The elements of texture

1. **Umbilic Lines in Orientational Order**
   Authors: Thomas Machon and Gareth P. Alexander
   Phys. Rev. X **6**, 011033 (2016); DOI: 10.1103/PhysRevX.6.011033
2. **Interpretation of saddle-splay and the Oseen-Frank free energy in liquid crystals**
   Authors: Jonathan V. Selinger
   Liquid Cryst. Rev. **6**, 129-142 (2019); arXiv:1901.06306
3. **Uniform distortions and generalized elasticity of liquid crystals**
   Authors: Epifanio G. Virga
   Phys. Rev. E **100**, 052701 (2019); arXiv:1908.09872

Recommended with a Commentary by Gregory M. Grason, UMass Amherst

Orientational order in liquid crystalline states is inherently malleable, which leads to the outstanding variety of *textures*, or spatial patterns of orientation, they display. Central to the understanding of liquid crystals for decades is the Oseen-Frank (OF) elastic theory that describes their free energy in terms of orientational gradients. A recent series of papers shows that an alternative approach for decomposing of gradient patterns greatly simplifies the classification of liquid crystalline textures.

In the standard OF formulation, the free energy density for distortion the director, $\mathbf{n}(\mathbf{x})$, from its uniform ground state describes all possible square gradients (i.e. second order in first derivatives of $\mathbf{n}$) consistent with nematic symmetry [1]:

$$F_{OF} = \frac{1}{2}K_{11}(\nabla\cdot\mathbf{n})^2+\frac{1}{2}K_{22}\big[\mathbf{n}\cdot(\nabla\times\mathbf{n})\big]^2+\frac{1}{2}K_{33}\big[(\mathbf{n}\cdot\nabla)\mathbf{n}\big]^2+K_{24}\,\nabla\cdot\big[(\mathbf{n}\cdot\nabla)\mathbf{n}-\mathbf{n}(\nabla\cdot\mathbf{n})\big]. \quad (1)$$

The first term of Eq. (1) describes the cost of *splayed* configurations, which can be measured by scalar $S \equiv \nabla\cdot\mathbf{n}$. The second penalizes *twisted* textures, where the director locally winds around some direction perpendicular (e.g. as in the uniaxial cholesteric texture), and is measured by a pseudo-scalar $T \equiv \mathbf{n}\cdot(\nabla\times\mathbf{n})$. The third term describes *bending* and is measured by the vector $\mathbf{B} = -(\mathbf{n}\cdot\nabla)\mathbf{n}$ (equal to the curvature times the normal to the field lines of $\mathbf{n}$). The final term is less widely known, and differs from the first 3 in that it is not positive definite. This "K_{24} term" is called the *saddle-splay* because, when $\mathbf{n}$ can be associated with the normal to a surface, the term is equal to its Gaussian curvature and is negative for saddle-shaped surfaces (i.e. favorable when $K_{24} > 0$). Because the K_{24}-term is a total divergence, it can be integrated to the boundary of the sample, and therefore is neglected in the vast majority of applications of the OF energy, where anchoring conditions fix $\mathbf{n}(\mathbf{x})$ at the boundary.

The free energy for material that realizes nematic symmetry includes only these square gradient terms *, distinguished by the values of Frank constants K_{11}, K_{22}, K_{33} and K_{24}. Notwithstanding its breadth, the formulation of Eq. (1) introduces some ambiguity about the status of saddle-splay as a boundary term vs. the "primary" bulk terms, splay, twist and bend. Indeed, there are prominent scenarios in which free boundaries become abundant, particularly where molecular geometry and interactions favor non-zero gradients everywhere. For example, in the liquid crystal blue phases [2], "doubly-twisted" director gradients (column 2 of Fig. 1) are preferred due to a linear term in T allowed for chiral molecules, but geometric compatibility enforces extensive disclinations arrays to thread through the bulk between local double-twist domains. In such cases, the contribution from the K_{24}-term at the defect cores is essential. Moreover, some textures have non-zero "saddle-splay energy", but have nothing to do with surfaces, saddles or otherwise. For example, there is no surface whose normal follows the "double-twist" texture favored in blue phases (Fig. 1), yet $\nabla \cdot \big[(\mathbf{n}\cdot\nabla)\mathbf{n} - \mathbf{n}(\nabla\cdot\mathbf{n})\big] \neq 0$ for that texture.

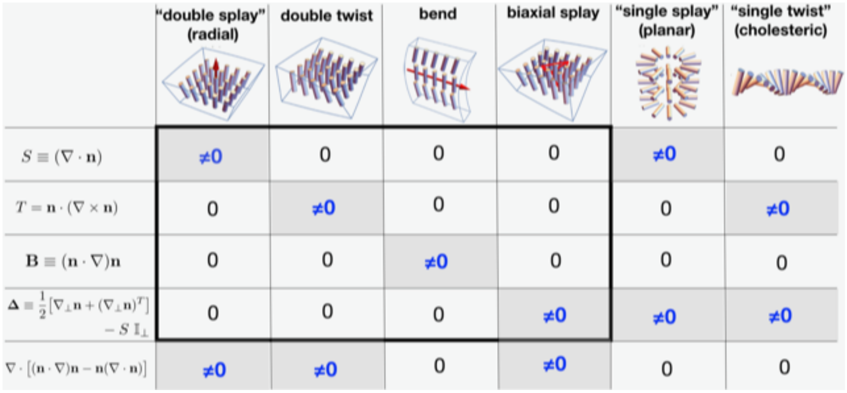
An alternative decomposition of gradient textures put forward by Machon and Alexander (MA) provides a means of resolving and reinterpreting these arguably unsavory aspects of the OF description. At the heart of the study of MA is a different, but related, question about complex field configurations that are topologically nontrivial, but nonsingular in terms of director pattern. Examples include skyrmion textures in 2D or so-called Hopfions in 3D [3, 4], where the director is everywhere smooth, yet the field configuration is topologically wound up in such a way that it can't be smoothly distorted back to a uniform one. For textures that are topologically non-trivial but smooth, where exactly does that topological information reside? To answer this, MA show that the gradient tensor of first derivatives $\nabla\mathbf{n}$ (from which F_{OF} is constructed) can be broken into 4 distinct and irreducible "elements". The first 3 are associated with the splay, twist and bend.

To understand the fourth "element", which I simply call "$\boldsymbol{\Delta}$", first consider the gradient tensor where the derivative along $\mathbf{n}$, i.e. bend, has been subtracted off, $\nabla_\perp\mathbf{n} \equiv \nabla\mathbf{n} - \mathbf{n}\mathbf{B}$. The tensor $\nabla_\perp\mathbf{n}$ only has non-zero components in the *plane perpendicular to the director*. It can then be represented by the 2×2 matrix of first derivatives of $\mathbf{n}$ in this perpendicular plane. The matrix can split up into 3 irreducible pieces. The first two of these – its trace and skew symmetric elements – simply correspond to S and T, respectively. Subtracting off the "tracefull" and antisymmetric parts of $\nabla_\perp\mathbf{n}$ then gives a symmetric, traceless (rank 2) matrix; this is Δ. Represented as a matrix the 2D plane perpendicular to $\mathbf{n}$

$$\nabla_\perp\mathbf{n} = \frac{S}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{T}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} \Delta_1 & \Delta_2 \\ \Delta_2 & -\Delta_1 \end{pmatrix}. \tag{2}$$

As a symmetric and traceless matrix, $\boldsymbol{\Delta}$ can be characterized by the equal and opposite eigenvalues and eigendirections in the plane. Fig. 1(fourth column) shows a "pure $\boldsymbol{\Delta}$" texture (i.e. $S = T = |\mathbf{B}| = 0$): along one of the eigendirection, the director splays outward, while in the orthogonal direction is splayed inward by an equal amount.

*That is, neglecting terms that are second-order (or higher) in derivatives of $\mathbf{n}$.



	"double splay" (radial)	double twist	bend	biaxial splay	"single splay" (planar)	"single twist" (cholesteric)
$S \equiv (\nabla \cdot \mathbf{n})$	≠0	0	0	0	≠0	0
$T = \mathbf{n} \cdot (\nabla \times \mathbf{n})$	0	≠0	0	0	0	≠0
$\mathbf{B} \equiv (\mathbf{n} \cdot \nabla)\mathbf{n}$	0	0	≠0	0	0	0
$\mathbf{\Delta} \equiv \frac{1}{2}[\nabla_\perp \mathbf{n} + (\nabla_\perp \mathbf{n})^T] - S\,\mathbb{I}_\perp$	0	0	0	≠0	≠0	≠0
$\nabla \cdot [(\mathbf{n} \cdot \nabla)\mathbf{n} - \mathbf{n}(\nabla \cdot \mathbf{n})]$	≠0	≠0	0	≠0	0	0

Figure 1: A schematic table showing how derivative operators "measure" gradients of $\mathbf{n}$ for different characteristic textures. The 4×4 block highlights the irreducible decomposition of MA. The last row illustrates that the "K_{24} -term" as a mixture of 3 "pure" modes, while the last two columns illustrate "single" splay and twist to pure "double" modes. Figures are adapted from Selinger (2019).

What can be gained from extracting the $\mathbf{\Delta}$ mode? For one, MA show that the topological structure of non-singular configurations are generically characterized by what they call "umbillic lines" in the field, places where $\mathbf{\Delta} = 0$ and in the plane perpendicular to $\mathbf{n}$, the gradient texture is (locally) isotropic. Like the umbillic points of surfaces (degeneracies in the principles curvatures), umbillics in nematics or vector fields can be characterized by the winding of the eigendirections around them, leading to a rich and natural framework to unify classification of a number of topologically complex and smooth textures as they describe in detail.

In a second paper, Selinger builds on this decomposition to recast the energetics of nematic elasticity, in a surprisingly simpler light. Notably, the four modes – splay, twist, bend and $\mathbf{\Delta}$ – are "normal" in the sense that tensor multiplication of unlike components $\nabla\mathbf{n}$ is zero. On these grounds, Selinger argues that breaking gradients up into these four irreducible elements provides a more natural description of the characteristic "modes". The free energy, eq. (1), can be rewritten,

$$F_{OF} = \frac{1}{2}\Big[K_S S^2 + K_T T^2 + K_B |\mathbf{B}|^2 + K_\Delta |\mathbf{\Delta}|^2\Big], \tag{3}$$

where $K_S = K_{11} - K_{24}$, $K_T = K_{22} - K_{24}$, $K_B = K_{33}$ and $K_\Delta = 2K_{24}$. In this way, the standard K_{24} gets split up into it constituent elements of splay, twist and $\mathbf{\Delta}$ – what Selinger calls *biaxial splay* – and in so doing, converts the free energy density into the sum of the squares of these four bulk "modes". As shown in the schematic table of Fig. 1, this not only reinterprets saddle-splay in terms of biaxial splay + splay + twist, but it also reinterprets the notion of what is "pure twist" and "pure splay" as local configurations which are strictly uniaxial in the plane perpendicular to $\mathbf{n}$ (and therefore have only T or S nonzero among the 4 modes). Hence, the canonical twisted texture, the cholesteric (e.g. with $\mathbf{n}$ winding a single fixed axis), is in fact a mixture of pure (double) twist and biaxial splay. Beyond its algebraic elegance, Selinger argues that this decomposition demystifies some implications of the K_{24} – specifically the stability of the blue phase as well as the spontaneous chirality for large K_{24} – in terms this of purely bulk elastic theory.

Maybe even more compelling is that this geometric decomposition of orientation gradients resets the framework to consider long-standing puzzles about the compatibility of Euclidean space with director patterns that favor *uniform gradients*. The classic example of this is indeed the chiral phases that due to the "screwy" symmetries of their molecular constituents favor everywhere $S = |\mathbf{B}| = |\mathbf{\Delta}| = 0$ but also constant twist, $T = T_0 \neq 0$. Because uniform, pure double twist is frustrated (in flat space) [2], constant T is only possible along 1D curves, and extending this texture to a "thicker" tubular region necessarily introduces other components (e.g bend). A third paper by Virga takes up this thread to answer the question, what are the possible textures in (flat) 3D space that allow uniform gradients (i.e. with splay, twist, bent and biaxial splay realizing uniform magnitudes)? The answer to this question is exactly one and only class of textures, known as the *heliconical* textures, which are splay free, but have constant, twist, bend and **Delta**. Heliconical textures are realized by tipping the directors of a cholesteric up along the its pitch axis by a constant angle. Meyer conjectured them long ago to be the optimal solution for the director field that favors constant bend but zero twist and splay [6], and more recently, they have been the subject of intense experimental interest in the context of *bent-core* mesogens [7].

The fact the only strict set of uniform gradient textures is possible is certainly a useful step in classifying the set of possible phases that could be exhibited by molecules of more complex shape preferences (e.g. a "target texture" favoring constant $\mathbf{\Delta} \neq 0$, but zero twist, bend and splay). But, in my view, this perspective largely sharpens what we don't know. Given that few possibilities exist for textures that satisfy strict conditions of "uniformity", what are the broader possibilities (beyond blue phases) for non-uniform energy density textures that can outcompete the uniform heliconical textures as energy minimizers for a given target texture? An alternative perspective might ask [8], if you can "bend the rules" of Euclidean spaces, which spatial curvatures are compatible with much broader (non-heliconical) class of uniform textures, and what can be learned by trying drag these rarified textures back down to the lowly flat 3D Euclidean space liquid crystals are force to live with?

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