Gnomonious projections for bend-free textures: thoughts on the splay-twist phase

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The Hopf fibration has inspired any number of geometric structures in physical systems, in particular, in chiral liquid crystalline materials. Because the Hopf fibration lives on the three sphere, $S^3$, some method of projection or distortion must be employed to realize textures in flat space. Here, we explore the geodesic-preserving gnomonic projection of the Hopf fibration, and show that this could be the basis for a new liquid crystalline texture with only splay and twist. We outline the structure and show that it is defined by the tangent vectors along the straight line rulings on a series of hyperboloids. The phase is defined by a lack of bend deformations in the texture, and is reminiscent of the splay-bend and twist-bend nematic phases. We show that domains of this phase may be stabilized through anchoring and saddle-splay.

1. Introduction

Topology and geometry have played an important role in illuminating the myriad textures that liquid crystals can make [1–4]. For instance, the blue phase of cholesteric liquid crystals has a frustrated texture in $\mathbb{R}^3$ with regions of double twist separated by a lattice of disclination lines [5,6]. The texture can be made frustration-free when placed in the curved space of $S^3$ [7]. Further, the smooth double twist structure in $S^3$ is tangent to a fascinating fibration of $S^3$ with great circles, known as the Hopf fibration [8,9]. In this paper, we take inspiration from this history to explore projections of the Hopf fibration for a twisted nematic texture that is bend-free. We show in §2 that in order to make a bend-free texture, we need a projection that preserves geodesics, the gnomonic projection. We call the texture which results from taking the gnomonic projection of the Hopf fibration ‘splay-twist’.
Figure 1. Here, we show the one-parameter family of projections that interpolates between the stereographic projection and the gnomonic projection, zoomed in near the origin. As $t$ changes from 0 to 1, the lines change from straight rulings on concentric hyperboloids to arcs of circles. (Online version in colour.)

Figure 2. Here, we show the one-parameter family of projections that interpolates between the stereographic projection and the gnomonic projection, at large distances. As $t$ grows from 0 to 1, the projection changes from pure splay, to a mixed state where some lines curl around into circles while others fly off to infinity as pure splay, and finally to the more common linked-loop projection of the Hopf fibration. (Online version in colour.)

The splay-twist texture is reminiscent of the twist-bend and splay-bend phases that lack splay and twist, respectively [10–12]. Given the existence of these two phases, it is not unreasonable to expect the existence of the third nematic phase. In the last few decades, the modulated nematic phase known as twist-bend has received attention due to its unique chiral symmetry breaking properties and giant flexoelectric constants both intrinsic [13,14] and structurally enhanced [15–20]. Furthermore, the splay nematic phase was recently discovered as the second modulated nematic phase in experiment [21]. Though liquid crystalline materials show a rich variety of structures and phases, only a few distinct nematic (chiral or not) phases have been discovered.

We show that ‘splay-twist’ domains consist of molecules following straight line rulings on the surface of a series of hyperboloids. The angle of the straight lines with the hyperboloid axis increases with increasing distance from the centre of the texture, allowing the architecture to be space-filling. The splay-twist texture is shown on the left-hand sides of figures 1 and 2. Furthermore, at large distances from the centre, the phase resembles a hedgehog nematic texture. In §3, we examine the elastic free energy of the splay-twist phase, and show that the phase can be stabilized with saddle-splay as in the blue phase, or with anchoring conditions, like hedgehog nematic textures.
2. The Hopf fibration and its gnomonic projection

Cholesteric liquid crystal blue phases are frustrated systems and consist of lattices of double twist regions separated by lattices of disclination lines. When the double twist structure is put in the curved space of $\mathbb{S}^3$, however, the system ceases to be frustrated, and its texture is space filling [7]. In $\mathbb{S}^3$, the nematic structure of the blue phase is tangent to a fibration of $\mathbb{S}^3$ with great circles, known as the Hopf fibration. Indeed, the imprint of the Hopf fibration can be seen in at least ‘seven different physical systems’ [22], and has previously been studied in the context of nematic liquid crystal defects [4,23].

In the following, $\mathbf{V} = (X, Y, Z) = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ are coordinates on $\mathbb{S}^2$, $(\tilde{x}, \tilde{y}, \tilde{z}, \tilde{w})$ are coordinates in $\mathbb{R}^4$ and $(x, y, z)$ are coordinates in $\mathbb{R}^3$. Recall that the Hopf fibration is a map from $\mathbb{S}^3 \to \mathbb{S}^2$. We parametrize $\mathbb{S}^3 \subset \mathbb{R}^4$ by $(\tilde{x}, \tilde{y}, \tilde{z}, \tilde{w})$ such that $\tilde{x}^2 + \tilde{y}^2 + \tilde{z}^2 + (\tilde{w} - 1)^2 = 1$ (a three-sphere in $\mathbb{R}^4$ sitting ‘above’ $\mathbb{S}^3$). The preimage of the vector $\mathbf{V}$ is then a great circle on $\mathbb{S}^3$ parametrized by an angle $\psi \in [-\pi, \pi)$,

\[
\begin{align*}
\tilde{x} &= \frac{(X \sin \psi - Y \cos \psi)}{\sqrt{2(1 + Z)}} \\
\tilde{y} &= \frac{(Y \sin \psi + X \cos \psi)}{\sqrt{2(1 + Z)}} \\
\tilde{z} &= \sqrt{\frac{1 + Z}{2}} \cos \psi \\
\tilde{w} &= \sqrt{\frac{1 + Z}{2}} \sin \psi + 1.
\end{align*}
\]

(2.1)

and

\[
(x, y, z) = (\tilde{x}, \tilde{y}, \tilde{z}) \left(\frac{1}{1 - \tilde{w}}\right).
\]

(2.2)

Recall that the gnomonic projection of $\mathbb{S}^2$ is a projection through the centre of the sphere to the two-dimensional plane upon which the sphere sits. It is similar to, but different from, the stereographic projection which projects from the same sphere to the same plane but through the north pole. In the latter, the entire sphere is conformally mapped to the Riemann sphere, $\mathbb{R}^2 \cup \{\infty\}$, sending circles to circles. In the gnomonic projection, however, only the southern hemisphere can be mapped to $\mathbb{R}^2$—the equator does not map to a unique point at infinity. However, if we consider a great circle on $\mathbb{S}^2$ then it lies in a plane with the sphere centre. That plane intersects $\mathbb{R}^2$ in a line—the gnomonic projection preserves geodesics! Similarly, the gnomonic projection from $\mathbb{S}^3$ to $\mathbb{R}^3$ will map great circles into straight lines (i.e. the intersection of $\mathbb{R}^2$ with $\mathbb{R}^3$ in $\mathbb{R}^4$ is a straight line). The appearance of the gnomonic projection is not surprising then, since we are looking for a texture without bend, which implies the presence of straight lines. This suggests that we look at a projection of the Hopf fibration that maps great circles to straight lines or, in other words, preserves geodesics. For a review of this and other projections of the sphere, see [24].

The projection from $\mathbb{S}^3$ to $\mathbb{R}^3$ is

\[
(x, y, z) = \frac{(\tilde{x}, \tilde{y}, \tilde{z})}{1 - \tilde{w}}.
\]

(2.2)

This can only project one hemisphere of $\mathbb{S}^3$ to $\mathbb{R}^3$ since $(1 - \tilde{w})$ vanishes on the equator of $\mathbb{S}^3$ where $\tilde{x}^2 + \tilde{y}^2 + \tilde{z}^2 = 1$. Employing the fibration in (2.1) we find $1 - \tilde{w} = \sqrt{(1/2)(1 + Z)} \sin \psi$ and so

\[
(x, y, z)_\mathbf{V} = \frac{1}{(1 + Z)} (X - Y \cot \psi, Y + X \cot \psi, (1 + Z) \cot \psi).
\]

(2.3)

For each $\mathbf{V}$ this is the equation for a straight line parametrized by $\cot \psi$ with $\psi \in [-\pi, 0]$ (the southern hemisphere) or $s \equiv \cot \psi \in (-\infty, \infty)$. The tangent to each of these lines defines the nematic director:

\[
n = \left[ -\sin \left(\frac{\theta_0}{2}\right) \sin \phi_0, \sin \left(\frac{\theta_0}{2}\right) \cos \phi_0, \cos \left(\frac{\theta_0}{2}\right) \right].
\]

(2.4)
Thus, the process of taking the preimage of the Hopf fibration and then a gnomonic projection amounts to a map that rotates the azimuthal angle by $\pi/2$ and halves the polar angle—a meron configuration on the two-sphere at infinity [25]. We can also think of the gnomonic projection as being generated by the method of characteristics. We can merely project from $S^3$ onto the $z = 0$ plane of $\mathbb{R}^3$ and then generate the characteristics generated by $(\mathbf{n} \cdot \nabla) \mathbf{n} = 0$. In the last section, we will discuss the conditions that prevent any shocks from occurring—when two characteristics collide. Note that although we draw the characteristics as lines, we are imagining here only a nematic texture made of short molecules. Were we considering, instead, polymer nematics, then we would have to account for the increased $K_1$ associated with splay-density coupling [26].

Continuing, we write $\rho^2 = x^2 + y^2$, and find

$$\rho^2 = (1 + z^2) \frac{X^2 + Y^2}{(1 + Z)^2} = (1 + z^2) \tan^2 \left( \frac{\theta_0}{2} \right), \tag{2.5}$$

and so we see that for each $\theta_0$ the Hopf fibration sweeps out a hyperboloid with a waist radius of $\tan(\theta_0/2)$. As $\theta_0$ grows from 0 to $\pi$ the hyperboloids nest with polar angle $\theta_0/2$, eventually forming an azimuthal defect in $\mathbf{n}$ at infinite $\rho$, when $\theta_0 = \pi$. To find $\theta_0$ as a function of $(x, y, z)$, we invert (2.3) and find

$$\begin{align*}
\frac{X}{1 + Z} &= \frac{x + yz}{1 + z^2} \\
\frac{Y}{1 + Z} &= \frac{y - xz}{1 + z^2}
\end{align*} \tag{2.6}$$

so that $\tan(\theta_0/2) = \sqrt{X^2 + Y^2}/(1 + Z) = \rho/\sqrt{1 + z^2}$ and $\cos(\theta_0/2) = \sqrt{1 + z^2}/\sqrt{1 + r^2}$ where $r^2 = x^2 + y^2 + z^2$. Finally, we get the nematic director field as a function of $(x, y, z)$:

$$
\mathbf{n} = \left[ \begin{array}{c}
\frac{-y + xz}{\sqrt{1 + z^2}\sqrt{1 + r^2}} \\
\frac{x + yz}{\sqrt{1 + z^2}\sqrt{1 + r^2}} \\
\frac{\sqrt{1 + z^2}}{\sqrt{1 + r^2}}
\end{array} \right]. \tag{2.7}
$$

Note that as $r \to \infty$, $\mathbf{n} \to (x/r, y/r, z/r)$ in the upper half-space ($z > 0$), as in a hedgehog configuration. For $z < 0$, however, $\mathbf{n} \to -(x/r, y/r, z/r)$. As a result, there is no net hedgehog charge in any finite volume. This is not a surprise since the core is defect-free. The difference between this configuration and the true hedgehog can be seen at $z = 0$. When $z = 0$, the texture is a meron configuration, with $\mathbf{n} = \hat{z}$ at the origin and a winding of +1 as $r \to \infty$ [25,27]. Were this texture a true hedgehog, there would be a radial defect at infinity. The winding near the $z = 0$ plane is responsible for zeroing the hedgehog charge. Finally, this configuration would be dilated or contracted had we projected from the three sphere of radius $\lambda \neq 1$. In this case, we would replace the $\mathbb{R}^3$ coordinates with $(x, y, z) \to (x, y, z)/\lambda$. We will only focus on $\lambda = 1$ in the following calculations since this just amounts to a change in overall scale.

To visualize this texture, it is instructive to consider a one-parameter family of projections that interpolates between the more familiar stereographic projection and the gnomonic projection. Using the parameter $t \in [0, 1]$, we have the projection from $S^3$ to $\mathbb{R}^3$:

$$[x(t), y(t), z(t)] = \frac{[\tilde{x}, \tilde{y}, \tilde{z}]}{(1 + t - \tilde{a})}, \tag{2.8}$$

where $t = 0$ is the gnomonic projection and $t = 1$ is the stereographic projection. In figure 1, we zoom in near the origin to see the projected textures. At $t = 0$ the lines are straight and they form concentric hyperboloids. As $t$ grows, the lines begin to curve until, at $t = 1$, they become arcs of circles. In figure 2, we show the far field. At large distances the $t = 0$ projection becomes pure splay, while at $t = 1$, we see the more common linked-loop projection of the Hopf fibration. In between, at $t = 0.9$ we can see a mixed state where some lines curl around into circles while others fly off to infinity as pure splay.
From (2.7), we calculate the splay, twist and bend of the Hopf projection and find
\[
\nabla \cdot \mathbf{n} = \frac{2z}{\sqrt{1+z^2}\sqrt{1+r^2}} \\
\mathbf{n} \cdot (\nabla \times \mathbf{n}) = \left( \frac{1}{1+z^2} + \frac{1}{1+r^2} \right) \\
and \\
(n \cdot \nabla) n = 0
\]
and we see that the bend vanishes, by construction. In addition, the saddle-splay does not vanish:
\[
\nabla \cdot \left[ \mathbf{n} (\nabla \cdot \mathbf{n}) - (\mathbf{n} \cdot \nabla) \mathbf{n} \right] = \frac{2}{1+r^2}.
\]

3. Geometry and stability

Under what conditions is this texture stable? Inspired by the ‘diabolo’ textures found in [28], we first consider a domain \( M \) contained within a hyperboloid as depicted in figure 3a. The director field is tangent to the hyperbola and intersects the discs at the top and the bottom in a swirl. Compared to the cholesteric state, these diabolos are not stable when saddle-splay is negligible. For a domain \( M \), the Frank free energy is
\[
F = \int_M d^3 x \left\{ K_1 \left[ \mathbf{n} (\nabla \cdot \mathbf{n}) \right]^2 + K_2 \left[ \mathbf{n} \cdot (\nabla \times \mathbf{n}) - q \right]^2 \right\} + \int_{\partial M} dA \left\{ W (\mathbf{v} \cdot \mathbf{n})^2 - K_{24} (\mathbf{v} \cdot \mathbf{n}) (\nabla \cdot \mathbf{n}) \right\},
\]
where \( \mathbf{v} \) is the outward pointing unit normal of \( M \). As usual, \( K_1, K_2, \) and \( K_{24} \) are the splay, twist, and saddle-splay elastic constants while \( W \) is the anchoring strength: negative \( W \) favours homeotropic alignment. We did not include the bend term as it vanishes identically. The pitch \( q \) allows for the possibility of a tendency to twist in the system. In the following, we calculate the free energy for \( K_1 = K_2, W = 0 \) and \( q = 1/2 \). The diabolo texture results in a stable domain as \( K_{24} \) grows as depicted in figure 4. Larger values of \( K_{24}/K_1 \) lead to larger regions of stability (we have chosen the sign of the saddle-splay coupling so that positive values of \( K_{24} \) favour this structure). Thus, for a diabolo system with saddle-splay and no explicit anchoring, the splay-twist may be more stable than a cholesteric. In this particular geometry, the surface alignment \( W \) leads to a complex contribution depending upon how the cholesteric phase sits in the diabolo and so, to demonstrate stability of this structure, we did not need to include it—no new geometric insight would be gained by these complexities.

Next, we consider the possibility of isolating a splay-twist structure in a spherical droplet, as is shown in figure 3b. This is evocative of how hedgehog nematic defects have been stabilized in liquid crystalline droplets with homeotropic anchoring, although in our case, with added twist [29]. The Frank free energy in (3.1) is shown for a spherical geometry in figure 5 and now we allow \( q \) to vary. In figure 5a, as the saddle-splay, \( K_{24}/K_1 \), grows and changes from negative to positive, the region of stability, as compared to a cholesteric, grows. Even for negative saddle-splay a region of stability is seen for high values of the pitch. The plot in figure 5b shows the regions of stability for non-zero anchoring and zero saddle-splay, when compared with a cholesteric. At low positive and small negative anchoring, the splay-twist is more stable than the cholesteric only for low values of the pitch \( q \). As anchoring becomes more negative, and favours homeotropic anchoring more strongly, the splay-twist is stable even for large values of the pitch.

We have seen that the gnomonic projection of the Hopf fibration gives a particular arrangement of space filling hyperboloids. However, the spacing of the hyperboloids can be distorted as long as no two helicoids intersect. We embellish (2.3) to
\[
(x, y, z) = (\chi, \zeta, 0) + \left[ -\zeta, \chi, c \left( \sqrt{\chi^2 + \zeta^2} \right) \right] s,
\]
Figure 3. In (a), we show a typical bundle shape. The bundle volume $M$ is defined by the hyperboloid generated by the outermost integral curves of the director. The tops and bottoms are chosen as flat discs to seal the volume. In (b), we show a typical spherical droplet with the splay-twist structure inside. (Online version in colour.)

Figure 4. The plot is for the diabolo structure, with $K_1 = K_2$ and $q = (1/2)$. We show the regions of stability as $K_{24}/K_1$ grows, with no anchoring. As the shading gets lighter, the stability region grows up to the contour line for each value, including all the darker regions.

where $c(\xi) > 0$. This representation generates a bend-free, twisted pattern with hyperboloids:

$$
\frac{\rho^2}{\xi^2} - \frac{z^2}{c^2(\xi)} = 1, \tag{3.3}
$$

with $\xi^2 = \chi^2 + \zeta^2$, reducing to the gnomonic case when $c = 1$ (or any constant). What are the constraints on $c(\xi)$ so that the integral curves of the director field do not intersect? Each
Figure 5. The plots are for the spherical droplet, with $K_1 = K_2$. In (a), we show the regions of stability as $K_{24}/K_1$ grows, with no anchoring. As the shading gets lighter, the stability region grows up to the contour line for each value, including all the darker regions. In (b), we show the regions of stability as $W/K_1$ becomes more negative for no saddle-splay, as compared with the free energy for a cholesteric of the same pitch.

hyperboloid is labelled by its waist radius $\xi_i$. If two hyperboloids $\xi_0$ and $\xi_1 > \xi_0$ intersect then they do so at the height $z$:

$$z^2 = \frac{\xi_1^2 - \xi_0^2}{\xi_0^2/c^2(\xi_0) - \xi_1^2/c^2(\xi_1)}.$$  

(3.4)

A solution exists when $z^2 \geq 0$ and so the hyperboloids avoid each other whenever

$$\frac{c(\xi_0)}{c(\xi_1)} > \frac{\xi_0}{\xi_1}.$$  

(3.5)

Equivalently, $c(\xi)/\sqrt{c^2(\xi) + \xi^2}$ is a decreasing function—the larger radii hyperboloids must tilt more and more towards the $xy$-plane. As mentioned previously, this means that the characteristic curves from the $z = 0$ plane never intersect. In a finite geometry, it is possible that a virtual intersection could occur outside the sample as discussed, for instance, in [30] in the context of viral rafts. In that and other cases (3.5) would be modified by the sample size. This also leads to the possibility of having a finite bundle such that at some radius $\bar{\xi}$ the $z$-component of the director field vanishes and thus the bundle stops. We will cross those bridges if we come to them.

Is the gnomonic projection special? Consider concentric discs of the diabolo at $z = 0$ of radii $\rho_1$ and $\rho_2$. At height $z$, these discs are at new spacings, $\rho'_i$ with

$$\frac{\pi(\rho'_1)^2 - \pi\rho_1^2}{\pi\rho_1^2} = \frac{c^2(\rho_2)}{c^2(\rho_1)} \frac{\pi(\rho'_2)^2 - \pi\rho_2^2}{\pi\rho_2^2},$$  

(3.6)

so that the isotropic expansion of each disc is not homogeneous unless $c(\rho_1) = c(\rho_2)$—precisely the gnomonic projection! Thus, we see that among all projections, the gnomonic projection creates uniform expansion of a bundle of rigid lines. In the liquid phase, the free energy is convex in the areal density of the lines (in the plane perpendicular to the $\hat{z}$-axis in this case) and thus a uniform density variation will minimize the free energy.

Each stable bundle might, in principle, act as a chiral constituent for a more complex arrangement as depicted in figure 6a. The chiral structure of the surface can lead to a chiral packing of each diabolo, something reminiscent of the observed packing of nucleosome core particles (NCPs) discovered by Livolant & Leforestier [28] shown in figure 6b. In that work, the NCPs formed a hexagonal columnar phase with two-dimensional crystalline order [31]. Because the plate-like stacking of the NCPs would enhance $K_3$ while doing little to the twist,
Figure 6. In (a), we show a possible packing of the chiral diabolos and compare to (b) images of nucleosome core particles (previously unpublished image courtesy of A. Leforestier and F. Livolant [28]). (Online version in colour.)

we might expect straight, chiral distortions in these phases, as seen in other chromonic systems [32]. Incorporating hexagonal order into the bundle at the waist, each successive z-slice is simply expanded uniformly by $\sqrt{1+z^2}$ with no shear, just a pure rotation. The crystalline elasticity thus contributes

$$F_{\text{xtal}} \sim \frac{B}{2} \int_{-h}^{h} dz \pi \tan^2 \left( \frac{\theta_0}{2} \right) z^2 = B \frac{\pi}{3} h^3 \tan^2 \left( \frac{\theta_0}{2} \right),$$

(3.7)

where $B$ is the bulk modulus. This would lead to stouter hyperboloids depending on the size of the twist penetration depth $\lambda = \sqrt{K_2/B}$.

4. Conclusion

We have shown how the gnomonic projection of the Hopf fibration gives us a series of hyperboloids, the tangent vectors to which define a nematic structure with no bend. This structure can be the third in a series of new nematic phases defined by combinations of splay, twist and bend deformations, the twist-bend, splay-bend, and now the splay-twist. Furthermore, the projection is one of a one-parameter family of projections that goes from a stereographic projection that produces pure bend at one end, to the gnomonic projection at the other end. We have explored two different geometries in which such a phase could be stabilized—a spherical droplet and a ‘diabolo’ structure seen in experimental work on chiral discotic columnar germs formed by nucleosome particles [28]. Finally, we have shown that a variation of bend-free structures is possible, one of which is the gnomonic projection of the Hopf fibration which can provide a basis for bulk-energy-minimizing bundles. It would be interesting to extend this projection to other textures on $S^3$ such as the Seifert fibrations considered in [4].

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