Line Defects in Cholesteric Liquid Crystals with Large Winding Number

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Introduction

Liquid crystals are optically anisotropic materials with uses in displays, photonics and optoelectric devices. They are able to contain defects (figure 1) which manifest as singularities in the director field. We can find cases where lines of singular points form in a material and analyse them using a local 2D cross-section for each point perpendicular to the line. On this 2D slice, we can calculate a winding number for the field, and find that this number is conserved throughout the volume via a topological effect. These singularities have high contribution to the energy of the system, so we look at the mechanics under which this energy cost can be reduced.

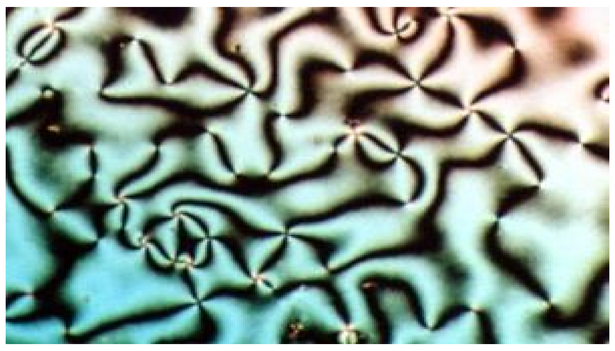

Figure 1: Optical texture of a nematic liquid crystal with defect points (from Wikipedia).

1) Frank Free Energy

The energetics of a cholesteric liquid crystal are described by the Frank Free Energy:

$$F = \int \frac{K_1}{2}(\nabla \cdot \mathbf{n})^2 + \frac{K_2}{2}(\mathbf{n} \cdot (\nabla \times \mathbf{n}) + c)^2 + \frac{K_3}{2}|(\mathbf{n} \cdot \nabla)\mathbf{n}|^2 dV. \qquad (1)$$

The case of a winding number 1 director with a singular line at the centre of the capillary is described by:

$$\mathbf{n} = \cos(\alpha(r))\,\mathbf{e}_z + \sin(\alpha(r))\,\mathbf{e}_r \qquad (2)$$

and minimised by the function $\alpha(r) = \pm 2\arctan(r/R)$. This is the 'escape' of a defect, with the + or - determining the escape direction (up or down).

2) Escape in Cholesterics

In cholesteric liquid crystals, the c in (1) is non-zero. This causes a high energy penalty for changes in the handedness of the director, encouraging defects to be resolved with a uniform handedness as seen in figure 2. In the winding number 1 case, such structures can lead to self-interference [1], but in the cases of higher winding number, the interference can be avoided. Figure 2 shows this for winding number 2, and our project aims to extend this to higher winding numbers.

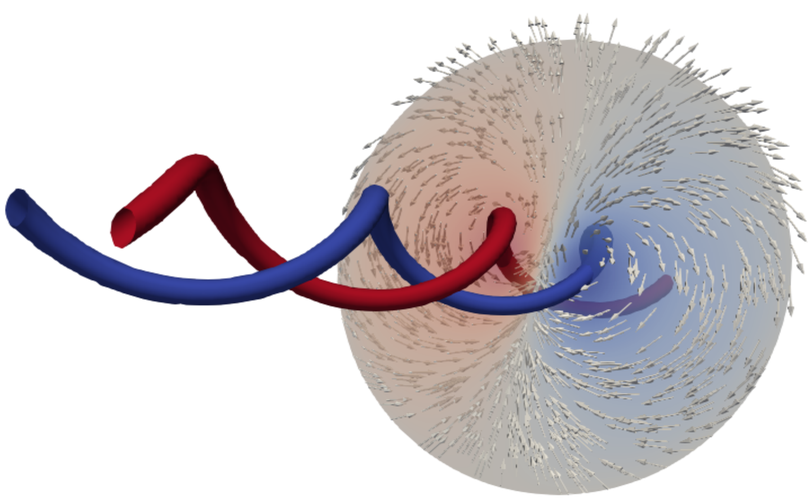

Figure 2: Numerical simulation of the $k = 2$ case with the escape up defect plotted in red and down in blue, and on the cross-section grey arrows representing the director field with areas of $n_z > 0$ tinted red and $n_z < 0$ blue.

We can express the local environment of a winding number k defect in a complex system using the function

$$m = e^{i\alpha} e^{iqz} \zeta^k \qquad (3)$$

This can naturally be unfolded into k different defects at different positions in the capillary tube, which will each escape in a predictable direction such that a uniform handedness may be maintained over the entire tube. We can use local analysis and various methods from contact topology to predict the directions and even the final outcomes of different unfoldings, and then investigate these predictions using numerical simulations which minimise the energy according to the Frank Free Energy in equation (1).

3) Symmetrical Unfoldings

An interesting unfolding to consider is one where we place the k defects uniformly around a circle centred on the original defect.

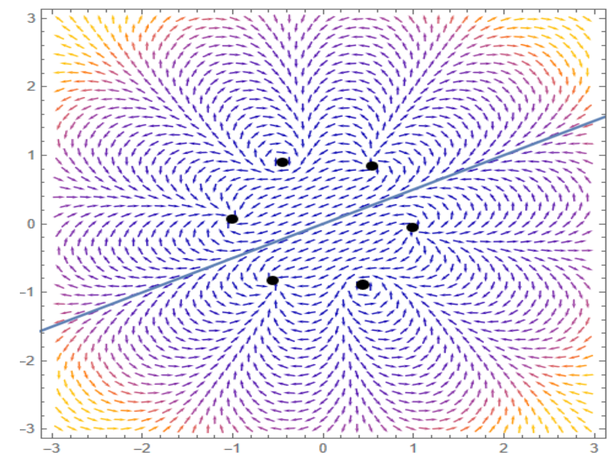

Figure 3: Theoretical prediction the unfolding of $k = 6$ symmetrically, with the defect positions plotted in black and the blue line dividing the defects into those that escape up and those that escape down (although not necessarily dividing the disc into the corresponding regions).

4) Simulation Results

We can use the symmetrical unfolding equation below in our numerical simulation,

$$m = e^{i\alpha} e^{iqz} \prod_{n=0}^{k-1} \left(\zeta - Re^{i\left(q'z + \frac{2\pi n}{k}\right)}\right), \qquad (4)$$

which results in figure 4. This doesn't match the prediction exactly, although all of the predicted features can still be found in these final forms.

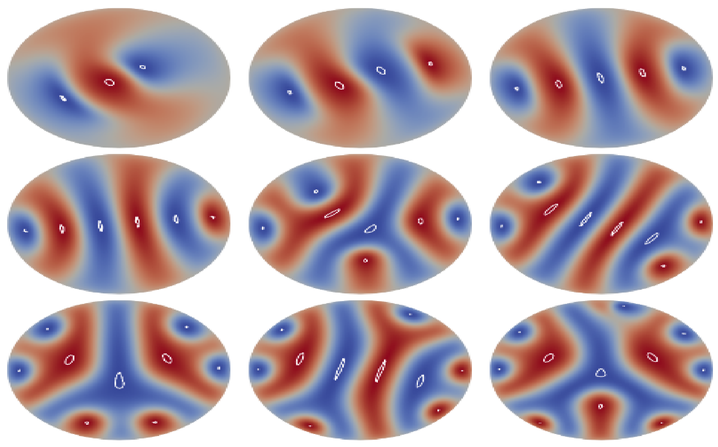

Figure 4: Cross sections of the stable results of symmetrical unfoldings with k from 3 to 11.

We do however, have some successful predictions for unfoldings, for example, if we consider 1 defect placed at the centre, and the other $k - 1$ placed uniformly about the centre, we have a very stable configuration of an escape up defect surrounded by escape down defects.

References

[1] J. Pollard and G. P. Alexander, "Escape into the Third Dimension in Cholesteric Liquid Crystals," *New J. Phys.*, vol. 26, 063027, 2024. DOI: 10.1088/1367-2630/ad5759.