Escape from the second dimension: A topological distinction between edge and screw dislocations

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Volterra's definition of dislocations in crystals geometrically distinguishes edge and screw defects according to whether the Burgers vector is perpendicular or parallel to the defect. A homotopy-theoretic analysis of dislocations as topological defects fails to differentiate edge and screw. Here we bridge the gap between the geometric and topological descriptions by demonstrating that there is a topological difference between screw and edge defects. Our construction distinguishes edge and screw based on the disclination-line pairs at the core of smectic dislocations. By exploiting the connection between topology and geometry in the form of Gaussian curvature, this analysis results in an invariant for dislocations in the saddle-splay vector. This construction can be generalized to crystals with triply periodic order.

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Introduction. It has been more than half a century since de Gennes's celebrated analogy between smectic liquid crystals and superconductors [1]. The relationship between the two systems has led to a greater understanding of smectic phases, prominently providing portent for the prediction of the twist grain boundary phase, an analogy to Abrikosov lattices in type II superconductors [2]. However, the structure of topological defects in smectics is profoundly different than that of the vortices in superconductors and superfluids. Not only do smectics enjoy disclinations, defects with no analog in superconductors, but smectics also differ from superconductors by breaking translational rather than internal symmetries [3]. The shortcomings of affording smectics only the complex order parameter of superconductors have also become apparent in recent numerical simulations of smectic defects [4,5]. Note, too, that vortex lines in superconductors have no special direction, but dislocations in smectics come in two types: edge and screw, defined via their geometry. On the other hand, the standard way of viewing dislocations in crystals-that of Volterra [6]-is much older than de Gennes's analogy. The Volterra process explicitly takes advantage of geometry by cutting, shifting, and gluing layers from a perfect crystal to create defects [7]. The direction of the Burgers vector with respect to the defect naturally falls out of this procedure, affording edge and screw dislocations their classical distinction: when the Burgers vector is parallel to the defect it is screw and when it is perpendicular it is edge.

While geometric constructions *alla* Volterra are useful for visualizing dislocations and disclinations, classification of defects and their properties falls within the realm of topology. Here is where a symmetry-based approach more akin to de Gennes's would shine, especially given the success of homotopy-theoretic descriptions of defects in superfluid

phases [8]. However, it was recognized that, in systems with broken translational order, the much-heralded homotopy theory approach to classify defects is inadequate: formally studying smectics as measured foliations, Poénaru proved that disclinations of charge q > 1 cannot coexist with evenly spaced smectic layers in two dimensions [9]. Disclinations in smectics thus do not form a group in the usual homotopy sense [3,10]. A homotopy-theoretic description of dislocations alone does, on the other hand, predict integer-valued Burgers charges. Still, it fails to distinguish between edge and screw dislocations [3], leaving their distinction to Volterra's geometric classification alone. In this paper we resolve this divide between the topological and geometric descriptions of dislocations by demonstrating that there is a topological distinction between screw and edge defects in smectics and, by extension, in all crystals. By studying the pair of disclinations unique to each dislocation core, we are able to detect the topological difference between edge and screw defects. In addition, an integral invariant involving the saddle-splay vector A allows us to measure this distinction away from the core. This relationship between the local defect set and boundary conditions in smectics also serves to answer the question, After inserting one defect in a sample, how do you decide whether the second defect is screw or edge? Should one use the local layer normal to define the Burgers displacement or the layer normal at infinity? The topology of the density wave that forms the smectic resolves this issue as well. We will also demonstrate that in the limit of a single defect in an otherwise perfect ground state, the geometric and topological determinations match.

Background. Smectic liquid crystals are phases with a one-dimensional density modulation $\rho(\mathbf{x}) = \rho_0 + \delta\rho \cos \Phi(\mathbf{x})$, where $\Phi(\mathbf{x})$ determines the phase of the modulation.¹ Density maxima, the level sets $\Phi = 2\pi \mathbb{Z}$,

¹It should not be confused with the volume fraction in "phase field"

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define the smectic layers with a director field parallel to the layer normal $\mathbf{N} = \nabla \Phi / |\nabla \Phi|$. A free energy density that leads to evenly spaced flat layers is, for instance [11],²

$$\mathcal{F} = \frac{B}{8} [(\nabla \Phi)^2 - 1]^2 + \frac{K}{2} (\nabla^2 \Phi)^2, \qquad (1)$$

where B is the bulk modulus controlling layer spacing and K is the bend modulus. This free energy density achieves an absolute minimum when $\Phi = \mathbf{k} \cdot \mathbf{x} + \phi$, where $|\mathbf{k}| = 1$ chooses the direction of the ordering and ϕ is a constant offset. The density wave is invariant under $\Phi \rightarrow \Phi + 2\pi$ and $\Phi \rightarrow -\Phi$. reflecting the discrete translational and rotational symmetries of the smectic. Together, these invariances dictate that the manifold of ground states, represented by different directions of **k** and offsets ϕ , is a Klein bottle for two-dimensional smectics [12] and a twisted circle bundle over $\mathbb{R}P^2$ for threedimensional smectics [13]. Dislocations are lines in three dimensions (or points in two dimensions) around which a Burgers circuit causes a displacement by some integer multiple of the lattice spacing. This winding in the layer labeling causes Φ to be ill defined on the dislocation. Since the density must be well-defined, this implies that $\delta \rho$ must vanish and so the smectic order melts at the defect core. As noted in Refs. [4,10,13-15], this melting can be avoided by breaking the dislocation into a disclination pair, with one disclination on a density maximum and the other on a density minimum.³ Explicitly, a rotation of **k** by π requires $\phi \rightarrow 2\pi n - \phi$ to preserve the symmetries of Φ : a translation by δ is equivalent to a rotation by π followed by a shift by $2\pi n - \delta$. Representing the rotation by π as \mathcal{F} and a shift by δ as \mathcal{S}_{δ} , we have $S_{\delta} = \mathcal{F}^{-1}S_{2\pi n-\delta}\mathcal{F}$ for all $n \in \mathbb{Z}$. From this relation we have $S_{2\pi} = S_{\pi}\mathcal{F}^{-1}S_{-\pi}\mathcal{F}$, that is, a dislocation that induces a shift by 2π and can be broken into a half shift, a rotation by $-\pi$, a half shift *backwards*, and a rotation by π . The net shift is 0 but is replaced by two rotations, i.e., disclinations. Whether this disclination pair or a melted dislocation core is observed in experiment is a matter of energetics-the core could melt into a nematic to lower the overall energy. However, from the topology of the phase field surrounding a melted dislocation core, we can always construct a smectic configuration with a disclination pair that fills the sample.

The disclination pairs are, however, different for an edge dislocation and a screw dislocation. The classic construction of two-dimensional edge dislocations in terms of a $+\frac{1}{2}/-\frac{1}{2}$ disclination dipole [16] extends to three-dimensional edge dislocations, where the core is comprised of a $+\frac{1}{2}$ and $-\frac{1}{2}$ disclination line in parallel. The screw dislocation, on the other hand, only exists in three dimensions. And, in contrast to edge dislocations, screw dislocation cores decompose into a pair of $+\frac{1}{2}$ disclination lines. The geometry of the disclination lines changes as well: were the two disclinations parallel to each other, the requisite screw symmetry of the dislocation would be broken. It follows that the two $+\frac{1}{2}$ disclinations



FIG. 1. Dislocations and the decomposition of their cores into disclination pairs, reproduced from Ref. [14]. (Left) Screw dislocation core composed of two helically winding $+\frac{1}{2}$ disclination lines. (Right) Edge dislocation comprised of a $\pm\frac{1}{2}$ disclination dipole. Both dislocations have Burgers scalar +10, and the insets show the infinite-compression phase structure of Φ_{screw} and Φ_{screw} before replacing their cores. Note the radial nature of the smectic layers entering the screw dislocation core, ensuring the geometry of a +1 disclination, compared to the disclination-charge-neutral edge dislocation.

wind around each other as a pair of regular helices as shown in Fig. 1, reproduced from [14].

Clearly the geometry of edge and screw dislocation cores, constructed as disclination pairs, is different. But are the two configurations topologically distinct? From the perspective of three-dimensional *nematics*, the defect geometries of the screw and edge core are topologically equivalent: recall that disclinations of a nematic director restricted to the plane are characterized by $\pi_1(\mathbb{R}P^1) = \mathbb{Z}$, while a three-dimensional nematic has disclinations characterized by $\pi_1(\mathbb{R}P^2) = \mathbb{Z}_2$. A pair of $+\frac{1}{2}$ nematic line disclinations thus *has no charge*—it escapes into the third dimension [17].

Distinguishing edge and screw. The topological equivalence of the dislocation cores viewed as nematic configurations does not carry over to the smectic phase. Among the extra conditions for smectics, the director, as a surface normal, must satisfy the Frobenius integrability condition $\mathbf{n} \cdot (\nabla \times \mathbf{n}) = 0$, i.e., there can be no twist. The transition of a nematic disclination from pure $+\frac{1}{2}$ to pure $-\frac{1}{2}$ geometries requires passing through intermediary states, known as wedge-twist and pure-twist disclinations, that have nonzero twist distortion. Hence the smooth transition from $a - \frac{1}{2}$ to $+\frac{1}{2}$ disclination is incompatible with smectic order. The disclination pairs at the cores of screw and edge dislocations are thus topologically distinct in the smectic phase. While the dislocation cores cannot transform continuously into each other, it is possible to construct a smectic configuration in which an edge dislocation transitions into a screw dislocation in space. As noted in [14], the transition requires a singular point where the $-\frac{1}{2}$ becomes a $+\frac{1}{2}$ disclination. At this point the Burgers' charge is unchanged, the winding of the phase field Φ is unchanged at large distances, but, importantly, the disclination geometry changes.

It is only because the smectic cannot transition smoothly from one disclination geometry to the other that we can exploit the dichotomy of dislocation cores. From this, it follows that we can distinguish a screw dislocation from an edge

²The normalization is chosen so that if we set $\Phi = z - u(\mathbf{x})$, we then arrive at the standard form of the free energy [7].

³When the Burgers displacement, measured in layer spacing, is even, both disclinations sit on density maxima or minima instead.

dislocation by examining the local texture of the layer normal around the disclination pair of which it comprises. Namely, screw dislocations can be distinguished from edge by their $+\frac{1}{2}$ disclination pair compared to the edge's disclinationcharge-neutral core. There is no need to reference a special direction for the Burgers charge, and, indeed, there is no real sense in which it is a vector in \mathbb{R}^3 —the phase field Φ does not transform under rotations. This is often obscured when one expands around a particular ground state so that $\Phi =$ $z - u(\mathbf{x})$, where the layers are normal to \hat{z} and where $u(\mathbf{x})$ is the standard Eulerian displacement field for a smectic [7]. In this case the transformation of z requires a concomitant transformation in $u(\mathbf{x})$. From a Lagrangian point of view, where we parametrize deformation of the ground state in terms of displacements from a fiducial ground state, it is far more compelling to view the Burgers charge as a vector, especially in the case of three-dimensional crystals (to which we will turn our attention in the following). The Volterra construction relies on this Lagrangian form of elasticity, and therein lies the need for it to distinguish edge and screw dislocations by global geometry.

Two- and three-dimensional crystals can also be described via phase fields: a *d*-dimensional crystal is created via $\rho(\mathbf{x}) =$ $\rho_0 + \delta \rho [\sum_{i=1}^{d} \cos(\Phi_i)]$ so that the lattice points sit at the maxima of all the density waves. Dislocations correspond to winding in one of the Φ_i and, in turn, this dislocation can be split, *mutatis mutandi*, into disclinations associated with that phase field. The remaining phase fields continue to provide a simple, periodic wave in the other directions, creating a dislocation with a Burgers charge in the *i*th phase field. More generally, a dislocation would be characterized by d dislocation charges, one for each phase field. In the ground state $\Phi_i = \mathbf{G}_i \cdot \mathbf{x} + \phi_i$, where \mathbf{G}_i are the reciprocal lattice vectors and ϕ_i set the origin of the crystal. The topological charges associated with each Φ_i are $2\pi n_i$ with $n_i \in \mathbb{Z}$ and can be converted into the Burgers vector $\mathbf{b} = \sum_{i} n_i \mathbf{e}_i$, where the \mathbf{e}_i are the basis vectors with $\mathbf{G}_i \cdot \mathbf{e}_i = 2\pi \delta_{ii}$.

From here, the discussion of splitting dislocations into disclination pairs proceeds as with the smectic for each density wave. It is essential to note that the disclinations are in the phase fields Φ_i and are *not* necessarily the geometric disclinations that the Volterra construction creates. In the case of a smectic they coincide, but in general, the phase disclinations and geometric disclinations are distinct [15]. Again, we can classify screw and edge based on the two topologically distinct disclination geometries that comprise the dislocation core. In an otherwise perfect ground state, the standard distinction between edge and screw (Burgers vector parallel or perpendicular to the dislocation line) provides the same classification as the topological character of their cores. What about adding a defect to a distorted ground state that is otherwise free of topological defects? If the distortions vanish at the boundary, then we can define asymptotic basis vectors \mathbf{e}_i from which to specify the Burgers vector. But a dislocation in the bulk need not remain a straight line-smooth deformations of a screw or edge dislocations may change the direction of the Burgers vector with respect to the asymptotic basis vectors. Any diffeomorphism of the sample preserves, however, the distinction between screw and edge, because the disclination

geometry at the defect core cannot change without twist and hence a change in topology of Φ . As an illustrative example, consider again the singular configuration in which an edge dislocation transforms at a point to a screw. Smooth deformations of the sample can move around the singular point at which the $+\frac{1}{2}$ disclination becomes a $-\frac{1}{2}$, changing the direction of the Burgers vector. However, the screw and edge character of the dislocations—defined by their local disclination geometry remains in character on either side of the singular point at all times. Even in cases like this, where expanding the Burgers vector in the asymptotic conflicts with the standard geometric classification of screw versus edge, our classification consistently defines screw and edge dislocations.

Gaussian curvature and the escape of smectic disclination charge. To make this discussion concrete and to demonstrate the effects of the distinction between screw and edge far from the defect core, we focus on the screw dislocation in a smectic. A screw dislocation of Burgers displacement *b* has the form $\Phi_{\text{screw}} = z - \frac{b}{2\pi} \arctan(y/x)$ at large distances. The Euler-Lagrange equation for (1) is

$$0 = \frac{1}{2}B\nabla \cdot [\nabla\Phi(|\nabla\Phi|^2 - 1)] - K\nabla^2\nabla^2\Phi.$$
 (2)

Because Φ_{screw} is harmonic in x and y and the gradient of the compression (radial) is orthogonal to the layer normal (azimuthal and along \hat{z}), it satisfies the necessary conditions for a minimum. However, all layers of a helicoid meet at the center to become one surface, yielding infinite compression energy at the screw defect core and a melting of the smectic order. To avoid this melting, the smectic may instead form a core of two $+\frac{1}{2}$ disclinations, shown in Fig. 1 (right). Here we briefly review the geometry of such a configuration, as described in Refs. [14,18]. The construction starts with a central helicoid upon which subsequent layers are built by pushing off a constant distance along the layer normal. By construction, this creates a family of evenly spaced layers with zero compression. However, just as with evolutes in two-dimensional curves, this family of surfaces will develop linelike cusps on either side of the initial helicoid, the first pair forming a double helix at a radius ρ_0 . These first cusps are precisely the location of the $+\frac{1}{2}$ disclination geometry. Thus a cylinder of radius ρ_0 can be constructed with zero compression and be used for the core of screw dislocation. An alternative way to visualize this and similar [19] constructions of screw defect cores is to take a pair of $+\frac{1}{2}$ smectic disclinations in two dimensions and create surfaces in three dimensions by continuously rotating the configuration as it is extended out of the plane. Here it is clear that the radial nature of the layers near the helicoidal core requires the geometry of +1 disclination charge.

Recall that two $+\frac{1}{2}$ disclinations cannot smoothly transform into a $\pm\frac{1}{2}$ pair in a smectic, suggesting that the +1 disclination charge of the screw dislocation core might be present throughout the system. This, however, cannot be the case: boundary conditions require that $\nabla \Phi$ be constant for both edge and screw dislocations, specifying no free disclination charge. We can track the behavior of the disclination geometry by analyzing the nematic director defined by $\nabla \Phi_{\text{screw}}$ at z = 0:

$$\mathbf{n} = \frac{\nabla \Phi_{\text{screw}}}{|\nabla \Phi_{\text{screw}}|} = \frac{1}{\sqrt{r^2 + b^2}} (-b\sin\theta, b\cos\theta, r), \quad (3)$$

where r, θ , and z are the usual cylindrical coördinates and $b \equiv b/(2\pi)$. This form of **n** has the geometry of a +1 disclination at the origin: looking down the screw axis of the helicoid yields normals that wind by 2π around the center, and hence the reason two +1/2 disclinations were required to build the core. However, in the smectic phase the director is not defined homogeneously throughout the sample but instead only normal to the layers. Rather than taking a projection for constant *z*, one only defines **n**||**N** on a surface of constant Φ . For instance, taking $\Phi_{\text{screw}} = 0$, i.e., $\theta = (2\pi/b)z$, yields

$$\mathbf{N} = \frac{1}{\sqrt{r^2 + b^2}} [-b\sin\left(z/b\right), b\cos\left(z/b\right), r]$$
(4)

at the point on the two-dimensional surface parameterized by r and θ , $\mathcal{P} = (r \cos \theta, r \sin \theta, b\theta)$.

As $r \to 0$ we see that the layer normal still rotates by 2π , and each full rotation is accompanied by a concomitant change in z: the Burgers displacement. The helicoid is simply connected, so in order to measure the disclination charge with a closed loop, we must rely on the density wave, which is well-defined everywhere, to fill in the remaining space with "virtual layers" between the density maxima. Only then do we see the nematic disclination on every constant z slice. However, as $r \to \infty$, $\mathbf{N} \to \hat{z}$ and $\mathbf{n} \to \hat{z}$. At constant height z a closed measuring circuit reports no disclination charge at large r, despite the charge at small r. Unable to flip one of its $+\frac{1}{2}$ disclinations, how is the smectic able to satisfy boundary conditions? Once again we can return to three-dimensional nematics for comparison. While a planar +1 disclination texture in a three-dimensional nematic may self-annihilate by splitting into two $+\frac{1}{2}$ disclinations and flipping one to a $-\frac{1}{2}$, a +1 disclination may also vanish by *escaping into the third* dimension [17].

In the smectic we find that the mechanism allowing the disclination charge of the screw dislocation's core to relax is the Gaussian curvature of the level sets of the smectic. Though the Gaussian curvature of a two-dimensional manifold interacts with the defects of director fields lying in the local tangent plane [20], here the situation is quite different; since the director is always normal to the surface, the director itself defines the surface. The fact that in the smectic-A phase the director and layer normal are one in the same is the key to connecting topological defects to Gaussian curvature: it allows us to construct a Gauss map for disclinations in the director field. Recall that the Gauss map is defined by taking the unit normal to a surface at a point and mapping it to the unit sphere. The collection of normals to a patch of the original surface sweeps out a corresponding signed area on the unit sphere, and the Jacobian that converts area on the manifold to area on the sphere is the Gaussian curvature [21].

With this in mind, consider a texture with the geometry of a +1 disclination line in a three-dimensional director field. The charge can be measured by a circle taken around the disclination. If the nematic director measured along this circle defined the normal to a smectic layer, we could use the director to to define a Gauss map. This measuring circuit may move between level sets while enclosing the defect, just like the measuring loop for the screw core. By definition, the director along the measuring circuit enclosing the +1



FIG. 2. The Gauss map on the helicoid for contours at varying distances from the core. (Top) Near the core the geometric texture of the director winds by 2π and maps the equator on the unit sphere. (Bottom) Far from the core the director and normals align along \hat{z} in accordance with boundary conditions. Connecting the two contours requires sweeping out the entire upper hemisphere under the Gauss map.

texture will be mapped to the equator of the unit sphere. Imposing the boundary conditions that the normals all point along \hat{z} at infinity, a contour stretched out to infinity must map to a point on the unit sphere (the North pole): as the contour is stretched continuously from the original measuring circuit to infinity, the Gauss map sweeps out area on the unit sphere and it follows that the surfaces must have Gaussian curvature. Indeed, by checking the relative orientation of the areas, we see that the surfaces must have a negative integrated Gaussian curvature. This is exactly what happens in the case of the screw dislocation, where the Gaussian curvature of the helicoid, $K = -b^2/(r^2 + b^2)^2$, allows for the equatorial loop on the unit sphere to be moved up along to a point infinitely far from the helicoid core (Fig. 2). Importantly, the +1 disclination charge is able to relax in this way without twist: the helicoidal surfaces ensure Φ remains well defined away from the core as the director conforms to boundary conditions.

Here we have arrived at the answer for how the screw dislocation, without allowing twist distortions, can have both the local geometry of two $+\frac{1}{2}$ disclinations and no disclination charge at infinity: the nematic director "escapes from the second dimension" by following smectic layers of negative integrated Gaussian curvature! For comparison, we can apply the same Gauss map procedure to an edge dislocation core. However, in this case the disclination-charge-neutral core already shows no winding; in order to match boundary conditions, the smectic layers around the edge dislocation must have exactly zero integrated Gaussian curvature. Under fixed boundary conditions, the integrated Gaussian curvature of the smectic layers is fixed: deformations to the system may add local curvature to surfaces, but the total integrated Gaussian curvature remains invariant. So, while edge and screw dislocations can be distinguished locally by the disclination geometry of their cores, the distinction between edge and screw leads to a global difference in their structure in the form of Gaussian curvature.

The topology of dislocation cores and commensurate Gaussian curvature-moderated escape of disclination charge in smectics are captured by the saddle-splay vector **A**. Recall that the saddle-splay term in the nematic is

$$F_{\rm ss} = -K_{24} \int d^3x \, \nabla \cdot \mathbf{A},\tag{5}$$

where $\mathbf{A} = \mathbf{n}(\nabla \cdot \mathbf{n}) - (\mathbf{n} \cdot \nabla)\mathbf{n}$. Because it is a total divergence it contributes only at boundaries, which include the cores of defects. While we have shown that disclinations can be arranged at dislocation cores so that the smectic need not melt, the disclinations themselves require vanishing of the nematic order since n becomes undefined. The saddle splay then integrates to the surface bounding the melted region. Note that for an *m*-fold, two-dimensional disclination, $\mathbf{n} = [\cos m\theta, \sin m\theta, 0]$ (with $m \in \frac{1}{2}\mathbb{Z}$), we find that $\mathbf{A} =$ $-m\hat{r}/r$ —it has a nonzero divergence at the origin and is singular when $m \neq 0$ (note, as well, that it is a true vector even when the defect is half-integer). Indeed, integrating around the inner boundary of the nematic (the disclination) in the xy plane, we find a total saddle splay of $2\pi m$. What is this quantity? Recall that the divergence of the saddle-splay vector is twice the Gaussian curvature of the smectic layers, $\nabla \cdot \mathbf{A} = 2K$. For a planar disclination of charge m = 1, the divergence of the saddle splay integrates to 2π . Similarly, twice the Gaussian curvature of a screw dislocation of +1 Burgers displacement integrated over the xy plane yields 2π . This can be calculated either by direct integration, by application of the Gauss map on the half-helicoid as in Fig. 2, or from the saddle splay. The final option corresponds precisely to the fact that the cross section of helicoidal layers in the xy plane has the geometry of a + 1 disclination. Indeed, the saddle-splay vector A reveals both the smectic disclination charge at the origin and the negative Gaussian curvature required to let it escape from the second dimension! This vector quantity is a measure

of the smectic complexion that allows us to distinguish the topology of screw from edge dislocations. Namely, for screw dislocations the divergence of the saddle splay must integrate to exactly 4π for each deck of the helicoid, and for edge dislocations it must integrate to zero. Again, to generalize to three-dimensional crystals it is only required to examine each phase field separately as discussed above. All the geometry and topology of the level sets follows the discussion for smectics.

Conclusion. By studying the topological properties of screw and edge dislocations according to their disclination cores, we provide a description of dislocations that both distinguishes screw from edge and unifies topological and geometric properties of dislocations. Our classification distinguishes screw and edge dislocations based on the $\pm \frac{1}{2}$ disclination geometry of the edge defect core compared to the topologically distinct pair of $+\frac{1}{2}$ disclinations of the screw core. Based on the need to satisfy boundary conditions, the disclination geometry of the dislocation cores forces the smectic layers to have a particular integrated Gaussian curvature, allowing the dislocations to be differentiated away from the core. The disinclination charge's "escape from the second dimension" plays a central role for screw dislocations, and its signature is captured by the saddle-splay vector A. This interpretation is essential when considering smooth deformations of crystals with embedded dislocations, as the local geometry can deviate from the crystalline axes specified by the boundary conditions. Whether further topological information regarding the entangling of dislocations and disclinations can be characterized is an open question.

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