

On the Analysis of Twisted Director Configurations

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A twist tensor (**T**-tensor) is introduced, which is defined for differentiable vector and director fields. Its eigensystem describes the local helical structure of the underlying field. It can have up to two nonzero eigenvalues, which indicate whether the local structure is untwisted, helical or double-twisted. The eigenvalues q_i , if real valued, are the helical wave numbers, and the corresponding eigenvectors represent the local twist axes. The **T**-tensor can serve as a tool to analyze director configurations in chiral nematic liquid crystals, and applications in computational fluid dynamics seem feasible.

1. Introduction

In this paper a twist tensor, derived from an at least once differentiable directional field, is defined and investigated. It is shown to be particularly useful as an instrument to analyze director fields of nematic liquid crystals.

The orientational order of a nematic liquid crystal is usually described by a *director field* indicating locally the preferred axis of orientation for the molecules. The director field is mathematically a directional field represented locally by a vector \mathbf{n} of unit length, i.e.

$$n_\mu n_\mu = 1. \quad (1)$$

Twisted nematics can be characterized by the (dimensionless) free energy per unit volume in the one-constant approximation [1]

$$f = n_{\mu,v} n_{\mu,v} + 2 q_0 \varepsilon_{\mu\nu\lambda} n_\mu n_{\lambda,v}. \quad (2)$$

We use the cartesian component notation, i.e. the gradient is written $n_{\mu,v} = \nabla_v n_\mu$ and the cross product is $\varepsilon_{\lambda\mu\nu} a_\mu b_\nu = (\mathbf{a} \times \mathbf{b})_\lambda$ with the total antisymmetric symbol ε . The first term in (2) is the elastic energy and the second one the chiral contribution; q_0 is the intrinsic helical wave number. The elastic part may be decomposed into four contributions using the identity [2]

$$n_{\mu,v} n_{\mu,v} = (\operatorname{div} \mathbf{n})^2 + (\mathbf{n} \cdot \operatorname{rot} \mathbf{n})^2 + (\mathbf{n} \times \operatorname{rot} \mathbf{n})^2 - \operatorname{div}(\mathbf{n} \times \operatorname{rot} \mathbf{n} + \mathbf{n} \operatorname{div} \mathbf{n}). \quad (3)$$

The four terms on the right hand side of (3) are referred to (in order of sequence) as *splay*, *twist*, *bend*, and *saddle-splay*. It is demonstrated in Sect. 4 that

some properties of the **T**-tensor are related to these partial energies.

A director field in equilibrium has to satisfy the Euler-Lagrange equation

$$n_{\mu,vv} + 2 q_0 \varepsilon_{\mu\nu\lambda} n_{v,\lambda} + \lambda n_\mu = 0, \quad (4)$$

where the Lagrange multiplier λ (needed to satisfy (1)) is found to be

$$\lambda = f. \quad (5)$$

In thin slabs with planar anchoring, the helical solution

$$\mathbf{n}(z) = (\sin qz, \cos qz, 0) \quad (6)$$

is usually encountered. In confined geometries like capillaries and droplets, however, the director fields are more complicated. In those cases it is not always easy to see whether there is single or double twist, in which direction the twist axis or axes point, and how large the local helical wave number(s) are.

This information can be extracted from the “twist-tensor” (referred to below as **T**-tensor). In the subsequent sections, twist axes and their corresponding wave numbers and the **T**-tensor are defined and illustrated by some examples. In Sect. 4, some mathematical properties of the **T**-tensor are derived. Section 5 contains the conclusions and acknowledgements.

2. Twist Axes and Wave Numbers

Given an arbitrary directional field \mathbf{n} , we define a twist axis at a given point to be an axis perpendicular to both the directional field and its directional derivative along this axis. Thus a unit vector \mathbf{t} defines the

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direction of a twist axis iff both

$$t_\mu n_{v,\mu} t_v = 0 \quad \text{and} \quad (7)$$

$$t_\mu n_\mu = 0 \quad (8)$$

hold true. The strength associated with the axis is defined to be the normalized modulus of the directional derivative

$$\pm \sqrt{\frac{t_\mu n_{v,\mu} t_\lambda n_{v,\lambda}}{n_\gamma n_\gamma}}, \quad (9)$$

where the sign is determined by the orientation of the helix. In the case of the helical solution (6), this equals the helical wave number q .

3. The Twist Tensor

A twist axis is defined by a direction, a strength and an orientation. Thus it yields three degrees of freedom and the question arises, whether it can be represented by a vector. This is not the case, as can be seen by considering a rotation by π around an axis perpendicular to the twist axis. Obviously, a vector changes sign, while the twist axis remains unchanged*. Thus the simplest representation is given by a second rank tensor, which, due to its transformation under space inversion, is actually a pseudo tensor.

Definition: The **T**-tensor field corresponding to a directional field \mathbf{n} is defined by

$$T_{\mu\nu} := \frac{\varepsilon_{\mu\kappa\lambda} n_\kappa n_{\lambda,\nu}}{n_\gamma n_\gamma}. \quad (10)$$

The solution of its eigenvalue problem

$$T_{\mu\nu} t_\nu^{(i)} = \lambda^{(i)} t_\mu^{(i)} \quad (11)$$

yields the twist axes. Let us call a real-valued nonzero eigenvalue of T a twist-eigenvalue. An eigenvector \mathbf{t} corresponding to a twist-eigenvalue λ represents a twist axis, with λ being the associated strength and the local helical wave number in direction of \mathbf{t} . Here and below, eigenvector means a right eigenvector as defined in (11). A straightforward calculation shows that this definition is consistent with the one given in the previous section in (7)–(9).

* This is the reason why you do not have to worry which way to put the nut on the bolt.

Let τ be the number of twist-eigenvalues of T . Then, there are three possibilities:

1. $\tau=0$. There is no local twist distortion at all, that is, $\mathbf{n} \cdot \text{rot } \mathbf{n} = 0$.
2. $\tau=1$. The local structure is helical. A specific example where the helical axis coincides with the z -axis has been given in (6).
3. $\tau=2$. The local structure is double twisted. A typical example is given below in (14).

The case $\tau=3$ does not occur, cf. Sect. 4.

An analogy to classical differential geometry should be mentioned: T can be considered as a generalized binormal \mathbf{b} to an integral curve Ψ of \mathbf{n} . Consider $T_{\mu\nu} w_\nu$: It specifies that the derivative occurring in (10) is taken in the direction of \mathbf{w} . Looking for twist axes means focusing on directions \mathbf{w} which are perpendicular to \mathbf{n} (see Sect. 4). In contrast, $\mathbf{w}=\mathbf{n}$ yields $T_{\mu\nu} n_\nu = k b_\mu$, where k is the curvature of Ψ . This analogy is interesting because the binormal \mathbf{b} contains information about the torsion of Ψ via Frenet-Serret's equations [3].

In the following we consider four examples of specific director fields and the associated twist tensor fields.

Example 1: the **T**-tensor of the helical director field (6) has the eigenvalues $\{0, 0, q\}$, and the eigenvector corresponding to q is $(0, 0, 1)$.

Example 2: chiral materials are in their ground state if the “double twist condition”

$$n_{j,k} + q \varepsilon_{ijk} n_i = 0 \quad (12)$$

is met. It has been shown by geometrical arguments that (12) can be fulfilled only locally [4]. At sites where (12) holds, the twist tensor has the form

$$T_{\mu\nu} = q(\delta_{\mu\nu} - n_\mu n_\nu). \quad (13)$$

This tensor has the multiple eigenvalues $\{q, q, 0\}$, and any vector perpendicular to \mathbf{n} is an eigenvector to q . Any two orthogonal eigenvectors to the eigenvalue q together with \mathbf{n} form an eigensystem.

Example 3: As an illustrating example, and in order to demonstrate the advantage of the **T**-tensor, the well-known double twist tube [4] is firstly presented by its director field, and secondly by its twist axes. The directors are represented by rods, and the eigensystem of the **T**-tensor by a parallelogram (which is a rectangle in this specific example). The edges are parallel

to the eigenvectors, and their lengths correspond to the eigenvalues. For single twist, the rectangle degenerates to a line. The director field used here is

$$\mathbf{n}(r, \phi) = (\sin \phi \sin qr, -\cos \phi \sin qr, \cos qr). \quad (14)$$

This is no equilibrium configuration satisfying (4), but it is quite similar to a known solution [5] in which qr is replaced by $2 \arctan r/R$. The above director field (14) has been chosen as an example because an analytical description of the eigensystem is available:

$$\lambda_1 = q, \quad \lambda_2 = \frac{\sin 2qr}{2r} \quad (15)$$

and

$$\mathbf{e}_1 = \begin{pmatrix} \cos \phi \\ \sin \phi \\ 0 \end{pmatrix}, \quad \mathbf{e}_2 = \begin{pmatrix} -\cos qr \sin \phi \\ \cos qr \cos \phi \\ \sin qr \end{pmatrix}. \quad (16)$$

Here \mathbf{e}_1 , \mathbf{e}_2 , and \mathbf{n} are mutually perpendicular, which, as will be shown in the next section, is not generally the case. See Figure 1.

In the \mathbf{T} -tensor representation, only the central region, where the director rotates by $\pi/2$, is depicted because outside the marked area the second helical wave number λ_2 becomes small, and one has effectively a single twist, cf. (15).

Although this director configuration is particularly simple due to its translational and rotational symmetry, it is not obvious in which directions the twist axes point, since only one layer is depicted. Showing more than one layer, however, would make the picture rather intricate.

Example 4: This is an example of an untwisted director field, namely the well known radial configuration which occurs in droplets with perpendicular boundary coupling. The director field

$$\mathbf{n} = \frac{\mathbf{r}}{\|\mathbf{r}\|} \quad (17)$$

is spherically symmetric with a point defect (a so-called hedgehog) in the center. The nonzero eigenvalues of the \mathbf{T} -tensor are

$$\lambda_{1/2} = \pm \frac{i}{r}, \quad (18)$$

where $i = \sqrt{-1}$ and $r = \|\mathbf{r}\|$. The radial configuration exhibits no twist (the twist energy is zero everywhere), and the saddle-splay energy is $-2/r^2$. A relationship between these two energies and the eigenvalues of the \mathbf{T} -tensor is derived in the subsequent section.

4. Properties of the Twist Tensor

The following properties hold for any directional field \mathbf{n} , which for simplicity is assumed to be normalized. The first three properties are of general interest, while the last three are especially related to director fields of chiral nematics. Proofs are omitted where straightforward.

1. Orthogonality between \mathbf{e} and \mathbf{n} : Let λ be a nonzero eigenvalue of \mathbf{T} , and \mathbf{e} the corresponding eigenvector. We have then $\mathbf{e} \perp \mathbf{n}$. It follows that the director can be easily deduced from the graphical representation of the \mathbf{T} -tensor as the layer normal of the rectangles (provided there is double twist).

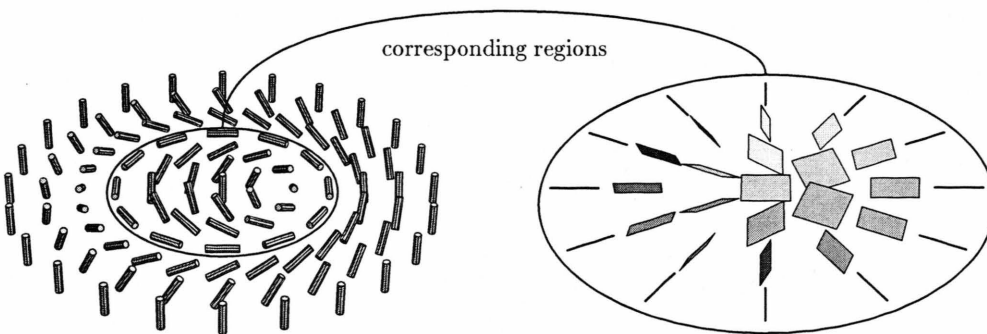


Fig. 1. Director field and \mathbf{T} -tensor field of a double-twist tube. The edges of the \mathbf{T} -tensor rectangles are parallel to the twist axes, and their lengths correspond to the local helical wave number. For single twist, the rectangles degenerate to lines. The \mathbf{T} -tensor representation is shown only for the central region where the director rotates by $\pi/2$.

- 2. Angle between e_1 and e_2 :** Let λ_1, λ_2 be nonzero eigenvalues of T , and e_1, e_2 the corresponding eigenvectors. In general, e_1 is not perpendicular to e_2 .

Proof: Let u_1, u_2, u_3 be three mutually orthogonal unit vectors defined by $u_1 := e_1$, $u_3 := n$, and $u_2 := u_3 \times u_1$. In this local base, T has the form

$$T = \begin{pmatrix} -n_{2,1} & -n_{2,2} & T_{13} \\ 0 & n_{1,2} & T_{23} \\ 0 & 0 & 0 \end{pmatrix}. \quad (19)$$

The components T_{13} and T_{23} need not to be specified, since the eigensystem does not depend on them. The eigenvalues are

$$\lambda_1 = T_{11} \equiv -n_{2,1}, \quad \lambda_2 = T_{22} \equiv n_{1,2}. \quad (20)$$

If $\lambda_1 \neq \lambda_2$ the corresponding eigenvectors are

$$e_1 = (1, 0, 0), \quad \text{and} \quad e_2 = \left(\frac{n_{2,2}}{\lambda_2 - \lambda_1}, 1, 0 \right). \quad (21)$$

It follows that $e_1 \perp e_2$ iff $n_{2,2} = 0$.

- 3. Determinant:** $\text{Det}(T) = 0$, cf. (19). As a consequence, the number of twist axes cannot exceed two.
- 4. Trace:** $\text{Tr}(T) = \varepsilon_{\mu\nu\lambda} n_\mu n_{\lambda,\nu}$ is a pseudoscalar proportional to the chiral contribution to the free energy density (2). The magnitude $-2q_0$ is a material property.
- 5. Norm:** The expression

$$\|T\| := \sqrt{\text{Tr}(T \cdot T)} \quad (22)$$

is a measure for the “overall twist”, at least if it is real-valued. Note that example 4 in the preceding section yields a negative value for $\|T\|^2$. Calculation of $\text{Tr}(T \cdot T)$ both in the cartesian representation (10) and in the eigen-representation (19) yields the interesting identity

$$\lambda_1^2 + \lambda_2^2 = n_{\mu,\nu} n_{\mu,\nu} - (n_{\mu,\mu})^2 - n_\mu n_\nu n_{\lambda,\mu} n_{\lambda,\nu}. \quad (23)$$

The first term on the right is the total elastic energy and the next two are the splay and the bend contribution to the energy with a negative sign, cf. (3). Accordingly, the sum of the squared eigenvalues is

proportional to the sum of the twist and the saddle-splay energies.

- 6. Equilibrium:** We will now assume that n is a director field in equilibrium, that is, (4) holds. It follows that

$$\begin{aligned} (\text{div } T)_\mu &= T_{\mu\nu,\nu} = 2q_0 \varepsilon_{\mu\nu\lambda} \varepsilon_{\kappa\gamma\lambda} n_\nu n_{\gamma,\kappa} \\ &= 2q_0 (n \times \text{rot } n)_\mu. \end{aligned} \quad (24)$$

Thus twist sources (or sinks) occur in relaxed director fields if both an intrinsic chirality ($q_0 \neq 0$) and a bend distortion exist.

5. Conclusions and Acknowledgements

A twist tensor associated with a differentiable directional field has been defined. For the director field of a chiral nematic liquid crystal it yields the twist axes and the corresponding twist wave numbers via its eigenvectors and eigenvalues. It can be used to analyze computed or modelled director fields, particularly in two and three dimensions, complementing the usual director representation. Also, it displays a number of interesting properties. The most remarkable one, from a liquid-crystal physicist's point of view, is that its norm depends not only on the twist, but also on the saddle-splay energy, which is basically a surface term and has therefore often been disregarded.

As an aside, the definition of the T -tensor $T_{\mu\nu}$ (cf. (10)) can be canonically generalized to cases where the alignment of the nematic phase cannot be described by a director, but rather must be represented by an alignment tensor $a_{\mu\nu}$ [6]:

$$T_{\mu\nu}^a = \varepsilon_{\mu\lambda\kappa} a_{\lambda\kappa} a_{\lambda\kappa,\nu}. \quad (25)$$

$T_{\mu\nu}^a$ simplifies to $T_{\mu\nu}$ when $a_{\mu\nu} = n_\mu n_\nu - \frac{1}{3} \delta_{\mu\nu}$. It can be employed to analyze twisted alignment tensor configurations, e.g. configurations describing the blue phases.

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