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# Singular Values, Nematic Disclinations, and Emergent Biaxiality

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Both uniaxial and biaxial nematic liquid crystals are defined by orientational ordering of their building blocks. While uniaxial nematics only orient the long molecular axis, biaxial order implies local order along three axes. As the natural degree of biaxiality and the associated frame, that can be extracted from the tensorial description of the nematic order, vanishes in the uniaxial phase, we extend the nematic director to a full biaxial frame by making use of a singular value decomposition of the gradient of the director field instead. New degrees of freedom are unveiled in the form of quasi-defects and the similarities and differences between the uniaxial and biaxial phase are analyzed by applying the algebraic rules of the quaternion group to the uniaxial phase.

Nematic liquid crystals are revered for their geometrically complex and visually compelling defect structures, stabilized by topological constraints [1]. The elementary rules of homotopy that govern these defects [2–8] imply ambiguities in defect classification when disclination lines are involved due to the action of the first homotopy group on itself and on the second homotopy group. Nematic defects have been probed in both nematic and cholesteric colloids and emulsions [9–12], highly confined geometries [13–15], and optically manipulated liquid crystals [16, 17]. So robust are they, that they can be manipulated to reproducibly form linked or knotted disclination lines [18–21] as well as other topologically interesting objects [22, 23]. Recall that uniaxial nematics can be interpreted as a highly symmetric special case of biaxial nematics [4, 6], suggesting an opportunity to study nematic defects with tools that are not available in the standard homotopy theory. In this letter, we explore the similarity between distortion patterns found in uniaxial nematics and defects in biaxial phases by introducing a new biaxial frame *derived entirely from deformations of the uniaxial director field* $\mathbf{n}$. Like the Frenet-Serret frame of a curve or the principal axes frame of a surface [24], our new frame has a well-defined (differential) geometric meaning and allows us to provide a topological characterization to the director geometry. The "quasi-defects" in this new frame allow us to apply the well-developed theory of biaxial nematics and to include the non-topological "escaped defect" [25] in our classification, embellishing, for instance, our understanding of the double-twist tube construction [26] of the blue phases. A motivation for this investigation is the study of similar quasi-defect structures in optics, where topological filaments in the derivative of a complex scalar field determine the topology of optical vortices [27, 28]. We demonstrate our technique on numerical models of blue phases and discuss the implications of newly extracted information.

Uniaxial nematics consist of elongated non-polar molecules that tend to align in a particular direction in space, taking directions in the manifold $\mathbb{R}P^2$. The *director* is specified by a unit vector $\mathbf{n}$ up to sign. As a result, uniaxial nematics accommodate both line defects (disclinations) and point defects [4, 8] since $\pi_1(\mathbb{R}P^2) = \mathbb{Z}_2$ and $\pi_2(\mathbb{R}P^2) = \mathbb{Z}$. While point defects can be oriented, a line defect, a disclination line, winds the director by $\pi$ leading to a sign inconsistency. Recall, however, that non-defect states exist as disclinations with a non-topological integer winding number. The famous escape into the third dimension renders these smooth [25] in $\mathbf{n}$. As a line field alone, the nematic director does not have an intrinsic biaxial nature. In order to define a biaxial structure, we turn to the tensor of gradients, $\partial_i n_j$, which provides the additional structure necessary to define an entire frame. Multiplying from the left by a unit vector extracts a directional derivative of $\mathbf{n}$; there are special orthogonal directions $[\mathbf{w}^1, \mathbf{w}^2, \mathbf{w}^3]$, in which the magnitudes $||w_i^\alpha \partial_i n_j||^2$ of the derivatives are extreme, which can also be seen as an eigenvalue problem. The derivatives in these directions take the form of $w_i^\alpha \partial_i n_j = \sigma_\alpha n_j^\alpha$ for each $\alpha \in \{1, 2, 3\}$, where $[\mathbf{n}^1, \mathbf{n}^2, \mathbf{n}^3]$ define a *different* orthonormal frame in the domain of the matrix in such a way, that the singular values $\sigma_\alpha$ are positive semi-definite and satisfy $\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq 0$. Because the director $\mathbf{n}$ is a unit vector, it is in the kernel of the derivative tensor, $(\partial_i n_j) n_j = 0$, which implies $\sigma_3 = 0$ and $\mathbf{n}^3 \equiv \mathbf{n}$. This makes the axes $\mathbf{n}^1$ and $\mathbf{n}^2$ orthogonal to $\mathbf{n}$ and decorate the uniaxial phase with a biaxial order! We thus decompose the gradient tensor as:

$$\partial_i n_j = \sigma_1 w_i^1 n_j^1 + \sigma_2 w_i^2 n_j^2 \tag{1}$$

By construction, the derivative of the director is largest in the direction $\mathbf{w}^1$, changing towards $\mathbf{n}^1$ with the rate of $\sigma_1$. The derivative in the direction $\mathbf{w}^2$ points towards $\mathbf{n}^2$ with a lower rate of $\sigma_2$. The remaining vector $\mathbf{w}^3 \equiv \mathbf{w}$ marks the direction in which the director is constant. This is known as the singular value decomposition (SVD) of the matrix $\partial_i n_j$ and proves to be just the thing we need.

It is amusing to note that the derivative tensor is intimately connected to the topological hedgehog charge through the Gauss integral: [8, 29],

$$\begin{aligned} q &= \frac{1}{4\pi}\iint \frac{1}{2}\epsilon_{ijk}\epsilon_{lmp}n_l\partial_j n_m \partial_k n_p \,\mathrm{d}S_i \\ &= \frac{1}{4\pi}\iint \sigma_1\sigma_2 \mathbf{w}\cdot \mathrm{d}\mathbf{S}. \end{aligned} \tag{2}$$

Thus the streamlines of the vector field $\tilde{\mathbf{w}} \equiv \sigma_1\sigma_2\mathbf{w}$ trace the preimage of a particular director orientation as a three-dimensional generalization of the schlieren texture [30] and the topological charge is simply the flux of these streamlines through the enclosing surface. The streamlines can only terminate on the singular nematic defects or where the $\tilde{\mathbf{w}}$ field disappears, *i.e.*, when $\sigma_2 = 0$. The latter are saddles in the derivative field, where the director is constant in two directions.

The SVD frame decorates the director field with two new vectors that encode the transverse degrees of freedom and can be interpreted as a coordinate in $\mathrm{SO}(3)/D_2$ to parameterize biaxial order. In regions where $\partial_i n_j$ does not vanish, the frame is continuous everywhere except on a one-dimensional set of points, which we collectively call line defects or disclinations in the SVD triad, as they are analogous to disclinations in biaxial nematics. There are two types of defects in this frame. On *native disclinations* – line and point defects in $\mathbf{n}$ (for simplicity, we can treat the point defects as small disclination loops [8]), the derivative tensor diverges and the frames and singular values are ill-defined. Away from the defects in $\mathbf{n}$, the SVD decomposition can still give a frame with degenerate axes wherever two singular values coincide; we call these locations *quasi-disclinations*. Both the $\mathbf{n}$-frame and the $\mathbf{w}$-frame share the defects, which are characterized by singularities and degeneracies in the singular values. Each disclination line is characterized by a *pair* of degenerate axes and by the amount of rotation of these axes around the remaining nondegenerate axis – the winding number of the disclination. We will draw an analogy with the biaxial phase and its first homotopy group – the quaternion group written in terms of unit quaternions, $\{\mathbb{1}, -\mathbb{1}, \pm\mathbb{i}, \pm\mathbb{j}, \pm\mathbb{k}\}$ [8, 31]. For the disclinations with half-integer winding number, we shall assign a unit quaternion $\mathbb{i}$ to a defect in axes $\{\mathbf{n}^2, \mathbf{n}\}$, $\mathbb{j}$ to a defect in $\{\mathbf{n}, \mathbf{n}^1\}$ and $\mathbb{k}$ to a defect in $\{\mathbf{n}^1, \mathbf{n}^2\}$. All disclinations with odd integer winding number belong to the class $-\mathbb{1}$, regardless of which pair of axes they involve. Finally, the disclinations with even integer winding number are all trivial, in the $\mathbb{1}$ class.

First, we study the native nematic disclinations. They all involve the director $\mathbf{n}$ as one of the degenerate axes. Moreover, on a tight circle around the disclination, the director rotates very rapidly in the plane defined by the two degenerate axes, so the singular value associated with this direction *diverges* at the defect core. Since the singular values are sorted by magnitude, all native nematic disclinations are, by construction, degenerate in the axes $\{\mathbf{n}, \mathbf{n}^1\}$. To see this, consider a plane perpendicular to the defect line. In this plane $\mathbf{n}$ winds around ever more rapidly as we approach the core. By definition, this rapid winding is into the $\mathbf{n}^1$ direction at all points, $w_i^1\partial_i n_j = \sigma_1 n_j^1$ with $\sigma_1$ diverging. Note that since $\mathbf{n}\cdot\mathbf{n}^1 = 0$, $w_i^1\partial_i n_j^1 = -\sigma_1 n_j + \gamma n_j^2$ where $\gamma$ is finite. It follows that the winding is between $\mathbf{n}$ and $\mathbf{n}^1$ and that the defects associated with the degeneracy of the smallest two singular values, $\sigma_2 = 0$, must be topologically trivial in the $\mathbf{n}$ frame. The disclinations with a half-integer winding number, already known from the homotopy theory of the bare director field, now also have the perpendicular axis $\mathbf{n}^1$ performing a half-integer turn (Fig. 1a). The addition of the perpendicular axes also reveals disclinations with an odd integer winding number, which are not topologically distinguished in the standard uniaxial setting, but are well-defined in our definition (Fig. 1b).

The line-like quasi-disclinations, on the other hand, have smooth director complexions, and so the degenerate axes with nonzero winding number must be the invisible perpendicular axes $\{\mathbf{n}^1, \mathbf{n}^2\}$. These disclinations are located where the singular values $\sigma_1 = \sigma_2$, precisely when we can no longer distinguish the two axes in the decomposition (1). These defects can have either half-integer or integer winding number (Fig. 1c,d).

The odd integer-winding-number disclinations all belong to the same $-\mathbb{1}$ class of biaxial disclinations and can transform one into the other: an unescaped integer winding number disclination with a singular core in $\mathbf{n}$ can escape into the third dimension, which removes the singularity, but still shows up as a defect in the perpendicular axes $\{\mathbf{n}^1, \mathbf{n}^2\}$ of the frame. Our construction therefore unambiguously locates both the escaped and unescaped integer nematic disclinations, which would be impossible to locate from the director field alone.

What about point defects in the uniaxial phase? Biaxial nematics cannot have point defects as $\pi_2[\mathrm{SO}(3)/D_2] = 0$. As we mentioned, to consider the biaxial structure we inflate all point defects into small disclination loops carrying the nontrivial element of $\pi_1(\mathbb{R}P^2)$. Each native disclination loop can either carry an odd or even topological point charge, measured by the second homotopy group, and it can be linked by an even or an odd number of other disclination loops [7, 8, 32, 33]. The half-integer native disclinations and all flavors of integer disclinations form an abelian subgroup $\mathbb{j}^\nu$, $\nu \in \mathbb{Z}_4$ of the quaternion group. This periodicity of four, consistent with the theoretical result given by the torus homotopy group [8, 32] is seen in the specialized form of self-linking numbers for $-1/2$ disclination loops [34]. The statement that the nematic hedgehog charge is a residual of linking a $-\mathbb{1}$ biaxial disclination [8] is intrinsic in our construction.

Unlike in proper biaxial nematics, the point defects are still present in our system – as small native disclination loops, linked by quasi-disclinations. To further

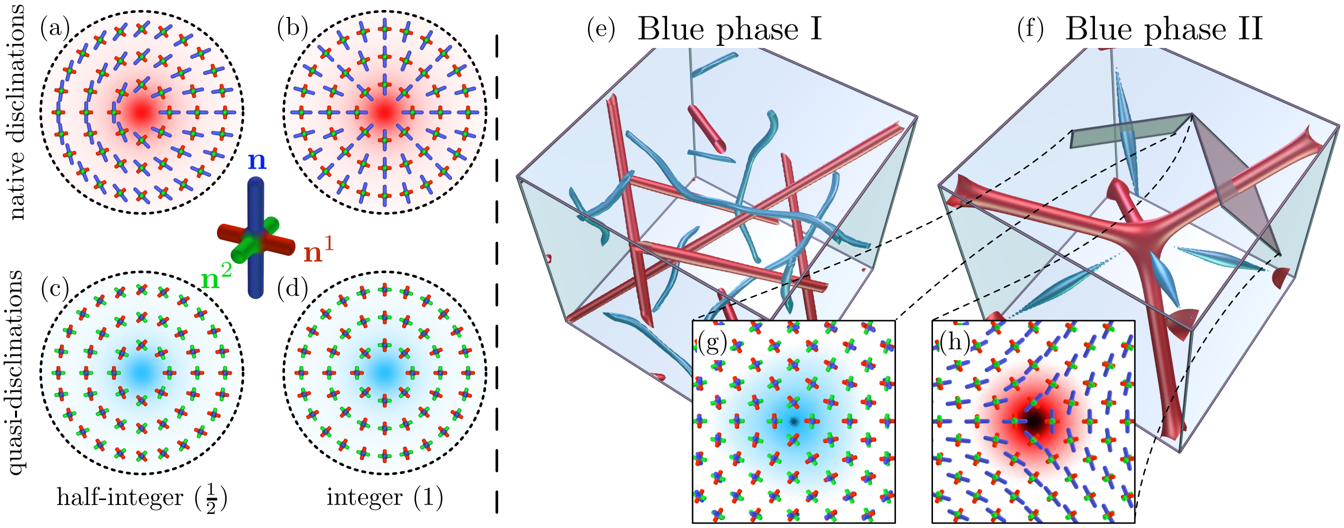


FIG. 1: (color) Sketched profiles for both native (a,b) and quasi-disclinations (c,d). The native disclinations involve half-integer (a) or integer (b) rotation of the director $\mathbf{n}$ and the perpendicular axis $\mathbf{n}^1$. The quasi-disclinations are similar, except the auxiliary axes $\{\mathbf{n}^1, \mathbf{n}^2\}$ are degenerate instead. Each depicted structure is just one of the many representatives of its class, as continuous rotations preserve the topology of the defects. (e,f) Numerical model of blue phases I and II with isosurfaces representing half-integer native (red) and quasi-(cyan) disclinations. BPI has the half-integer quasi-disclinations running along the axes of double twist cylinders, extending infinitely along each lattice direction. BPII has four native disclinations and four half-integer quasi-disclinations meeting at the center, spanning all the diagonals of the cube in an alternating order. (g) At the quasi-disclinations, the axes $\mathbf{n}^1$ (red) and $\mathbf{n}^2$ (green) rotate by $-\pi$ around $\mathbf{n}$ (blue). (h) At the native disclinations, the $\mathbf{n}$ and $\mathbf{n}^1$ axes show a similar behavior, producing a characteristic $-1/2$ disclination profile. (f,g,h) In BPII, exchanging $\mathbf{n}$ and $\mathbf{n}^2$ exchanges the disclinations and effectively rotates the unit cell by $\pi/2$.

explore the connection between the point charge and the threading of the native loops, recall that the topological charge $q$ in nematics is the degree of mapping $\mathbb{R}^3 \to \mathbb{R}P^2$ from a closed measuring surface in the nematic medium to the unit sphere. The director $\mathbf{n}$ on this enclosing surface is in fact a $q$-covered sphere, which by the Riemann-Hurwitz theorem has the Euler characteristic of $\chi = 2q$. The transverse axes $\{\mathbf{n}^1, \mathbf{n}^2\}$ form a tangent plane to $\mathbb{R}P^2$ and so, by the Poincaré-Brouwer theorem, the total winding number of their surface defects must be equal to the Euler characteristic. Every sphere that encloses a point defect is penetrated by quasi-disclinations, with the sum of their winding numbers equal to $2q$. All quasi-disclinations terminate on the point defects and thread native disclination loops that carry a topological charge.

Similarly to the native disclinations, the half-integer quasi-disclinations form a distinct $\mathbb{k}^\nu$ subgroup, with the same algebraic structure and linking rules that we found for the native nematic disclinations. However, the coexistence of half-integer disclinations of both flavors reveals the nonabelian nature of the quaternion group: the $\mathbb{j}$ and $\mathbb{k}$ disclination loops cannot link without creating a $-\mathbb{1}$ line connecting the loops [35]. An additional feature of our gradient framing is the *absence* of $\mathbb{i}$ quaternions representing the impossible disclinations with a degenerate pair of axes $\{\mathbf{n}^2, \mathbf{n}\}$, as discussed above. This is a variation of Poénaru's theorem [36] that limits the merging of defects in gradient fields, as in smectics [37]. Were a half-integer quasi-disclination ($\mathbb{k}$) to merge with a half-integer native disclination ($\mathbb{j}$), the resulting defect would have the impossible signature $\mathbb{i}$, so the quasi-and native defects naturally avoid each other. They can only meet at discrete points – at point defects, which we have shown act as sources or sinks for the quasi-disclinations. As in systems with broken translational symmetry [4, 37], the missing quaternion causes the homotopic description to be incomplete in this case: the $\pm\mathbb{i}$ elements of the fundamental group have no realization in the sample.

We selected a numerical model of blue phases to showcase the SVD construction. Blue phases are a suitable system for studying the biaxial defects on practical data, as they show nonuniform behavior without complicated boundary conditions. We use the finite difference relaxation method, based on the Landau-de Gennes model and material parameters adopted from Ref. [38]. As the existence of quasi-disclinations is topologically conditioned, the precise choice of material parameters plays little role, as long as the blue phase remains stable. The Q-tensor field was used to retrieve the order parameter $S$, and the director field $\mathbf{n}$, which was subsequently differentiated and decomposed with SVD, giving singular values and framing information for each point in space. A large resolution of 80 points along each direction was used to counteract noise caused by discrete approximation of the derivatives. The zeroes of the order parameter $S$ were used to locate the native disclinations, while the zeroes of a functional $\sigma_1 - \sigma_2$ were used to find the quasi-disclinations.

Both blue phases form a periodic cubic lattice. The blue phase I consists of straight native disclinations, extending infinitely in the direction of body diagonals and offset by half of the cell spacing to avoid each other. The rest of the bulk can be roughly explained as mutually perpendicular double-twist cylinders, extending in the direction of main coordinate axes [31]. Plotting the near-zero isosurfaces of $\sigma_1 - \sigma_2$ reveals infinitely extending quasi-disclinations that approximately follow the double-twist cylinders, which is not unexpected, as $\sigma_1 = \sigma_2$ condition implies the rate of change is equal in two directions, which is likely to occur near the axis of a double twist cylinder (Fig. 1e). In particular, the geometric pattern of the cross section has a half-integer winding number and looks like a characteristic three-fold profile of a $-1/2$ nematic disclination line in the axes $\mathbf{n}^1$ and $\mathbf{n}^2$.

The blue phase II consists of a cross-linked network of disclinations. The unit cell contains two junctions where four diagonal native disclinations meet in a tetrahedral formation. The quasi-disclinations also extend from one junction to the other in straight diagonal lines, forming a tetrahedral structure, dual to the native one (Fig. 1f). The junctions are thus highly degenerate meeting points of four native and four half-integer quasi-disclinations, extending to all 8 vertices of the unit cube. An inspection of the disclination cross sections again reveals that both the native and the quasi-disclinations have a three-fold profile (Fig. 1g,h). Furthermore, the cross sections of both disclination types are exact copies of each other, with the axes $\mathbf{n}$ and $\mathbf{n}^2$ in exchanged roles. In fact, the framing across the entire space possesses such a symmetry, that an exchange of these axes has the same effect as a rotation of the unit cell by $90°$. Even though the point symmetry group around the central point is the tetrahedral group, the $\mathbf{n}^1$ axis has a full cubic symmetry, up to a small perturbation that depends on the difference in the free energy costs of native and quasi-defects and could therefore be used as a model director field for a periodic cubic structure with an eight-way central junction of half-integer disclinations [39]. In general, the adjoint fields $\mathbf{n}^1$ and $\mathbf{n}^2$ always have equal or higher symmetry as the original director.

In this letter, we explored the uniaxial nematic as a special kind of biaxial nematic with hidden perpendicular degrees of freedom. Instead of using the eigenvectors of the tensorial order parameter, which is highly degenerate in the uniaxial phase, we retrieved the missing perpendicular axes by using the SVD decomposition of the director derivative, treating the disclination lines as simple defects in the biaxial frame. This frame is nevertheless related to the frame, retrieved from the $Q$-tensor, as the first encodes the spatial variations of the director and the latter describes thermal fluctuations of the molecular director. Both frames are coupled through the free energy functional, allowing the use of director derivatives to estimate the otherwise minute biaxial components of the $Q$-tensor [40]. Continuity of the director field and integrability conditions near singular defects give rise to rules that restrict the set of allowed defects, resulting in an intricate structure that is similar, yet not equivalent to that of general biaxial defects. Beside the native uniaxial nematic disclinations, known from the conventional homotopy analysis, we uncover another type of disclinations that arise through hidden biaxial order – topologically unavoidable patterns in the elastic response, such as the escaped integer disclination lines, which were impossible to treat topologically in bare nematic director fields, but can now be computationally detected. The significance of quasi-disclinations is primarily topological and unlike native disclinations, they have no singular core with associated free energy cost, as they do not represent a divergence of the Q-tensor itself. Such non-energetic topological defect structures are common in other physical systems, such as those in optics. With the elusive defects pinpointed deterministically, the complete set of linking rules for disclination lines emerges and unifies the line and point defects under the same formalism.

The SVD decomposition has a potential use in numerical and analytic calculations, as it couples the free energy with topology via the singular values. The $\mathbf{n}$-frame we focused on in this paper, can be taken as a convenient choice of frame in the Mermin-Ho construction [24]. Additionally, the conjugate $\mathbf{w}$-frame also constitutes a biaxial frame that can be investigated in the future. As a visualization technique, the singular values help to locate the escaped defects and other characteristic features without resorting to visualization of vector fields.

The technique illuminates an intricate link between geometry and topology independent of the physical meaning of the order parameter. In addition to extending the investigation of double-twist structures in blue phases, which we briefly outlined in this letter, the underlying biaxial field can extract hidden degrees of freedom for a wide variety of materials that allow parametrization by an orthogonal frame. Of particular interest for future research are patterns and defects in chiral nematics, smectic liquid crystals and fields of polarized light, building on the connection between local differential structure and the traditional homotopy of defects.

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