Quasi-stable configurations of liquid crystals in polyhedral geometries

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ABSTRACT

Bistable director configurations are of great interest in liquid crystal display technologies, offering the possibility of higher resolution combined with reduced power consumption. One way to achieve such bistability is to use the cell geometry. As part of an ongoing programme to analyze quasi-stable configurations of liquid crystals in polyhedral geometries, we construct a topological classification scheme of unit-vector fields in convex polyhedra subject to tangential boundary conditions and obtain a general lower bound on the energy of these configurations. We also study the specific case of a unit cube, where we obtain lower and upper bounds for the energies of a family of topological types.

1. INTRODUCTION

Our problem is motivated by the study of liquid crystals in confined geometries. Confined geometries may require the liquid crystal molecules to satisfy certain material-dependent boundary conditions, amongst which tangential boundary conditions are one possibility. A stable configuration of a nematic liquid crystal may be described by a unit-vector field that minimizes the energy, the so-called Frank elastic energy [1] subject to the imposed boundary conditions. Such configurations satisfy the associated Euler-Lagrange equations – a non-linear system of elliptic partial differential equations.

Simple geometries may support only one stable configuration. Display technologies based on such geometries need a constant source of power to maintain optical contrast. On the other hand, more complex polyhedral geometries can support multiple stable configurations with distinct optical properties [3]. Such geometries form the basis of one class of bistable display technologies, in which power is required only to switch between optically contrasting states but not to maintain them. Our study of these geometries includes a complete topological classification of the admissible configurations along with an analysis of the energies of the stable (or metastable) states of different topological types.

2. TOPOLOGICAL CLASSIFICATION [4]

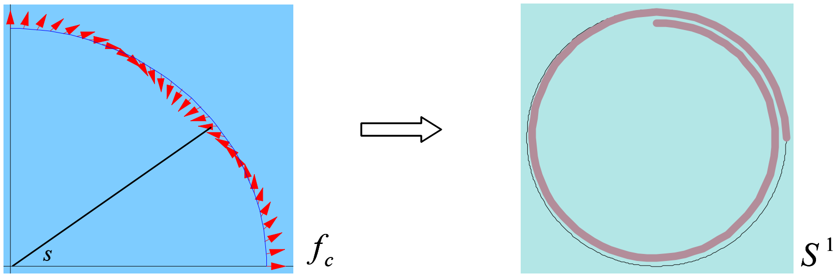
Consider unit-vector fields, $\hat{\varphi}$, in a three-dimensional convex polyhedron, P, subject to tangential boundary conditions. Tangential boundary conditions implies that on the faces of P, $\hat{\varphi}$ is tangent to the faces. Consequently on the edges of P, $\hat{\varphi}$ is parallel to the edges and therefore, necessarily discontinuous at the vertices. We require that, away from the vertices, $\hat{\varphi}$ is continuous (thus we do not consider defects in the bulk).

Two vector fields, $\hat{\varphi}$ and $\hat{\varphi}'$, are said to be homotopic if one can be continuously deformed into the other whilst preserving the boundary conditions. We want to determine the homotopy classes of such vector fields. These classes are labelled by a complete set of integer invariants, which we call **edge orientations, kink numbers,** and **wrapping numbers.** The values of these invariants are constrained by certain sum rules. It turns out that $\hat{\varphi}$ and $\hat{\varphi}'$ are homotopic if and only if their invariants are the same.

Below we give a brief and informal description of these invariants. See [4] for details.

The **edge orientations,** $E_b(\hat{\varphi})$, are just the values of $\hat{\varphi}$ on the edges e_b (they are determined up to a sign).

Kink numbers. Consider a path $P_{b,b'}(t), 0 \le t \le 1$, on a face of the polyhedron, denoted by f_c, which connects a pair of adjacent edges, e_b and $e_{b'}$, on f_c. Tangential boundary conditions imply that, along $P_{b,b'}(t)$, $\hat{\varphi}$ is constrained to lie in the unit circle tangent to f_c. The associated kink number, $k_{b,b'}(\hat{\varphi})$, counts the number of times $\hat{\varphi}(P_{b,b'}(t))$ winds around this circle relative to the shortest arc joining the values of $\hat{\varphi}$ at the endpoints, namely $E_b(\hat{\varphi})$ and $E_{b'}(\hat{\varphi})$.

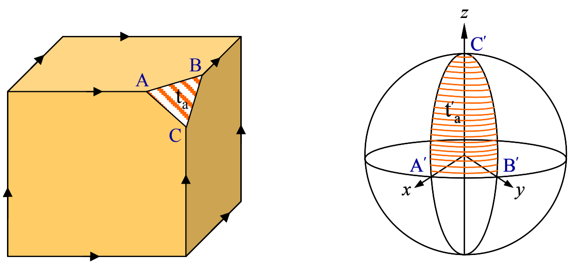


The vector field traverses the tangent unit circle once along a path joining the initial and final states.

Figure 1

Continuity implies that the kink numbers on each face satisfy a sum rule, which depends on the edge orientations (the form can be worked out explicitly).

Wrapping numbers. Let t_a be a surface which isolates one of the vertices, v_a, from the others. The wrapping number $w_a(\hat{\varphi})$ is a signed count of the number of times $\hat{\varphi}(t_a)$ covers, or wraps, around the unit sphere relative to some conventionally defined reference configuration. Continuity implies that the wrapping numbers sum to zero.



$\hat{\varphi}$ being a unit-vector field, takes its values on the unit sphere as shown in Figure 2.The reference configuration has $t_a{}'$ as the image of t_a (wrapping number zero).

Figure 2

3. LOWER BOUNDS FOR THE ENERGY [5]

In the one-constant approximation, the Frank energy is given by

$$E = \iiint_P |\nabla \hat{\varphi}|^2 \, dV .$$

Let E_I denote the minimal energy for configurations of a given topological type, characterised by a set of values I of the edge orientations, kink numbers and wrapping numbers. We extend methods from [2] to unit-vector fields satisfying tangent boundary conditions, to obtain a lower bound for E_I - this lower bound is a function of the topological invariants. Below we give a brief description of the argument and the result. For details see [5].

Let $\hat{\varphi}$ be a unit-vector field of topological type I with continuous second partial derivatives. A unit-vector field is a mapping from P to the two-sphere, S^2. Let *D* denote the vector dual to the pullback, $\hat{\varphi}^*(\omega)$, of the area-form, ω, on S^2 i.e.

$$D^{\alpha} = \frac{1}{2}\varepsilon_{\alpha\beta\gamma}\,\varepsilon_{\rho\mu\nu}\,\hat{\varphi}^{\rho}\partial_{\beta}\,\hat{\varphi}^{\mu}\,\partial_{\gamma}\,\hat{\varphi}^{\nu} \qquad \textbf{(1)}$$

where $\varepsilon_{\alpha\beta\gamma}$ is the antisymmetric tensor and the subscripts β,γ denote partial derivatives. Thus, the flux of *D* through a surface Σ in P is the signed area of $\hat{\varphi}(\Sigma)$ on S^2. It follows that **div** *D* = 0 in the interior of P, and one can check the following inequality,

$$|D| \le \frac{1}{2}|\nabla\hat{\varphi}|^2. \qquad \textbf{(2)}$$

.

Consequently, E_I is bounded from below by

$$E_I \ge 2\iiint\limits_P |D|\,dV \qquad \textbf{(3)}$$

Now, let $\xi(r)$ be any real-valued Lipschitz function on an arbitrary bounded domain $\Omega \subset R^3$ with Lipschitz constant less than or equal to 1 i.e. $|\xi(r_1) - \xi(r_2)| \le |r_1 - r_2|$. Then the following holds for a vector field *A* with continuous partial derivatives

$$\iiint\limits_{\Omega} |A|\,dV \ge -\iiint\limits_{\Omega} \xi\nabla\cdot A\,dV \quad + \oiint\limits_{\partial\Omega} \xi\, A\cdot dS \qquad \textbf{(4)}$$

(Note that **(4)** follows directly from integration by parts for a continuously differentiable $\xi(r)$ with $|\nabla\xi| \le 1$.)

We apply **(4)** to the case $A = D$, taking Ω to be a subset $\hat{P}$ of P, obtained by removing small neighbourhoods of each of its vertices. Using the properties that **div** *D* = 0 in $\hat{P}$ and $D = 0$ on the truncated faces of $\hat{P}$ [4], we obtain

$$E_I \ge \max 8\pi \sum_{v_a} Q_a(\hat{\varphi})\xi(v_a). \qquad \textbf{(5)}$$

Here $4\pi Q_a(\hat{\varphi})$ is the flux of *D* through a small surface in *P* isolating the vertex v_a from the other vertices (eg. t_a to Figure**2**). In fact, $Q_a(\hat{\varphi})$ depends only on the topology of $\hat{\varphi}$; it is by itself a homotopy invariant independent of any convention. An explicit expression in terms of the invariants I is given in [4]. Note that, in general, $Q_a(\hat{\varphi})$ is not an integer in contrast to the related notion of the integer-valued degree of a map $\hat{f}: S^2 \to S^2$ The continuity of $\hat{\varphi}$ in the bulk implies that

$$\sum_{v_a} Q_a(\hat{\varphi}) = 0. \qquad \textbf{(6)}$$

Let S_+ (respectively S_-) denote the set of vertices v_a where $Q_a(\hat{\varphi}) > 0$ (respectively $Q_a(\hat{\varphi}) < 0$). We now use the Kantorovich theorem [2] to deduce that the energy is bounded by the minimum of the following linear function:

$$E_I \ge \min 8\pi \sum_{i\in S_+,\, j\in S_-} a_{ij}\,|v_i - v_j|,. \qquad \textbf{(7)}$$

where $a_{ij} \ge 0$, and

$$\sum_{j\in S_-} a_{ij} = Q_i(\hat{\varphi}), \sum_{i\in S_+} a_{ij} = | Q_j(\hat{\varphi}) |$$

This gives a lower bound for the energy in terms of the solution of **(7)**. Such problems can be easily solved for given values of $Q_a(\hat{\varphi})$ and $| v_i - v_j |$.

4. THE MODEL CONFIGURATIONS [6]

We introduce a 2-parameter family of unit-vector fields, $\hat{\varphi}_{m,n}$, contained in a unit cube, subject to tangential boundary conditions, labelled by two integers *m* and *n*, called the **(m,n)-wrapion** configurations. For definiteness, take a unit cube to be the region of space $\{(x,y,z) \,|\, 0 \le x,y,z \le 1\}$. We parameterise physical space by polar coordinates, θ and ϕ, with respect to the origin and define the vector field in the first octant by

$$\hat{\varphi}^*_{m,n} = (\sin(2m+1)\theta\cos(2n+1)\phi, \sin(2m+1)\theta\sin(2n+1)\phi, \cos(2m+1)\theta) \quad 0 \le x,y,z \le \frac{1}{2}. \quad \textbf{(8)}$$

Elsewhere, $\hat{\varphi}_{m,n}(x,y,z) = \hat{\varphi}^*_{m,n}(h(x),h(y),h(z))$ where $h(t) = \begin{cases} t & 0 \le t \le 1/2 \\ 1-t & 1/2 \le t \le 1 \end{cases}$.

4.1 The associated invariants.

1.**Edge orientations**: Let $\hat{E}_x, \hat{E}_y, \hat{E}_z$ denote the edge orientations on the edges along the positive *x,y* and z axes respectively. Then, it follows from **(1)** above that

$$\hat{E}_x = (-1)^m \hat{x}, \hat{E}_y = (-1)^{m+n} \hat{y}, \hat{E}_z = \hat{z}$$

$\hat{\varphi}_{m,n}$ is identified on pairs of parallel edges so that the corresponding edge orientations are equal.

2. **Kink numbers**: We have three kink numbers associated with the origin, one for each of the coordinate planes, labelled by $k_{x,y}, k_{y,z}, k_{z,x}$ respectively.

$k_{x,y}$	$-\left[\frac{n}{2}\right] - \left(\frac{1-(-1)^n}{2}\right)$
$k_{y,z}$	$(-1)^n\left(\left[\frac{m}{2}\right] + \left(\frac{1-(-1)^m}{2}\right)\right)$
$k_{z,x}$	$-\left(\left[\frac{m}{2}\right] + \left(\frac{1-(-1)^m}{2}\right)\right)$

[X] denotes the integer part of the quantity X.

At vertices other than the origin, with coordinates $(\varepsilon_x, \varepsilon_y, \varepsilon_z)$, the kink numbers change by a sign $(-1)^{\varepsilon_x + \varepsilon_y + \varepsilon_z}$.

3. **Wrapping numbers**: The wrapion-wrapping number relative to the origin, w_0, is shown below for two distinct cases – *n* even and *n* odd.

n	w_0
n even	$\left[\frac{n}{2}\right]$
n odd	$\left[\frac{n}{2}\right]+1$

The wrapping numbers associated with the other vertices are of the same magnitude as w_0 but alternate in sign.

4.2 Lower bounds.

Let $E^0_{m,n}$ denote the total energy of the **(m,n)-wrapion** configuration. Then $E_{I(m,n)}$ is the minimal energy in the **(m,n)-homotopy class** – the class of all vector fields which are homotopic to the **(m,n)-wrapion** state. Firstly, we calculate lower bounds for $E_{I(m,n)}$.

The symmetry of these configurations implies that $Q_a(\hat{\varphi})$ is of equal magnitude for all the vertices v_a, but alternates in sign. $Q_a(\hat{\varphi})$ is explicitly calculated to be $(2n+1)/8$. It follows from **(6)** that there four positive and four negative vertices respectively; these are paired together to minimize the sum **(7)**. This yields the following lower bound

$$E_{I(m,n)} \geq 4\pi(2n+1) \quad . \tag{9}$$

Note that this lower bound is linear in the parameter n.

4.3. Upper bounds.

$E^0_{m,n}$ is itself an upper bound for $E_{I(m,n)}$. By symmetry, all octants of the cube make an equal contribution to $E^0_{m,n}$ and it, therefore, suffices to consider only the first octant, namely, $0 \leq x, y, z \leq (1/2)$. $|\nabla\hat{\varphi}_{m,n}|^2$ is explicitly calculated to be

$$|\nabla\hat{\varphi}_{m,n}|^2 = \frac{(2m+1)^2}{r^2} + \frac{(2n+1)^2}{r^2}\frac{\sin^2(2m+1)\theta}{\sin^2\theta} \tag{10}$$

We have analytically computed the integral of **(10)** over a unit cube; the expression involves the Appell hypergeometric functions of two variables, $F_2(\alpha,\beta,\beta',\gamma,\gamma';x,y)$, for a suitable choice of the parameters and is shown below.

$$\begin{aligned}
&\int_{0\leq x,y,z\leq 1} |\nabla\hat{\varphi}_{m,n}|^2 dV \\
&= 8\{\sum_{p_1,p_2=0}^{m}\sum_{p_3=0}^{p_1+p_2}\binom{2m+1}{2p_1+1}\binom{2m+1}{2p_2+1}\binom{p_1+p_2}{p_3}(-1)^{p_1+p_2} \\
&\frac{F_2(2m+1,p_3+1/2,2m-p_1-p_2+1/2,p_3+3/2,2m-p_1-p_2+3/2;-1,-1)}{(2p_3+1)(2(2m-p_1-p_2)+1)} \\
&+\sum_{p_1,p_2=0}^{m}\sum_{p_3=0}^{p_1+p_2}\binom{2m+1}{2p_1+1}\binom{2m+1}{2p_2+1}\binom{p_1+p_2}{p_3}(-1)^{p_1+p_2} \\
&\frac{F_2(2m+1,p_1+p_2-p_3+1/2,p_3+1/2,p_1+p_2-p_3+3/2,p_3+3/2;-1,-1)}{(2p_3+1)(2(p_1+p_2-p_3)+1)}\}
\end{aligned} \tag{11}$$

$E^0_{m,n}$ can also be represented in terms of a double infinite series or a single infinite series involving the Gauss hypergeometric function of one variable. The detailed calculations are presented in [6].

A simple approximation is obtained by inscribing the octant of the cube within an octant of a ball of radius $\sqrt{3}/2$. This yields the following upper bound for the minimal energy

$$E_{I(m,n)} \leq E^0_{m,n} \leq 2\sqrt{3}\pi(2m+1)^2 + 2\sqrt{3}\pi(2n+1)^2 C_m$$
$$C_0 = 1\ ,\ C_m = \left(\frac{1}{2}\ln(m) + \frac{23}{15}\right) + O\left(\frac{1}{m}\right) \quad m \neq 0 \qquad \textbf{(12)}$$

Note that **(12)** contains quadratic terms in both the parameters *m* and *n*. This indicates that there will be a large difference between the lower **(9)** and upper **(12)** bounds with increasing values of *m* and *n*.

We have also carried out some preliminary numerical analysis of the **(m,n)-wrapion** configurations using **FEMLAB** – Finite Element Modelling LABoratory, a commercial PDE solver package. Some early results in this context are

(m,n)	$E_{m,n}$	The energy of the corresponding FEMLAB solution	Lower bound using **(9)**
(0,0)	15.2	14.8	12.6
(0,1)	78.8	49.8	37.7
(1,0)	74.9	67.8	12.6
(1,1)	164.2	122.9	37.7

We see that **(9)** suggests that the minimal energy is completely determined by the parameter *n*.

5. FURTHER WORK

Ongoing work includes a study of the minimizing configurations and trying to obtain refined estimates of the minimal energy in the different homotopy classes. We also aim to extend our study to other topological classes and arbitrary polyhedra.

Further extensions of this work are to incorporate defects in our set-up, either in the bulk or on the surface of the polyhedron, construct similar classification schemes for normal and periodic boundary conditions and deal with more complex (non-convex) geometries.

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