{\alpha} \times \left[\boldsymbol{v} + {}^{\alpha}\boldsymbol{V}\right]\right), \end{aligned} \tag{6.4}$$

making transparent the relative nature of the dislocation and director incompatibility velocities.

The equations in (6.4) are capable of geometrically representing loop expansion as demonstrated in Section 7 of [Ach03] for the dislocation density. As a simple special case, the loop is assumed to be planar, with ${}^{\alpha}\boldsymbol{V}$ in-plane with the dislocation loop, being of constant magnitude V and pointwise perpendicular to it. Within this *ansatz*, it is interesting to note that the tensorial system $(6.4)_2$ reduces to the eikonal equation for front propagation of a scalar field π in two space dimensions and time, (x, y, t), given by

$$(\pi_t)^2 = V^2\left[(\pi_x)^2 + (\pi_y)^2\right].$$

In (6.1) and (6.3), we have not included possible solenoidal nucleation terms for the director incompatibility and dislocation density fields for simplicity. At this level of generality, they are easily admitted. However, the possibility of nucleation as a dynamical instability [DB06] is obviously not ruled out within the framework and it may even be expected to be the norm in liquid crystalline materials.

7 Consequences of frame-indifference and Ericksen's identity for this theory

In preparation for deducing constitutive guidance on elastic response and dissipative driving forces, we consider a consequence of frame-indifference on the free energy density function, ψ, where ψ depends on $\boldsymbol{n}, \boldsymbol{E}, \boldsymbol{W}, \boldsymbol{\alpha}, \boldsymbol{\beta}$. We adapt the presentation of [ACF99] for this purpose. Frame indifference requires that ψ satisfy

$$\psi\left(\boldsymbol{n}, \boldsymbol{E}, \boldsymbol{W}, \boldsymbol{\alpha}, \boldsymbol{\beta}\right) = \psi\left(\tilde{\boldsymbol{R}}\boldsymbol{n}, \tilde{\boldsymbol{R}}\boldsymbol{E}\tilde{\boldsymbol{R}}^T, \boldsymbol{W}\tilde{\boldsymbol{R}}^T, \boldsymbol{\alpha}\tilde{\boldsymbol{R}}^T, \tilde{\boldsymbol{R}}\boldsymbol{\beta}\tilde{\boldsymbol{R}}^T\right) \tag{7.1}$$

for all proper orthogonal $\tilde{\boldsymbol{R}}$ and for all elements $\boldsymbol{n}, \boldsymbol{E}, \boldsymbol{W}, \boldsymbol{\alpha}, \boldsymbol{\beta}$ in the domain of the function ψ. In particular, (7.1) has to apply for all functions $s \to \tilde{\boldsymbol{R}}(s), 0 \leq s \in \mathbb{R}$, with

$$\tilde{\boldsymbol{R}}(0) = \boldsymbol{I}; \quad \frac{d\tilde{\boldsymbol{R}}}{ds}(0) = \boldsymbol{S} = -\frac{d\tilde{\boldsymbol{R}}^T}{ds}(0)$$

and $\boldsymbol{S}$ is an arbitrary fixed skew tensor. Differentiating (7.1) and then evaluating it at $s = 0$ implies

$$\left[\frac{\partial \psi}{\partial \boldsymbol{n}} \otimes \boldsymbol{n} + \frac{\partial \psi}{\partial \boldsymbol{E}}\boldsymbol{E}^T - \boldsymbol{E}^T\frac{\partial \psi}{\partial \boldsymbol{E}} - \boldsymbol{W}^T\frac{\partial \psi}{\partial \boldsymbol{W}} - \boldsymbol{\alpha}^T\frac{\partial \psi}{\partial \boldsymbol{\alpha}} + \frac{\partial \psi}{\partial \boldsymbol{\beta}}\boldsymbol{\beta}^T - \boldsymbol{\beta}^T\frac{\partial \psi}{\partial \boldsymbol{\beta}}\right] : \boldsymbol{S} = 0$$

and due to the arbitrariness of $\boldsymbol{S}$ we obtain Ericksen's identity for our model:

$$\left(\frac{\partial\psi}{\partial\boldsymbol{n}}\otimes\boldsymbol{n}\right)_{\text{skw}}=-\left(\frac{\partial\psi}{\partial\boldsymbol{E}}\boldsymbol{E}^T-\boldsymbol{E}^T\frac{\partial\psi}{\partial\boldsymbol{E}}\right)_{\text{skw}}+\left(\boldsymbol{W}^T\frac{\partial\psi}{\partial\boldsymbol{W}}\right)_{\text{skw}}+\left(\boldsymbol{\alpha}^T\frac{\partial\psi}{\partial\boldsymbol{\alpha}}\right)_{\text{skw}}-\left(\frac{\partial\psi}{\partial\boldsymbol{\beta}}\boldsymbol{\beta}^T-\boldsymbol{\beta}^T\frac{\partial\psi}{\partial\boldsymbol{\beta}}\right)_{\text{skw}}. \tag{7.2}$$

In the next section we will use the transformation rule for the partial derivatives of ψ; we record this rule for only one case below as the rest are similar. Denoting the partial derivative of ψ with respect to its second argument as $\partial_E\psi$, (7.1) implies

$$\partial_E\psi\left(\boldsymbol{n},\boldsymbol{E},\boldsymbol{W},\boldsymbol{\alpha},\boldsymbol{\beta}\right)=\tilde{\boldsymbol{R}}^T\partial_E\psi\left(\tilde{\boldsymbol{R}}\boldsymbol{n},\tilde{\boldsymbol{R}}\boldsymbol{E}\tilde{\boldsymbol{R}}^T,\boldsymbol{W}\tilde{\boldsymbol{R}}^T,\boldsymbol{\alpha}\tilde{\boldsymbol{R}}^T,\tilde{\boldsymbol{R}}\boldsymbol{\beta}\tilde{\boldsymbol{R}}^T\right)\tilde{\boldsymbol{R}}. \tag{7.3}$$

We also note that if

$$\boldsymbol{X}:(\boldsymbol{A}\boldsymbol{B})=\boldsymbol{d}$$

for second-order tensors $\boldsymbol{A},\boldsymbol{B}$ and a vector $\boldsymbol{d}$ then

$$\boldsymbol{X}:\left(\tilde{\boldsymbol{R}}\boldsymbol{A}\tilde{\boldsymbol{R}}^T\tilde{\boldsymbol{R}}\boldsymbol{B}\tilde{\boldsymbol{R}}^T\right)=\tilde{\boldsymbol{R}}\boldsymbol{d}, \tag{7.4}$$

which is a direct consequence of the preservation of angles between, and magnitudes of, vectors under the action of an orthogonal tensor.

8 Constitutive guidance for reversible response and driving forces

Assuming a free energy density function ψ with arguments as discussed in Section 7, we now re-examine the mechanical dissipation D in (3.2). We first compute the material time derivative of ψ:

$$\begin{aligned}\dot{\psi}&=\frac{\partial\psi}{\partial\boldsymbol{n}}\cdot\dot{\boldsymbol{n}}+\frac{\partial\psi}{\partial\boldsymbol{E}}:\dot{\boldsymbol{E}}+\frac{\partial\psi}{\partial\boldsymbol{W}}:\dot{\boldsymbol{W}}+\frac{\partial\psi}{\partial\boldsymbol{\alpha}}:\dot{\boldsymbol{\alpha}}+\frac{\partial\psi}{\partial\boldsymbol{\beta}}:\dot{\boldsymbol{\beta}}\\&=-\frac{\partial\psi}{\partial\boldsymbol{n}}\otimes\boldsymbol{n}:\boldsymbol{\Gamma}\\&\quad+\frac{\partial\psi}{\partial\boldsymbol{E}}:\left(-\boldsymbol{\beta}\times{}^{\beta}\boldsymbol{V}-(\boldsymbol{E}-\boldsymbol{G})\boldsymbol{L}+\dot{\boldsymbol{G}}-\boldsymbol{\Gamma}(\boldsymbol{E}-\boldsymbol{G})\right)\\&\quad+\frac{\partial\psi}{\partial\boldsymbol{W}}:(-\boldsymbol{\alpha}\times{}^{\alpha}\boldsymbol{V}+\operatorname{grad}\boldsymbol{p}-\boldsymbol{W}\boldsymbol{L})\\&\quad+\frac{\partial\psi}{\partial\boldsymbol{\alpha}}:\left(-\operatorname{div}\boldsymbol{v}\boldsymbol{\alpha}+\boldsymbol{\alpha}\boldsymbol{L}^T-\operatorname{curl}\left(\boldsymbol{\alpha}\times{}^{\alpha}\boldsymbol{V}\right)\right)\\&\quad+\frac{\partial\psi}{\partial\boldsymbol{\beta}}:\left(-\operatorname{div}\boldsymbol{v}\boldsymbol{\beta}+\boldsymbol{\beta}\boldsymbol{L}^T-\operatorname{curl}\left(\boldsymbol{\beta}\times{}^{\beta}\boldsymbol{V}+\boldsymbol{\Gamma}(\boldsymbol{E}-\boldsymbol{G})\right)\right).\end{aligned} \tag{8.1}$$

Some useful formulae for subsequent use are

$$\begin{aligned}&\dot{\boldsymbol{G}}=\dot{\overline{\operatorname{grad}\boldsymbol{n}}}=\operatorname{grad}\dot{\boldsymbol{n}}-\boldsymbol{G}\boldsymbol{L},\\&\boldsymbol{A}:\operatorname{grad}\dot{\boldsymbol{n}}=(\boldsymbol{X}:(\boldsymbol{n}\otimes\boldsymbol{A})):\boldsymbol{M}-\left(\boldsymbol{A}\boldsymbol{G}^T\right):\boldsymbol{\Gamma}=e_{jki}n_kA_{ip}M_{jp}-A_{ip}G_{kp}\Gamma_{ik}\end{aligned}$$

for an arbitrary second-order tensor $\boldsymbol{A}$, and

$$\rho\frac{\partial\psi}{\partial\boldsymbol{\beta}}:\operatorname{curl}\left(\boldsymbol{\Gamma}(\boldsymbol{E}-\boldsymbol{G})\right)=-\rho\left(\frac{\partial\psi}{\partial\boldsymbol{\beta}}-\operatorname{tr}\left[\frac{\partial\psi}{\partial\boldsymbol{\beta}}\right]\boldsymbol{I}\right)(\boldsymbol{E}-\boldsymbol{G})^T:\boldsymbol{M}+\left(\rho\frac{\partial\psi}{\partial\boldsymbol{\beta}}\right)\boldsymbol{\beta}^T:\boldsymbol{\Gamma}.$$

Recalling the dissipation (3.2)

$$D = \int_{V(t)} \left(\boldsymbol{T} : \boldsymbol{L} + \boldsymbol{\Lambda} : \boldsymbol{M} + \boldsymbol{T} : \boldsymbol{\Gamma} - \rho \dot{\psi} \right) \, dv,$$

we collect the terms multiplying $\boldsymbol{L}, \boldsymbol{\Gamma}, \boldsymbol{M}$ respectively:

$$\int_{V(t)} \left(\boldsymbol{T} - \rho \left[-\boldsymbol{E}^T \frac{\partial \psi}{\partial \boldsymbol{E}} - \boldsymbol{W}^T \frac{\partial \psi}{\partial \boldsymbol{W}} - \left(\frac{\partial \psi}{\partial \boldsymbol{\alpha}} : \boldsymbol{\alpha} + \frac{\partial \psi}{\partial \boldsymbol{\beta}} : \boldsymbol{\beta} \right) \boldsymbol{I} + \left(\frac{\partial \psi}{\partial \boldsymbol{\alpha}} \right)^T \boldsymbol{\alpha} + \left(\frac{\partial \psi}{\partial \boldsymbol{\beta}} \right)^T \boldsymbol{\beta} \right] \right) : \boldsymbol{L} \, dv,$$

$$\int_{V(t)} \left(\boldsymbol{T} - \left[-\rho \frac{\partial \psi}{\partial \boldsymbol{n}} \otimes \boldsymbol{n} - \rho \frac{\partial \psi}{\partial \boldsymbol{E}} \boldsymbol{E}^T - \rho \frac{\partial \psi}{\partial \boldsymbol{\beta}} \boldsymbol{\beta}^T \right] \right)_{\text{skw}} : \boldsymbol{\Gamma} \, dv,$$

$$\int_{V(t)} \left(\boldsymbol{\Lambda} - \boldsymbol{X} : \left[\boldsymbol{n} \otimes \frac{\partial \psi}{\partial \boldsymbol{E}} \right] - \rho \left[\frac{\partial \psi}{\partial \boldsymbol{\beta}} - \operatorname{tr} \left(\frac{\partial \psi}{\partial \boldsymbol{\beta}} \right) \boldsymbol{I} \right] (\boldsymbol{E} - \boldsymbol{G})^T \right) : \boldsymbol{M} \, dv.$$

The remaining contributions to the dissipation are:

$$\begin{aligned}
&\int_{V(t)} \left(\boldsymbol{X} : \left[\left(\rho \frac{\partial \psi}{\partial \boldsymbol{E}} + \operatorname{curl} \left[\rho \frac{\partial \psi}{\partial \boldsymbol{\beta}} \right] \right)^T \boldsymbol{\beta} \right] \right) \cdot {}^{\beta}\boldsymbol{V} \, dv + \int_{\partial V(t)} -\rho \frac{\partial \psi}{\partial \boldsymbol{\beta}} : \left(\left[\boldsymbol{\beta} \times {}^{\beta}\boldsymbol{V} \right] \times \boldsymbol{\nu} \right) \, da, \\
&\int_{V(t)} \left(\boldsymbol{X} : \left[\left(-\rho \frac{\partial \psi}{\partial \boldsymbol{W}} + \operatorname{curl} \left[\rho \frac{\partial \psi}{\partial \boldsymbol{\alpha}} \right] \right)^T \boldsymbol{\alpha} \right] \right) \cdot {}^{\alpha}\boldsymbol{V} \, dv + \int_{\partial V(t)} -\rho \frac{\partial \psi}{\partial \boldsymbol{\alpha}} : \left(\left[\boldsymbol{\alpha} \times {}^{\alpha}\boldsymbol{V} \right] \times \boldsymbol{\nu} \right) \, da, \qquad (8.2) \\
&\text{and} \quad \int_{V(t)} -\frac{\partial \psi}{\partial \boldsymbol{W}} : \operatorname{grad} \boldsymbol{p} \, dv.
\end{aligned}$$

In the spirit of generalizing EL theory, we make the constitutive assumption for the equilibrium part $\boldsymbol{T}^e$ of the total stress $\boldsymbol{T} = \boldsymbol{T}^e + \boldsymbol{T}^d$ as

$$\boldsymbol{T}^e = \rho \left(-\boldsymbol{E}^T \frac{\partial \psi}{\partial \boldsymbol{E}} - \boldsymbol{W}^T \frac{\partial \psi}{\partial \boldsymbol{W}} - \left(\frac{\partial \psi}{\partial \boldsymbol{\alpha}} : \boldsymbol{\alpha} + \frac{\partial \psi}{\partial \boldsymbol{\beta}} : \boldsymbol{\beta} \right) \boldsymbol{I} + \left(\frac{\partial \psi}{\partial \boldsymbol{\alpha}} \right)^T \boldsymbol{\alpha} + \left(\frac{\partial \psi}{\partial \boldsymbol{\beta}} \right)^T \boldsymbol{\beta} \right), \qquad (8.3)$$

and the couple-stress tensor as

$$\boldsymbol{\Lambda} = \boldsymbol{X} : \left[\boldsymbol{n} \otimes \frac{\partial \psi}{\partial \boldsymbol{E}} \right] + \rho \left[\frac{\partial \psi}{\partial \boldsymbol{\beta}} - \operatorname{tr} \left(\frac{\partial \psi}{\partial \boldsymbol{\beta}} \right) \boldsymbol{I} \right] (\boldsymbol{E} - \boldsymbol{G})^T. \qquad (8.4)$$

Incorporating these assumptions, the dissipation can now be expressed as

$$\begin{aligned}
&\int_{V(t)} \boldsymbol{T}^d_{\text{sym}} : \boldsymbol{D} \, dv + \int_{V(t)} \boldsymbol{T}^d_{\text{skw}} : \left(\boldsymbol{\Omega} - \boldsymbol{\Gamma}^T \right) \, dv \\
&+ \int_{V(t)} \left(\boldsymbol{T}^e + \rho \frac{\partial \psi}{\partial \boldsymbol{n}} \otimes \boldsymbol{n} + \rho \frac{\partial \psi}{\partial \boldsymbol{E}} \boldsymbol{E}^T + \rho \frac{\partial \psi}{\partial \boldsymbol{\beta}} \boldsymbol{\beta}^T \right)_{\text{skw}} : \boldsymbol{\Gamma} \, dv \qquad (8.5) \\
&+ \text{terms displayed in (8.2)}.
\end{aligned}$$

We first consider the two boundary terms in (8.2). The dependence of the free energy on $\boldsymbol{\alpha}, \boldsymbol{\beta}$ accounts for the energy content of individual defect cores, beyond the elastic energy in their stress-fields. Mathematically, they act as regularization [cf. Ach10; AMZ10]. For instance, the dislocation core energy contribution may look like $\mu b^2 \boldsymbol{\alpha} : \boldsymbol{\alpha}$ where μ is a shear modulus and b is of the order of the interatomic spacing. Thus, the terms $\frac{\partial \psi}{\partial \boldsymbol{\beta}}, \frac{\partial \psi}{\partial \boldsymbol{\alpha}}$ are expected to be small away from cores in comparison to typical

derivatives of ψ with respect to $\boldsymbol{E}$ or $\boldsymbol{W}$. Consequently, constitutive guidelines to ensure non-negative dissipation in the model will be based only on the bulk terms in the expression for the dissipation.

The procedure used in [E97; Ste07] to find the driving force for permeation uses integration-by-parts and subsequent neglect of the boundary term. For the term related to permeation in (8.2) we do not follow this procedure as it is unclear that the boundary term can be estimated to be small in comparison to the other dissipative contributions.

An essential requirement is that the dissipation in the model be frame-indifferent or objective[4]. Given that the director field transforms as $\boldsymbol{n} \to \tilde{\boldsymbol{R}}\boldsymbol{n}$ under a superposed rigid body motion characterized by the time-dependent, spatially uniform orthogonal tensor field $\tilde{\boldsymbol{R}}$, it can be seen that T^d_{sym}, T^d_{skw}, $\boldsymbol{D}$, $\boldsymbol{\Omega} - \boldsymbol{\Gamma}^T$ transform objectively, i.e. follow the transformation rule $(\cdot) \mapsto \tilde{\boldsymbol{R}}(\cdot)\tilde{\boldsymbol{R}}^T$. Thus, the first two terms in (8.5) transform as objective scalars, i.e. remain invariant under superposed rigid body motions.

By their physical definitions, the director incompatibility and dislocation velocities (with respect to the material), ${}^{\beta}\boldsymbol{V}, {}^{\alpha}\boldsymbol{V}$, are objective vector fields on the current configuration and therefore have to transform by the rule $(\cdot) \mapsto \tilde{\boldsymbol{R}}(\cdot)$ under superposed rigid body motions. Due to its two-point nature, $\operatorname{grad}\boldsymbol{p}$ transforms as $(\cdot) \mapsto (\cdot)\tilde{\boldsymbol{R}}^T$. Using the discussion surrounding (7.3) and (7.4), the bulk terms in (8.2) transform as objective scalars.

To ensure frame-indifferent dissipation, only the third integral in (8.5) remains. Denoting by $\boldsymbol{S}(t) := \dot{\tilde{\boldsymbol{R}}}(t)\tilde{\boldsymbol{R}}^T(t)$, $\boldsymbol{\Gamma}$ transforms as

$$\boldsymbol{\Gamma} \mapsto -\boldsymbol{S} + \tilde{\boldsymbol{R}}\boldsymbol{\Gamma}\tilde{\boldsymbol{R}}^T$$

under superposed rigid body motions, where arbitrary $\boldsymbol{S}$ generate corresponding funtions $\tilde{\boldsymbol{R}}$. Since the coefficient of $\boldsymbol{\Gamma}$ in (8.5) transforms objectively, it has to vanish for the dissipation to transform as an objective scalar. If not, the dissipation can be made to take arbitrarily different values in motions that differ only by superposed rigid-body motions generated by varying $\boldsymbol{S}$. To avoid imposing any constraints on the function ψ beyond those due to frame-indifference and material symmetry[5], it is necessary that the coefficient of $\boldsymbol{\Gamma}$ in (8.5) vanish for all admissible choices of ψ. This is a strong constraint and its satisfaction validates the mechanical structure of the theory. Using (7.2), (8.3) and that $\left(\boldsymbol{A}^T\boldsymbol{B} + \boldsymbol{B}^T\boldsymbol{A}\right)_{\text{skw}} = \boldsymbol{0}$ for any second order tensors $\boldsymbol{A}, \boldsymbol{B}$, we see that the requirement is indeed satisfied for all frame-indifferent ψ.

We emphasize that the presence of the last two terms in the coefficient of $\boldsymbol{\Gamma}$ in (8.5) is a direct consequence of the geometric source term in (4.2). Hence, these terms play a crucial role in ensuring the frame-indifference of the theory. Since we are working with a 3-d body in 3-d Euclidean space the tangent space of a material point is always the same vector space. Consequently, there is no ambiguity in defining material time derivatives of tensor fields unlike in tensor calculus on manifolds. Curiously, however, frame-indifference forces the consideration of geometrically 'proper' convected derivatives in ordinary, 'flat-space', 3-d continuum mechanics as in (4.5).

Usually, the bulk terms in an expression for dissipation like (8.2) directly indicate the driving forces for director incompatibility velocity, the dislocation velocity and the permeation velocity gradient as the coefficients of ${}^{\beta}\boldsymbol{V}, {}^{\alpha}\boldsymbol{V}, \operatorname{grad}\boldsymbol{p}$, respectively, in the sense that the absence of these forces render the corresponding dissipative mechanisms non-operational. Also, the simplest constitutive equations ensuring non-negative dissipation are constructed by assigning linear relations between members of dissipative power-conjugate pairs. But here we face an obstacle with the last integral in (8.2). The driving force for

[4]These are notions we use interchangeably with invariance under superposed rigid body motions.

[5]Note in (8.5) that T^e_{skw} is also expressed in terms of ψ and its derivatives.

the permeation velocity gradient, as it stands, is not necessarily a gradient of a vector field. Moreover, as mentioned above, there is no justification to integrate this term by parts and ignore the resulting boundary contribution.

We deal with this by using a Stokes-Helmholtz decomposition for $-\frac{\partial \psi}{\partial \boldsymbol{W}} =: \boldsymbol{P}$ stated as

$$
\begin{aligned}
&-\operatorname{div}\operatorname{grad}\boldsymbol{H}_P = \operatorname{curl}\boldsymbol{P}; \quad \operatorname{div}\boldsymbol{H}_P = \boldsymbol{0} \text{ on } V\\
&\boldsymbol{H}_P \times \boldsymbol{n} = \boldsymbol{0} \text{ on } \partial V\\
&\operatorname{div}\operatorname{grad}\boldsymbol{g}_P = \operatorname{div}\boldsymbol{P}; \quad (\operatorname{grad}\boldsymbol{g}_P - \boldsymbol{P})\,\boldsymbol{n} = \boldsymbol{0} \text{ on } \partial V \text{ and}\\
&\boldsymbol{P} = \operatorname{curl}\boldsymbol{H}_P + \operatorname{grad}\boldsymbol{g}_P \text{ on } V.
\end{aligned}
$$

Given a square-integrable tensor field $\boldsymbol{P}$ with square-integrable gradients on the body, the decomposition guarantees the existence of a unique tensor field $\boldsymbol{H}_P$ and a unique (up to a constant) vector field $\boldsymbol{g}_P$. Utilizing this decomposition

$$
\int_{V(t)} -\frac{\partial \psi}{\partial \boldsymbol{W}} : \operatorname{grad}\boldsymbol{p}\, dv = \int_{V(t)} \operatorname{grad}\boldsymbol{g}_P : \operatorname{grad}\boldsymbol{p}\, dv
$$

where the boundary condition on $\boldsymbol{H}_P$ in the Stokes-Helmholtz decomposition is crucial. Consequently, we consider $\operatorname{grad}\boldsymbol{g}_P$ as the driving force for the permeation velocity gradient $\operatorname{grad}\boldsymbol{p}$. For ${}^{\alpha}\boldsymbol{V}, {}^{\beta}\boldsymbol{V}$ we identify driving forces directly from the bulk expressions in (8.2).

In ending this section, we note the decidedly nonlocal nature of the non-negative dissipation arguments. Clearly, positive dissipation is guaranteed only in a global sense over the entire body.

9 Constitutive structure and the modeling of common classes of liquid crystalline materials

The quantities $\psi, \boldsymbol{T}, \boldsymbol{\Lambda}, {}^{\alpha}\boldsymbol{V}, {}^{\beta}\boldsymbol{V}, \operatorname{grad}\boldsymbol{p}$ require constitutive specification. The constitutive choices

$$
\begin{aligned}
&\boldsymbol{T} = \boldsymbol{T}^e + \boldsymbol{T}^d,\\
&\boldsymbol{T}^e = \rho\left(-\boldsymbol{E}^T\frac{\partial\psi}{\partial\boldsymbol{E}} - \boldsymbol{W}^T\frac{\partial\psi}{\partial\boldsymbol{W}} - \left(\frac{\partial\psi}{\partial\boldsymbol{\alpha}}:\boldsymbol{\alpha} + \frac{\partial\psi}{\partial\boldsymbol{\beta}}:\boldsymbol{\beta}\right)\boldsymbol{I} + \left(\frac{\partial\psi}{\partial\boldsymbol{\alpha}}\right)^T\boldsymbol{\alpha} + \left(\frac{\partial\psi}{\partial\boldsymbol{\beta}}\right)^T\boldsymbol{\beta}\right),\\
&\boldsymbol{T}^d_{\text{sym}} = \text{ identical to restrictions of Ericksen-Leslie theory [Les92]},\\
&\boldsymbol{\Lambda} = \boldsymbol{X} : \left[\boldsymbol{n}\otimes\frac{\partial\psi}{\partial\boldsymbol{E}}\right] + \rho\left[\frac{\partial\psi}{\partial\boldsymbol{\beta}} - \operatorname{tr}\left(\frac{\partial\psi}{\partial\boldsymbol{\beta}}\right)\boldsymbol{I}\right](\boldsymbol{E}-\boldsymbol{G})^T,\\
&{}^{\beta}\boldsymbol{V} \text{ in the direction of } \boldsymbol{X} : \left[\left(\rho\frac{\partial\psi}{\partial\boldsymbol{E}} + \operatorname{curl}\left[\rho\frac{\partial\psi}{\partial\boldsymbol{\beta}}\right]\right)^T\boldsymbol{\beta}\right] =: \boldsymbol{f}^{\beta},\\
&{}^{\alpha}\boldsymbol{V} \text{ in the direction of } \boldsymbol{X} : \left[\left(-\rho\frac{\partial\psi}{\partial\boldsymbol{W}} + \operatorname{curl}\left[\rho\frac{\partial\psi}{\partial\boldsymbol{\alpha}}\right]\right)^T\boldsymbol{\alpha}\right] =: \boldsymbol{f}^{\alpha},
\end{aligned}
\tag{9.1}
$$

achieve non-negative dissipation in the model. Reasonable constitutive equations for defect motion may be assumed to be

$$
{}^{\beta}\boldsymbol{V} = m^{\beta}\frac{\boldsymbol{f}^{\beta}}{|\boldsymbol{f}^{\beta}|}; \quad {}^{\alpha}\boldsymbol{V} = m^{\alpha}\frac{\boldsymbol{f}^{\alpha}}{|\boldsymbol{f}^{\alpha}|},
$$

where $m^\alpha, m^\beta \geq 0$ are frame-indifferent scalar functions. For example, $m^\alpha = \frac{|\boldsymbol{f}^\alpha|}{B^\alpha|\boldsymbol{\alpha}|}$ with B^α a material constant that characterizes the dislocation drag that arises from energy dissipated at scales that are not resolved by the continuum fields.

We note that non-negative dissipation and frame-indifference are the only constraints on the kinetic functions for the defect velocity specification.

With regard to a constitutive equation for $\operatorname{grad} \boldsymbol{p}$, any gradient of a vector field on the body satisfies the constraint

$$\int_{V(t)} \operatorname{grad} \boldsymbol{g}_P : \operatorname{grad} \boldsymbol{p} \, dv \geq 0$$

and transforms as $(\cdot) \mapsto (\cdot)\tilde{\boldsymbol{R}}^T$ under superposed rigid-body motions of the current configuration suffices; the notion is not empty as a reasonable and simple choice is

$$\operatorname{grad} \boldsymbol{p} = \frac{1}{B^P} \operatorname{grad} \boldsymbol{g}_P; \; B^P > 0,$$

where B^P is a material viscosity constant related to the permeation mechanism.

As examples, we record possible forms of constitutive assumptions for modeling various classes of liquid crystalline materials. We account for our relaxation of the unit magnitude constraint on $\boldsymbol{n}$ by the rescaling:

$$\tilde{\boldsymbol{n}} := \frac{\boldsymbol{n}}{l}; \quad \tilde{\boldsymbol{E}} := \frac{\boldsymbol{E}}{l}; \quad \tilde{\boldsymbol{\beta}} := \frac{\boldsymbol{\beta}}{l} \tag{9.2}$$

9.1 The nematic liquid with director defects

A proposed model is the standard Ericksen-Leslie nematic liquid augmented with a treatment of director defects. We make the choices

$$\frac{\partial \psi}{\partial \boldsymbol{W}} \equiv \boldsymbol{0}, \frac{\partial \psi}{\partial \boldsymbol{\alpha}} \equiv \boldsymbol{0}, \frac{\partial \boldsymbol{p}}{\partial \boldsymbol{x}} \equiv \boldsymbol{0}, {}^\alpha\boldsymbol{V} \equiv \boldsymbol{0}.$$

Then, $(6.1)_5$ is simply the kinematic compatibility relationship between the deformation gradient map of the current configuration from any arbitrarily fixed reference configuration and the velocity gradient field on the current configuration. Denoting the deformation gradient from this arbitrary reference as $\boldsymbol{F} := \boldsymbol{W}^{-1}$, we note that

$$\dot{\boldsymbol{W}} = -\boldsymbol{W}\boldsymbol{L} \Leftrightarrow \dot{\boldsymbol{F}}\boldsymbol{F}^{-1} = \boldsymbol{L}.$$

Thus, this equation is identically satisfied if the current configuration is achieved by a motion of the body that is compatible with the reference at all instant of time.

If the nematic is further assumed to be incompressible, one adds a term $-P\boldsymbol{I}$ to $(9.1)_1$ to account for the incompressibility constraint

$$\operatorname{div} \boldsymbol{v} = 0$$

and the latter is an additional equation to be solved. Here P is a constitutively undetermined pressure field that is determined by the field equations and boundary conditions.

For the free energy density, one could adopt the OZF form [Ose33; Zoc33; Fra58] augmented by a simple defect core energy:

$$\psi_n = \frac{1}{2\rho_0}\left(\begin{array}{l} k_1\left(\tilde{\boldsymbol{E}}:\boldsymbol{I}\right)^2 + k_2\left(\tilde{\boldsymbol{n}}\cdot\left(\boldsymbol{X}:\tilde{\boldsymbol{E}}\right)\right)^2 + k_3\left|\tilde{\boldsymbol{n}}\times\left(\boldsymbol{X}:\tilde{\boldsymbol{E}}\right)\right|^2 \\ +(k_2+k_4)\left(\left(\tilde{\boldsymbol{E}}\right)^2:\boldsymbol{I}-\left(\tilde{\boldsymbol{E}}:\boldsymbol{I}\right)^2\right)+k_5 l_\beta^2\left(\tilde{\boldsymbol{\beta}}:\tilde{\boldsymbol{\beta}}\right) \end{array}\right) + p\left(|\tilde{\boldsymbol{n}}|-1\right)^2. \tag{9.3}$$

Here, k_1, k_2, k_3 are the splay, twist, and bend constants; (k_2+k_4) is the saddle-splay constant and k_5 is a modulus related to defect core energies, expected to be of the order of the other standard moduli; l_β is a length of the order of the spatial extent of the cross section of the defect core; and l is the length of the nematic molecule along the director. $\boldsymbol{E}$ is naturally assumed to be dimensionless (following $\boldsymbol{G}$) and the various moduli have the physical units of force or energy per unit length [see e.g. Hal72; Ste04]. ρ_0 is the density of the state in which the measurement of the moduli were made and $p>0$ is a penalty moduli with units of stress to impose the fixed-length constraint on the director.

We note that while the energy density (9.3) is essentially the same as the OZF energy in the absence of defects, it deviates from the OZF energy in the presence of defects due to the fact that $\operatorname{grad}\boldsymbol{n}\neq\boldsymbol{E}$, even when $\boldsymbol{n}$ is locally close to a unit vector field and the core term is ignored. Maintaining the correspondence in the presence of defects appears to be difficult, primarily because of the ambiguity in defining a director field that corresponds to an $\boldsymbol{E}$ in the presence of defects.

In correspondence with the elasticity of solids, it is natural to expect that the OZF energy displays non-convexity in the director distortion at large magnitudes to reflect a breakdown in director elastic strength with increasing director deformation.

A constitutive equation for ${}^{\beta}\boldsymbol{V}$ is required, and a simple form that may be assumed is

$${}^{\beta}\boldsymbol{V} = \frac{\boldsymbol{f}^{\beta}}{B^{\beta}g\left(|\boldsymbol{\beta}|\right)}; \quad g\left(|\boldsymbol{\beta}|\right)=1 \text{ or } |\boldsymbol{\beta}|$$

where B^{β} is a defect drag coefficient.

Finally, the viscous stress can follow the EL theory [e.g. Ste04]:

$$\boldsymbol{T}^d = \alpha_1\left(\tilde{\boldsymbol{n}}\cdot\boldsymbol{D}\tilde{\boldsymbol{n}}\right)\tilde{\boldsymbol{n}}\otimes\tilde{\boldsymbol{n}}+\alpha_2\left(\dot{\tilde{\boldsymbol{n}}}-\boldsymbol{\Omega}\tilde{\boldsymbol{n}}\right)\otimes\tilde{\boldsymbol{n}}+\alpha_3\tilde{\boldsymbol{n}}\otimes\left(\dot{\tilde{\boldsymbol{n}}}-\boldsymbol{\Omega}\tilde{\boldsymbol{n}}\right)+\alpha_4\boldsymbol{D}+\alpha_5\left(\boldsymbol{D}\tilde{\boldsymbol{n}}\right)\otimes\tilde{\boldsymbol{n}}+\alpha_6\tilde{\boldsymbol{n}}\otimes\boldsymbol{D}\tilde{\boldsymbol{n}}.$$

The various $\alpha_{(\cdot)}$ are the well-established Leslie viscosities.

9.2 The cholesteric liquid with director defects

The model is structurally the same as for the nematic, except for the replacement of $k_2\left(\tilde{\boldsymbol{n}}\cdot\left(\boldsymbol{X}:\tilde{\boldsymbol{E}}\right)\right)^2$ by $k_2\left(t_0+\tilde{\boldsymbol{n}}\cdot\left(\boldsymbol{X}:\tilde{\boldsymbol{E}}\right)\right)^2$ in the nematic energy (9.3).

9.3 The smectic-A phase with director defects and dislocations

The liquid-like response remains the same as for the nematic. However, there is additionally a solid-like response due to the positional ordering of the smectic layers.

Our model is motivated by those in [E97; Ste07]. We posit an undeformed director $\boldsymbol{a}_0$ that characterizes the smectic layer normal in the undistorted elastic reference (Section 5) with $|\boldsymbol{a}_0|$ being the undistorted inter-layer spacing. Now define the deformed layer normal as

$$\boldsymbol{a} = \boldsymbol{W}^T \boldsymbol{a}_0.$$

Then a simple phenomenological energy density for the smectic is

$$\psi_s = \psi_n + \psi_e\left(|\boldsymbol{a}| - |\boldsymbol{a}_0|\right) + \frac{1}{2}\rho_0 p_s \left(1 - \left(\frac{\boldsymbol{n}\cdot\boldsymbol{a}}{|\boldsymbol{n}|\,|\boldsymbol{a}|}\right)^2\right) + \frac{1}{2}\rho_0 \mu b^2 \boldsymbol{\alpha} : \boldsymbol{\alpha}. \tag{9.4}$$

Here, ψ_e is a positive scalar function characterizing (positional) elasticity of the smectic layers that penalizes changes in interlayer spacing. The third term penalizes orientations of the layer normal that are not aligned with the director, with p_s a penalty modulus with units of stress. In the fourth term, μ is a typical modulus related to the elasticity of layer deformation and b is a length scale of the order of the cross-section of the dislocation core.

A simple constitutive equation for the dislocation velocity ${}^{\alpha}\boldsymbol{V}$ that may be assumed is

$${}^{\alpha}\boldsymbol{V} = \frac{\boldsymbol{f}^{\alpha}}{B^{\alpha} g\left(|\boldsymbol{\alpha}|\right)}; \quad g\left(|\boldsymbol{\alpha}|\right) = 1 \text{ or } |\boldsymbol{\alpha}|,$$

where B^{α} is a dislocation drag coefficient.

The fluid viscous response, i.e. the specification for $\boldsymbol{T}^d$, is as in nematics. However, a distinguishing feature of flow in smectics is a very high flow viscosity [Hel69]. In crystalline materials, the primary source of non-Newtonian viscosity is slip deformations in the lattice. Extending that analogy to the smectic case, a simple constitutive equation might be

$$\operatorname{grad} \boldsymbol{p} = m^P \operatorname{grad} \boldsymbol{g}_P$$

where m^P is a permeation mobility constant that is set to reflect the higher observed viscosity due to permeation.

9.4 The Smectic-C phase with director defects and dislocations

The model is identical to the Smectic A except the third term in (9.4) is replaced:

$$\frac{1}{2}\rho_0 p_s \left(1 - \left(\frac{\boldsymbol{n}\cdot\boldsymbol{a}}{|\boldsymbol{n}|\,|\boldsymbol{a}|}\right)^2\right) \quad \text{changes to} \quad \frac{1}{2}\rho_0 p_s \left((\cos\theta_0)^2 - \left(\frac{\boldsymbol{n}\cdot\boldsymbol{a}}{|\boldsymbol{n}|\,|\boldsymbol{a}|}\right)^2\right)$$

where θ_0 is the angle between the smectic-C layer normal and the director.

9.5 The nematic, cholesteric, and smectic A/C liquid crystal elastomers with dislocations and director defects

We set $\boldsymbol{T}^d = \boldsymbol{0}$ in the various liquid crystal models as well as $m^P = 0$ for the smectics. We then add an appropriate solid free energy response for the elastomer to obtain a nematic liquid crystal elastomer. A

possible choice for this additional energy is the neo-classical energy density of Bladon et al. [BWT94]:

$$\psi_{nc} = \frac{1}{2}\mu \left[\left(\boldsymbol{l}\left(\tilde{\boldsymbol{n}}_0\right) \boldsymbol{W}^{-T} \boldsymbol{l}^{-1}\left(\tilde{\boldsymbol{n}}\right) \boldsymbol{W}^{-1} \right) : \boldsymbol{I} \right],$$

where $\boldsymbol{l}$ is a given symmetric invertible tensor-valued function of $\tilde{\boldsymbol{n}}$, and $\tilde{\boldsymbol{n}}_0$ is a known reference director field that remains unchanged under superposed rigid body motions.

9.6 Columnar Liquid Crystals

Columnar liquid crystals have two distinguished directions, $\boldsymbol{a}_0$ and $\boldsymbol{b}_0$ in the reference [KL03]. Hence, in the deformed configuration, $\boldsymbol{a} = \boldsymbol{W}^{-1}\boldsymbol{a}_0, \boldsymbol{b} = \boldsymbol{W}^{-1}\boldsymbol{b}_0$. The positional elastic strain energy density will depend on $\boldsymbol{a}, \boldsymbol{b}$ in a frame-indifferent way. Closely analogous to smectics (9.4), the free energy will contain penalties to impose the co-directionality between $\boldsymbol{n}$ and $\boldsymbol{a} \times \boldsymbol{b}$.

10 Conclusion

We have relied on four primary design criteria in developing this model:

1. Defects are introduced through geometrically rigorous spatial densities (Euclidean-space analogs of 1-, 2- and 3-forms) and the consequent conservation laws.
2. In the absence of defects, the model for liquid crystalline materials should reduce to the Ericksen-Leslie model.
3. The specification of nematic elasticity response must depend only on the current configuration (both positional and orientational) of the body and not prior states.
4. Defects should be identified as localizations in fields and it should not be necessary to deal with them as individual entities in specifying the rules of dynamic evolution.

Criterion 1, though fairly general and therefore weak, has some significant implications. For example, consider a second-order tensor order parameter $\boldsymbol{A}$ which is not known or defined to be a spatial density, i.e., it is not an object that can be integrated along curves, or areas, or volumes. Then, even if one were to write a conservation law for it, the nature of the flux of $\boldsymbol{A}$ is not clear. For instance, if $\boldsymbol{A}$ was the volume-density of a (second order) tensor field (i.e. a second order tensor-valued 3-form), the appropriate rate of change of $\boldsymbol{A}$ would be the divergence of a third order tensor flux field that represents a second order tensor-valued 2-form. On the other hand, if $\boldsymbol{A}$ were an areal density of a vector field (a vector-valued 2-form), the appropriate time derivative would be the curl of a second order tensor flux field that represents a vector-valued 1-form. Moreover, the appropriate convected time derivatives also take very different forms in the two cases[6]. For this reason, despite our high regard for Ericksen's intuition for the mechanics of liquid crystals and his seminal contributions to the understanding of these materials,

[6]The (back-leg) convected derivative, with respect to a flow, of a 2-form (2.1) is naturally different from that of a 1-form (4.4). For a 3-form a, it equals $\dot{a} + a \operatorname{div} \boldsymbol{v}$. Essentially, they arise from transport theorems for areas, curves, and volumes, respectively.

we have reservations about the balance law for the degree of orientation field, S, in [Eri91]: it is not physically clear to us what the generalized momentum P (corresponding to S) represents. A similar comment applies to the corresponding flux, T, although, from the mathematical balance law it is clear that the generalized momentum P is intended to be a scalar-valued 3-form (a volume density of a scalar) and its flux, therefore, is a scalar valued 2-form (an areal density of a scalar).

Criterion 1 also has practical implications for computation. Conservation forms have advantages for the design of numerical approximation schemes, e.g. based on the finite volume method in computational fluid dynamics [LeV02], or providing natural weak forms for the finite element method [LW02]. In combination with Criterion 4, the regularized nature of the auxiliary fields permits us to bypass the explicit tracking of individual defects in contrast to configurational force treatments as in, e.g., [SSF09; AK91b; PB03]. We emphasize, however, that the kinetic relation between the defect velocity and the driving force can, in principle, be as complex as necessary to model the material, in marked contrast to conventional regularizations of defect motion as demonstrated in, e.g., [AK91a]. This enables a temporal multiscale strategy that can easily incorporate kinetic laws from molecular calculations [e.g. following the procedure outlined in DJ09]. Finally, Criteria 1 and 4 allow a clear separation between the defect kinetics and the energetics even with the regularization of defects.

Criterion 2 has important practical consequences as the EL model has been thoroughly validated and there is a wealth of information about these features of the model. There also exists a comprehensive literature on experimental measurements of the material constants [e.g. Lar99]. The practical difficulties in going to a format far-removed from the EL model can be appreciated from a reading of Sonnet et al. [SMV04].

Criterion 3 is, to us, a physical requirement that can be justified from a molecular basis. In adhering to this, our model stands at odds with that presented in [ACF99].

With respect to Smectic A response, our elastic response function for the couple stress tensor differs from that given in [Ste07]. This is a direct consequence of the integration-by-parts carried out there, as discussed in Section 8 surrounding (8.5). The flow viscosity coefficients admitted in [Ste07] are more general than in EL theory and consequently ours. Stewart's smectic A model is a mechanically sound generalization of E's model [E97], making clear the manner in which balance of angular momentum and the couple stress tensor are to be understood in the latter theory. A fundamental construct of both models is a field equation for the 'layer variable' whose evolution uses a newly-introduced 'permeation force at the boundary' [E97], that expends power associated with the evolution of the layer variable. This model has been effectively used to study the dynamics of filaments during the isotropic-smectic A phase transition [EPM99]. Smectic A response represents a gradual transition of the liquid crystalline material towards positional order characteristic of solids and defects in such ordering, and we believe that the 'extra-nematic' response is best posed in the context of positional kinematics and elasticity of solids.

A very interesting recent paper by Klein et al. [KLGCC08], in accord with Criterion 4 above, demonstrates a practical theory for liquid crystal polymers that is capable of predicting the occurrence of disclinations in flows. Their model is motivated from the microscopic theory due to Doi [Doi81]. An averaging procedure with several closure assumptions provides an evolution equation for the second moment of the distribution function in Doi's theory. An asymmetric stress tensor for a non-simple material is introduced, following Feng et al. [FSL00], and a result from Doi and Edwards [DE88] is used to justify a 'body torque' that balances the torque produced by the skew symmetric part of the stress. A similar model is utilized to understand defect morphology and dynamics in Yang et al. [YFMW09]. The fundamental basis of our model is obviously very different from these approaches, especially the treatment

of angular momentum balance and the operational dissipative mechanisms. However, our model shares features with these works in being able to deal with defects, seamless interpolation between the solid and liquid-like states, and the relative ease (expected, in our case) of practical computation. Hence, it would be useful to compare future predictions that emerge from a numerical implementation of our model.

We believe that this work is the first to lay out a geometrically exact framework for the study of both orientational and positional defects in liquid crystal materials. This can enable the study of a rich class of theoretical questions and physical phenomena in liquid crystalline materials spanning the liquid to the solid state. For example, Fried and Sellers [FS06] show that the inverse elastic distortion (here $\boldsymbol{W}$) in a liquid crystal elastomer can become incompatible in the presence of a radial hedgehog defect in the nematic director field. In conventional liquid crystal elastomer models, this is a serious practical problem as an incompatible total deformation requires abandoning the fundamental kinematics; this leads Fried and Sellers to question the validity of the assumed defect structure or the constitutive equations in their static calculations. In our setting, this merely describes a dislocation defect in the positional order associated with a hedgehog defect in the orientational order, and what persists in time is decided by dynamics that is, at the least, approximately computable. As is known, disclinations in bulk are observed in liquid crystal polymers (LCP) both in the liquid [GM84] and solid [DWH06] phases. An important mechanism of time-dependent deformation for polymers is nonlinear viscoelasticity, and this can be modeled within our framework by a straightforward augmentation following the ideas of [Doi81] and [BB98].

Important open questions yet remain in our formulation. First, to clarify the kinematic connection between our defect fields $\boldsymbol{\beta}$, $\boldsymbol{E}$ and the powerful DeGennes $\boldsymbol{Q}$ tensor, particularly since the latter automatically respects the head-to-tail symmetry of the director field. Second, the related question of a kinematic connection between $\boldsymbol{\beta}$, $\boldsymbol{E}$ and the notion of disclinations as topological objects with fixed angular deficits. Third, also related, is the problem of going both from an observed director field to $\boldsymbol{n}$, $\boldsymbol{E}$ and reconstructing a physically useful director field from $\boldsymbol{n}$, $\boldsymbol{E}$. These questions are the focus of our current research.

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A Geometric motivation for the director incompatibility balance law

For those unfamiliar with the notion of convected (generalized Lie) derivatives, we begin with an example specific to our context that exposes the geometric structure of these time derivatives. Recalling the definition of the orthogonal tensor field $\boldsymbol{R}$ and defining its initial condition as

$$\dot{\boldsymbol{R}}\boldsymbol{R}^T = -\boldsymbol{\Gamma}; \quad \boldsymbol{R}(s) = \boldsymbol{I},$$

the left side of (4.5) can be expressed as

$$\left[\boldsymbol{R}^T\boldsymbol{\Gamma}(\boldsymbol{E}-\boldsymbol{G})\boldsymbol{F}+\boldsymbol{R}^T\overset{\cdot}{\overline{(\boldsymbol{E}-\boldsymbol{G})}}\boldsymbol{F}+\boldsymbol{R}^T(\boldsymbol{E}-\boldsymbol{G})\boldsymbol{L}\boldsymbol{F}\right]_{t=s}=\left[\boldsymbol{R}\left(\overset{\cdot}{\overline{\boldsymbol{R}^T(\boldsymbol{E}-\boldsymbol{G})\boldsymbol{F}}}\right)\boldsymbol{F}^{-1}\right]_{t=s}=\overset{\odot}{\overline{(\boldsymbol{E}-\boldsymbol{G})}}\,.$$

Thus, $\overset{\odot}{\overline{(\boldsymbol{E}-\boldsymbol{G})}}$ represents the push-forward of the time derivative of the pull-back of $\boldsymbol{E}-\boldsymbol{G}$ by the pointwise time-dependent tensor functions $\boldsymbol{R}$ (front-leg) and $\boldsymbol{F}^{-T}$ (back-leg), evaluated at $s=t$. Thus it is a mixed, covariant convected derivative which cannot be viewed as a Lie derivative because of the fact that two (more-or-less) unrelated time-dependent tensor functions are involved in the pull-back and push-forward operations, one of which (i.e., $\boldsymbol{R}$) may not lend itself to interpretation as a deformation gradient of *any* flow of the basic manifold. To see the resulting convected derivative transparently, consider two sets of time-dependent bases

$$\boldsymbol{c}_i(t)=\boldsymbol{R}(t)\boldsymbol{c}_i(s);\quad \boldsymbol{e}_i(t)=\boldsymbol{F}(t)\boldsymbol{e}_i(s),$$

where s is an arbitrarily fixed instant of time. The corresponding dual bases are denoted as $(\boldsymbol{c}^i:i=1,2,3)$ and $(\boldsymbol{e}^i:i=1,2,3)$ with $\boldsymbol{c}^i(t)=\boldsymbol{R}(t)\boldsymbol{c}^i(s)$ and $\boldsymbol{e}^i(t)=\boldsymbol{F}^{-T}(t)\boldsymbol{e}^i(s)$. We write the tensor $(\boldsymbol{E}-\boldsymbol{G})$ on these mixed bases:

$$(\boldsymbol{E}-\boldsymbol{G})=(E-G)_{ij}\boldsymbol{c}^i\otimes\boldsymbol{e}^j;\quad (E-G)_{ij}=\boldsymbol{c}_i\cdot(\boldsymbol{E}-\boldsymbol{G})\boldsymbol{e}_j.$$

Then,

$$\overset{\odot}{\overline{(\boldsymbol{E}-\boldsymbol{G})}}=\left[\overset{\cdot}{\overline{(E-G)_{ij}}}\boldsymbol{c}^i\otimes\boldsymbol{e}^j\right]_{t=s}=\left[\boldsymbol{R}\left(\overset{\cdot}{\overline{(E-G)_{ij}\boldsymbol{R}^T\boldsymbol{c}^i\otimes\boldsymbol{F}^T\boldsymbol{e}^j}}\right)\boldsymbol{F}^{-1}\right]_{t=s}.$$

It is because of this *pull-back* $\rightarrow$ *time derivative* $\rightarrow$ *push forward* structure that these derivatives are useful to differentiate a one-parameter family of tensors where the elements of the family do not belong to the same linear space.

We now provide the motivation behind stating the director incompatibility balance in the form (4.2). The preliminary notion is a desire to write a balance law for densities of lines in the form

$$\overset{\cdot}{\overline{\int_{a(t)}\boldsymbol{\beta}\boldsymbol{\nu}\,da}}=-\int_{c(t)}\boldsymbol{\beta}\times\boldsymbol{V}\,d\boldsymbol{x}.$$

Localization of the integral balance produces the term $\mathring{\boldsymbol{\beta}}$ on the left side. However, from its definition, $\boldsymbol{\beta}(\boldsymbol{x},t)$ is a tensor that maps a time-evolving tangent space at a point on the current configuration to itself. Thus, simply adopting a 'back-leg' convected derivative for $\boldsymbol{\beta}$ does not make rigorous geometric sense. Since we are working in Euclidean space, a valid meaning can still be attached to such a derivative, and we could accept such an object if it did not interfere with the overall structure of the theory[7]. However, in the situation with director incompatibility, such a device does not work; if the free energy density is a function of $\boldsymbol{E}$, as it is for the materials considered here, the dissipation of the model is not frame-indifferent. Summing vectors from tangent spaces of different base points of a manifold, as implied in the writing of an integral, also does not make rigorous geometric sense: however, again, the Euclidean structure allows a meaning to be attached to the integral and, in this case, such an operation does not interfere with frame-indifference down the road.

[7]Balance of linear momentum is an example of a widely-accepted physical equation that contains a time derivative that is not frame-indifferent.

Hence, we define the auxiliary (front-leg) pulled-back, two-point tensor field

$$\operatorname{curl}\left(\boldsymbol{R}^T(\boldsymbol{E}-\boldsymbol{G})\right) =: \boldsymbol{\beta}^s, \tag{A.1}$$

where s is still the arbitrarily fixed instant of time introduced in connection with (4.3). Now consider a conservation law for $\boldsymbol{\beta}^s$ in the form

$$\overset{\cdot}{\int_{a(t)} \boldsymbol{\beta}^s \boldsymbol{\nu}\, da} = -\int_{c(t)} \boldsymbol{\beta}^s \times \boldsymbol{V}^s\, d\boldsymbol{x} \quad \forall t,$$

where $\boldsymbol{V}^s$ is the velocity of the $\boldsymbol{\beta}^s$ at time t. With arguments similar to (4.3), we arrive at

$$\boldsymbol{R}^T\boldsymbol{\Gamma}(\boldsymbol{E}-\boldsymbol{G})\boldsymbol{F} + \boldsymbol{R}^T\overset{\cdot}{(\boldsymbol{E}-\boldsymbol{G})}\boldsymbol{F} + \boldsymbol{R}^T(\boldsymbol{E}-\boldsymbol{G})\boldsymbol{L}\boldsymbol{F} = -\boldsymbol{\beta}^s \times \boldsymbol{V}^s \quad \text{for all } t \text{ with } s \text{ held fixed.} \tag{A.2}$$

From a mathematical standpoint this is a reasonable expression; however, physically it has the shortcoming that it involves an arbitrary history dependence through the definition of $\boldsymbol{R}, \boldsymbol{F}$ that cannot be relevant in describing the evolution of director distortion or incompatibility. This is not an obstacle, as we evaluate (A.2) at $s = t$, since s was fixed arbitrarily. Moreover, the procedure can be repeated for all values of s, fixing s first, performing the time derivative, and then evaluating for $s = t$, i.e. choosing the current configuration as the reference. Consequently, we arrive at the evolution equation for director distortion (4.5).

On asking the question of what integral balance law is consistent with (4.5) *for all instants of time*, one simply reverses the computation of arriving at (4.5) from (4.1) and (4.2) to observe that (4.2), with its specific geometric source term, is the correct statement.

An interesting fact is that from the point of view of using an objective time rate, $\boldsymbol{F}^{-1}$ instead of $\boldsymbol{R}^T$ could just as well have been used for the pull-back in (A.1). However, this would not suffice for the frame indifference arguments in Section 8. Physically, $\boldsymbol{R}$ is the obvious tensor to pull back the 'front-leg' of $(\boldsymbol{E}-\boldsymbol{G})$.

B Analytical solution for non-singular axial disclinations

In this appendix, we use our approach to construct a solution to a family of wedge disclinations for the 1-constant OZF energy.

For the sake of analysis, very often the equations governing statics of nematics is converted to an angle parametrization. This is more so in the analysis of defects, where all analysis is done for such equations, e.g. [dGP95; Ste04]. We demonstrate our ideas on the possibility of finite energy axial disclinations within the context of such angle parametrized equations and within the standard 1-constant OZF energy.

The governing equations are obtained under the ansatz $\boldsymbol{n} = \cos\theta(x_1, x_2)\boldsymbol{e}_1 + \sin\theta(x_1, x_2)\boldsymbol{e}_2$. Here, θ is the angle measured from the x_1 axis. Within the context outlined, it is a standard result [dGP95; Ste04] that equilibrium for planar nematic configurations is governed by the equation $\operatorname{div}\operatorname{grad}\theta = 0$. Following our strategy of replacing the director gradient field with an incompatible director "gradient", we introduce the vector fields $\boldsymbol{E}^\theta, \boldsymbol{\beta}^\theta$ in the angle-parametrized formulation with the governing equations:

$$\operatorname{curl}\boldsymbol{E}^\theta = \boldsymbol{\beta}^\theta, \quad \operatorname{div}\boldsymbol{E}^\theta = 0 \tag{B.1}$$

These are exactly the equations that are satisfied by the incompatible, antiplane displacement "gradient" of the screw dislocation in the linear theory of continuously distributed dislocations. Non-singular solutions to these have been worked out in [Ach01] using the formalism of the Riemann Graves integral for solving exterior differential equations, and we simply translate that solution to the current context. For modeling of finite-energy axial disclinations, we impose the following class of $\boldsymbol{\beta}^\theta$ field:

$$\boldsymbol{\beta}^\theta(x_1,x_2)=\begin{cases}\phi(r)\boldsymbol{e}_3, r<r_0\\ \mathbf{0}, r\geq r_0\end{cases};r=(x_1^2+x_2^2)^{\frac{1}{2}} \tag{B.2}$$

with the stipulation that

$$2k\pi=\int_0^{2\pi}\int_0^{r_0}\phi(r)\,dr\,rd\psi\Rightarrow k=\int_0^{r_0}\phi(r)\,rdr \tag{B.3}$$

where k is the strength of the disclination and r_0 is a core radius. Then following Section 5.2 in [Ach01], we have the solution

$$\begin{aligned}&\text{For } r<r_0: \quad E_1^\theta=\frac{-x_2}{r^2}\int_0^r\phi(s)s\,ds, E_2^\theta=\frac{x_1}{r^2}\int_0^r\phi(s)s\,ds\\ &\text{For } r\geq r_0: \quad E_1^\theta=k\frac{-x_2}{r^2}, E_2^\theta=k\frac{x_1}{r^2}\end{aligned} \tag{B.4}$$

It can be checked that this solution indeed satisfies the governing equations (B.1) for any ϕ satisfying the given conditions. For the choice

$$\phi(r)=\begin{cases}\frac{2k}{r_0}\left(\frac{1}{r}-\frac{1}{r_0}\right), r\leq r_0\\ 0, r>r_0\end{cases} \tag{B.5}$$

the inside-core solution evaluates to

$$\text{For } r\leq r_0: \quad E_1^\theta=\frac{-x_2}{r^2}\left(\frac{2k}{r_0}\left[r-\frac{r^2}{2r_0}\right]\right), E_2^\theta=\frac{x_1}{r^2}\left(\frac{2k}{r_0}\left[r-\frac{r^2}{2r_0}\right]\right) \tag{B.6}$$

while the outside-core distribution remains unchanged.

The classical singular solutions due to Frank for these axial wedge-disclination problems are given as [dGP95; Ste04]:

$$\theta(x_1,x_2)=k\arctan\left(\frac{x_2}{x_1}\right)+\phi_0 \tag{B.7}$$

where ϕ_0 is a constant, and it can be checked that the gradient of this field matches our outside-core solution. As mentioned in [Ach01], for any axially-symmetric core incompatibility distribution whose singularity is stronger than in (B.5) results in singular angle-distortion field $\boldsymbol{E}^\theta$ with singularity at $r=0$, while anything weaker results in vanishing distortion at $r=0$. Of course, the classical result due to Frank can be recovered by choosing ϕ as a Dirac distribution centered at $r=0$.

It is also a standard (but perhaps not so well-known) result of potential theory [Bâr05] that the outside-core, irrotational angle-distortion field (essentially on a doubly connected domain arising from excluding the core) corresponds to the gradient of an infinite family of angle fields (resulting in corresponding director fields), some of which are given by (B.7), for varying ϕ_0.

Thus, it becomes clear that the classical singular solutions necessarily entail non-uniqueness and singularity. On the other hand, the problem posed in terms of the distortion is better-posed and devoid of

singularity, which is physically desirable. In fact, this desirable feature is what lead to the discovery of the famous "escape" solutions [CK72] for $+1$ strength axial disclinations. Of course, no physical configuration can be expected to have infinite energy and what we have demonstrated here is the possibility of such solutions within our theory, regardless of the strength of the disclination. For this reason we consider this demonstration as an improvement in the status of the theory of liquid crystals. In some sense, we have exchanged singularity and non-uniqueness for a multiple-scale theory through the introduction of a locally concentrated, but nonsingular, incompatibility field. On the question of whether such locally-concentrated equilibrium or very-slowly evolving configurations of incompatibility can arise dynamically within our model, we refer to [AMZ10; AT11] which deal with model equations that would arise from our model where an affirmative answer is provided.

A heuristic observation is in order here. Note that in the core region where the incompatibility does not vanish, an angle parametrization cannot be defined. This may be interpreted as suggesting that the representation of the state requires more than a single parameter, a feature embedded in the representation of state by the distortion vector (instead of the gradient of a scalar field). In fact, a model of a biaxial core surrounding a uniaxial disclination line as a model of the $k = \frac{1}{2}$ disclination is demonstrated in [KL03].

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