Quasi-Stable configurations of liquid crystals in polyhedral geometries[+]

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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 have constructed a topological classification scheme of unit-vector fields in convex polyhedra subject to tangential boundary conditions, and have carried out numerical and analytical calculations of the energy and stability properties of certain test configurations contained in a unit cube.

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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 have constructed a topological classification scheme of unit-vector fields in convex polyhedra subject to tangential boundary conditions, and have carried out numerical and analytical calculations of the energy and stability properties of certain test configurations contained in a unit cube.

INTRODUCTION.

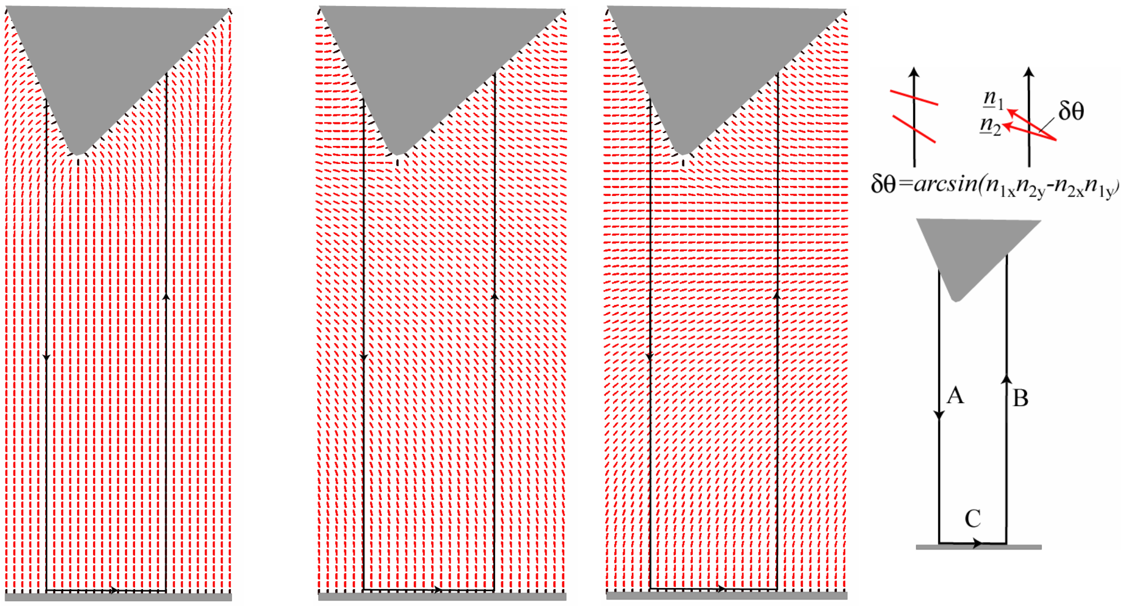
In the continuum model of liquid crystals, the mean orientation of the molecules is described by a director field, a unit-vector field determined up to an overall sign. Quasi-stable configurations, or stable configurations for short, are director fields that are local minimizers of an energy functional, the so-called Frank's energy [1]. These are the configurations one expects to find in the absence of external fields. The optical properties of a medium, in particular its transmissivity as a function of the wave vector and polarisation, are determined by the director field.

Liquid crystal cells in simple geometries may support only one stable configuration. Display technologies based on such geometries require a constant source of power to produce configurations with optical contrast. On the other hand, more complex polyhedral geometries can support multiple stable states 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. A theoretical study of these geometries includes a topological classification of the admissible director fields along with an analysis of the minimizing director fields of given topological types.

As an illustration of a two–dimensional classification scheme, we look at zenithally bistable nematic cells (ZBN). ZBN displays use a monograting on one side of the cell and a planar surface on the other, with both surfaces treated to be homeotropic, so that the director field is normal to the surface. When modelling in two dimensions, three stable states are found [3]. These are illustrated here together with their topological classifications. These states do not continuously transform into each other. This can be explained in terms of their topological non-equivalence – the distinct states are distinguished by their different winding numbers.

Normal boundary conditions fix the director field at the top and bottom of the cell. In between, it can wind some number of times. There are separate left and right winding numbers associated with the paths A and B. These must be the same as those for the reference non-defect state (shown below) unless there are discontinuities in the director field (either at the tip of the obstacle or in the bulk). The periodic boundary conditions on the sides allow for an additional winding number across the cell, but this is always fixed to be zero owing to the homeotropic alignment of the director field at the bottom (C). Therefore, we deduce that the topology is completely determined by the left and right winding numbers – the topological invariants for this two dimensional problem.



Numerical results for angular changes along the contours

	A	B
Non-defect state	63	45
Defect state	-117	45
Higher energy defect state	63	-135

As shown above, the director field rotates by different angles along paths A and B in all three cases. In the non-defect state, it turns by the minimal angle, in the positive sense, between the fixed orientations at the grating and planar surface. On the other hand, the remaining configurations show some non-trivial intermediate behaviour, indicating the presence of defects. The higher-energy defect state is not observed experimentally, or when modelling in three dimensions [4]. We believe this to be a consequence of the restriction to two dimensions. It 'untwists' or 'unwinds' in real space and ceases to exist.

Before attempting the topological classification of director fields in three dimensions, we deal with a simplified problem - classifying unit-vector fields in convex polyhedra with tangential boundary conditions. A topological classification scheme of the admissible configurations is constructed. Further, we consider some model configurations in a unit cube with specified topologies and analytically compute the corresponding energies. Lower bounds for the associated energy are also evaluated using methods similar to [2].

THE TOPOLOGICAL CLASSIFICATION.

We now look for a complete set of topological invariants for a unit-vector field, φ, in a three-dimensional convex polyhedron, P_0, satisfying planar boundary conditions. This particular choice of boundary conditions implies that the values of φ on the faces are tangential and, consequently, parallel to the edges. φ is necessarily discontinuous at the vertices but is required to be smooth everywhere else as our model does not include bulk defects.

If one vector field can be continuously deformed into another while preserving the boundary conditions, they necessarily have the same set of values for the topological invariants and are said to be homotopic to one another.

Consider a convex polyhedron P_0 with V vertices, E edges, and F faces. Denote the vertices by v_a, a = 1 ...V, the edges by e_b, b = 1 ... E and the faces by f_c, c = 1 ... F. We further assign a unit vector $\hat{e}_b$ to each edge e_b, parallel to it. $\hat{e}_b$ is determined up to a sign, which we fix arbitrarily. The outward unit normal $\hat{f}_c$ to the face f_c determines its orientation. In what follows, let $P = P_0 - \sum_{a=1}^{V} v_a$ denote the polyhedron with vertices removed; then φ is continuous on *P*.

The vector field φ assigns to each point in physical space a unit vector and can, therefore, be regarded as a map from the polyhedron P to the unit sphere S^2 subject to the constraint $\varphi \mid_{f_c} \bullet \hat{f}_c = 0$. Let C be the space of all such continuous maps.

The construction of a suitable topological classification scheme for such a three-dimensional configuration has the following distinct stages –

1. **Definition of the Invariants:**
   Two maps φ , $\psi \in$ C are said to be homotopic only if there is a continuous path in C that connects them. A path in the space C is simply a map $\varphi_t : [0,1] \to C$, or equivalently, $\varphi_t(x) : [0,1] \times P \to S^2$. The path $\varphi_t, 0 \le t \le 1$, is continuous if and only if $\varphi_t(x)$ is continuous in both *x* and *t*. A topological invariant is a function defined on C that is constant for all path-connected components or takes equal values for all homotopic maps.

A set of topological invariants $I_\alpha(\varphi)$ = {edge signs, kink numbers, wrapping numbers} is introduced in the following section.

2. **Characterization: -**
   Maps labelled by the same set of invariants are homotopic to one another. Quantitatively this is expressed as
   $$I_\alpha(\varphi) = I_\alpha(\varphi') \Leftrightarrow \varphi \sim \varphi'.$$
   These invariants serve to label the distinct homotopy classes or, equivalently, partition the allowed configurations into disjoint equivalence classes.

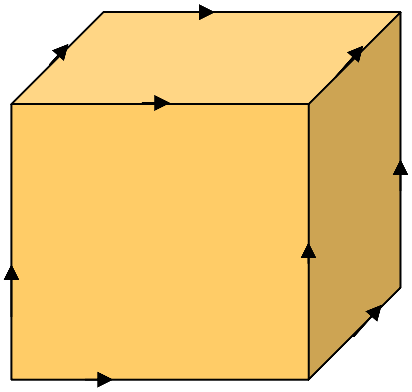
3. **Representatives: -**
   Given a set of edge signs, kink numbers, wrapping numbers, $I = \left(E_b, K_{b,c}, W_a\right)$, we construct a map $\varphi_I \in C$ with these invariants.

INVARIANTS

We now define the edge signs, kink numbers and wrapping numbers mentioned above, noting that the continuity of the vector field in P will impose restrictions on the possible values of these invariants. These restrictions will take the form of sum rules for the kink and wrapping numbers.

Edge Signs.

Edge signs –Tangential boundary conditions require that $\varphi(e_b) = E_b(\varphi)\ \hat{e}_b$, where $E_b(\varphi) = \pm 1$. These edge signs $E_b(\varphi)$ determine the orientation of φ on the corresponding edges.

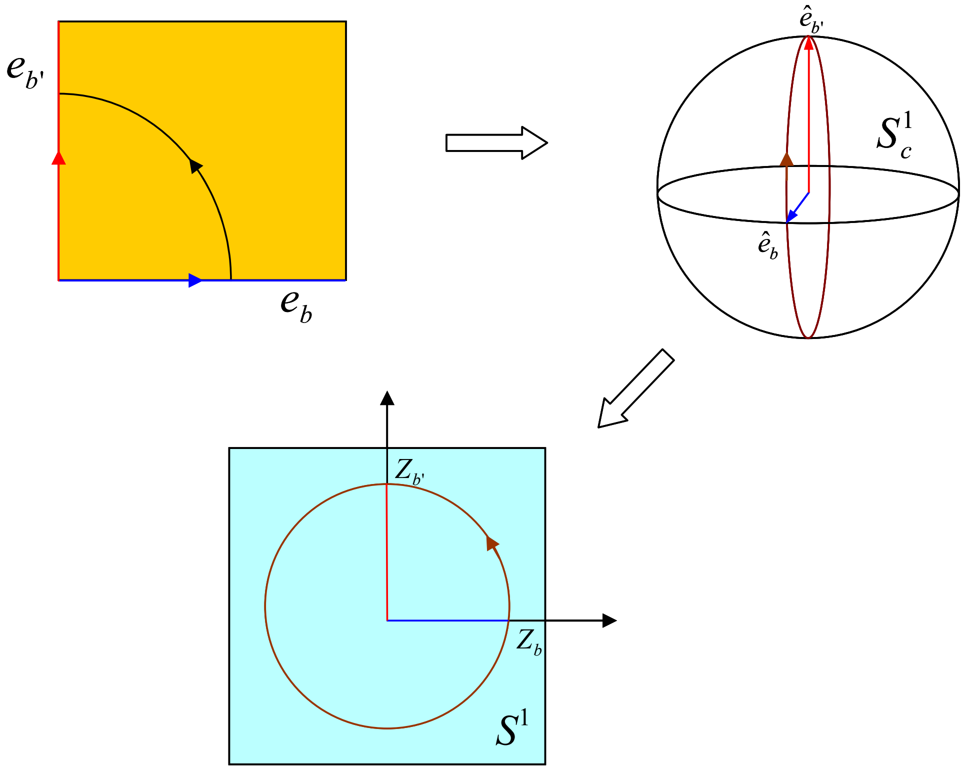


Kink Numbers.

These are generalized winding numbers associated with pairs of adjacent edges. The planar boundary conditions imply that the vector field φ, as evaluated on a face f_c, takes its values on the great circle S_c^1 in the plane orthogonal to $\hat{f}_c$. This great circle may be identified with a unit circle S^1 in the complex plane. φ, restricted to f_c, can, therefore, be alternatively viewed as a complex-valued function.

Next, consider a pair of adjacent edges e_b and $e_{b'}$ and trace out a smooth path $P_{b,b'}(t)$, $0 \le t \le 1$ between them on the face f_c. With respect to the previous identification $S_c^1 \cong S^1$, let $\hat{e}_b$ and $\hat{e}_{b'}$ correspond to complex numbers Z_b and $Z_{b'}$ of unit modulus. The vector field along the path $P_{b,b'}(t)$ is described by $z_{b,b'}(t)$, where $|z_{b,b'}(t)| = 1$.

This inter-relation between physical space, the target sphere and the complex plane is illustrated in the diagram below.



The associated kink number $k_{b,b'}$ is given by

$$k_{b,b'} = \frac{1}{2\pi}\left(\int_0^1 \operatorname{Im}\frac{\dot{z}_{b,b'}}{z_{b,b'}}\partial t - \left(\arg\left(E_{b'}\, Z_{b'}\right) - \arg\left(E_b\, Z_b\right)\right)\right).$$

It represents the winding number of $z_{b,b'}(t)$ relative to a reference path joining ($E_b\, Z_b$) to $\left(E_{b'}\, Z_{b'}\right)$ and is independent of the choice of the path $P_{b,b'}(t)$.

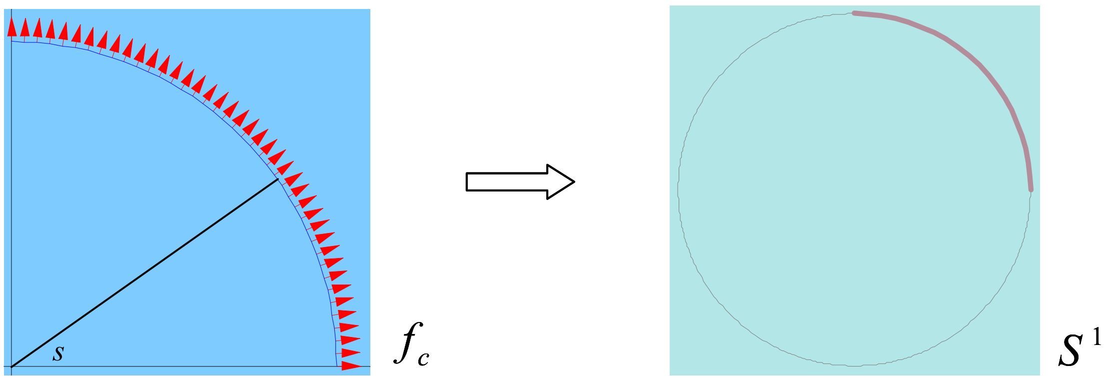
The kink numbers around a given face are constrained by a sum rule, as we now show. For simplicity, assume that the various paths connecting pairs of adjacent edges have coincident endpoints and, therefore, can be concatenated to obtain a closed curve $q(t)$ on f_c. The winding number of φ around $q(t)$ is just the sum of the kink numbers on the c^{th} face. Since $q(t)$ can be contracted on this face without encountering any vertices and φ is continuous away from the vertices, we infer that this winding number must vanish. The corresponding sum rule can be stated as

$$\sum_{e_b, e_{b'} \in f_c} k_{b,b'} = 0.$$

An interesting point is that omission of the second term from the integral expression for $k_{b,b'}$ results in a well-defined invariant with real, not integer values. This modified expression for $k_{b,b'}$ would represent a fractional line defect at the common vertex of the adjacent pair of edges and may be used in future discussions.

As an illustration, we consider two simple configurations –

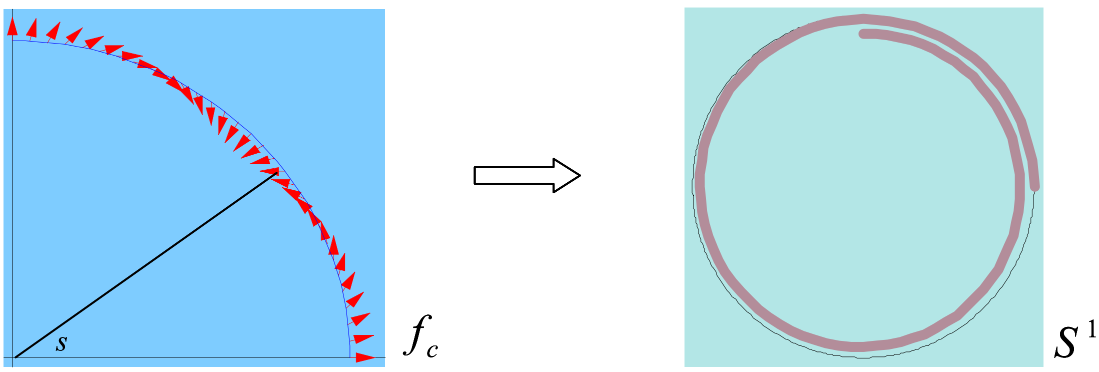
1) $\varphi = (\cos s, 0, \sin s) \quad 0 \le s \le \frac{\pi}{2}$



Kink number zero.

Zero winding is conventionally taken to be a single anticlockwise turn from Z_b to $Z_{b'}$, along S^1, as demonstrated above. The vector field moves around a quarter of the corresponding great circle, S_C^1, on the unit sphere, to reach its final state.

2) $\varphi = (\cos 5s, 0, \sin 5s) \quad 0 \le s \le \frac{\pi}{2}$

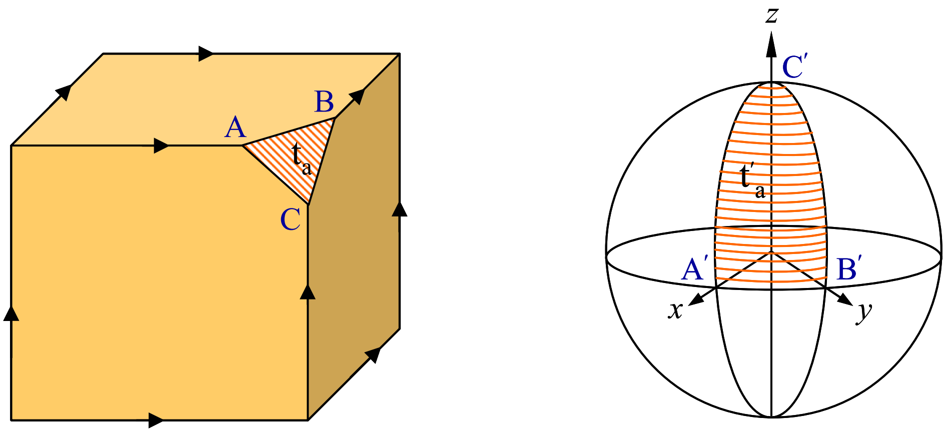


Kink number +1.

This vector field is assigned kink number **+1**. It does one complete anticlockwise turn of the great circle before traversing the segment connecting the initial and final states. The associated behaviour on S^1 is shown above on the right.

Wrapping numbers.

Wrapping numbers are integer-valued invariants associated with vertices. The simplest description of its physical meaning is as follows –we truncate P by removing neighbourhoods of each of its vertices as shown below. Let t_a be a planar surface isolating the vertex v_a from the remaining vertices. The associated wrapping number w_a counts the signed number of times the image of φ restricted to t_a covers or wraps around the unit sphere relative to some reference configuration.



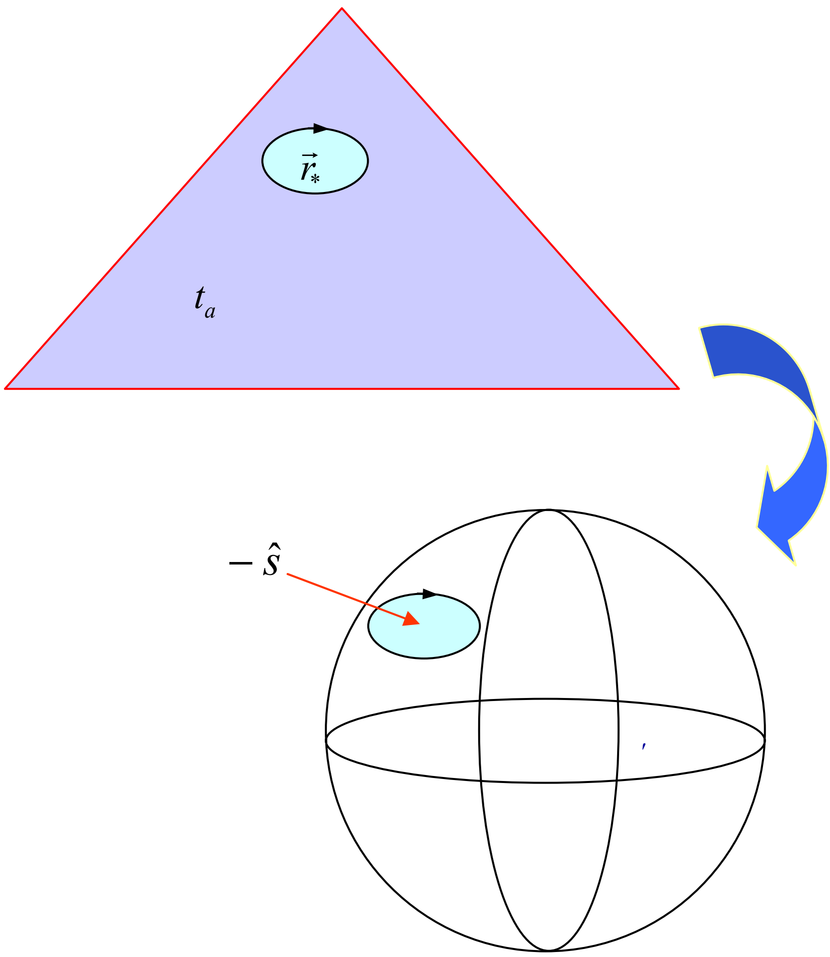
The reference configuration (wrapping number zero) has t_a' as the image of t_a. For more convoluted or wrapped configurations, t_a gets mapped onto $t_a' + m\,S^2$, for some integer m. This corresponds to a wrapping number of '+m'.

Quantitatively speaking, choose a reference unit vector $\hat{s}$ that is not tangential to any of the faces of P. Let α and β denote polar coordinates on the unit sphere with north pole at $\hat{s}$ (so that $\hat{s}$ corresponds to $\alpha = 0$ and $-\hat{s}$ to $\alpha = \pi$). Then, $\varphi(r)$ has polar angles $\alpha(r)$ and $\beta(r)$. The wrapping number w_a assigned to vertex v_a is defined by

$$w_a = \frac{1}{4\pi}\left(\int_{t_a} \sin\alpha \left(\nabla\alpha \times \nabla\beta\right) \bullet d\vec{S} \quad - \quad \int_{\partial t_a} \left(1 - \cos\alpha\right)\nabla\beta \bullet d\vec{L} \right),$$

where ∂t_a denotes the boundary of t_a, $d\vec{S}$ is the outward-oriented area element on t_a and $d\vec{L}$ is the line element along its boundary ∂t_a.

The contributions from the surface integral and the line integral cancel each other at all points (by virtue of Stokes' theorem) except those where the vector field is aligned along $-\hat{s}$. w_a counts the number of such points $\vec{r}_*$ inside t_a with a sign, determined by whether φ preserves or reverses the orientation of the outward element $d\vec{S}(\vec{r}_*)$.

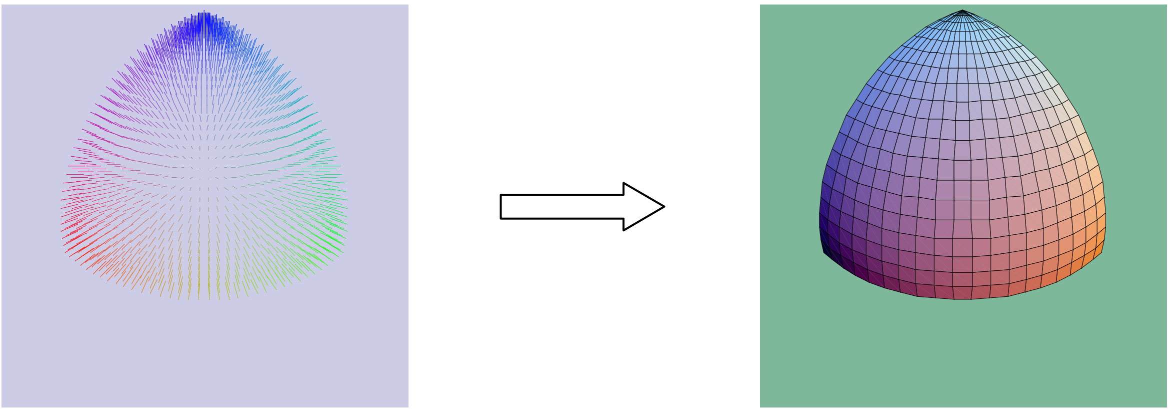


A few simple illustrations might shed further light on this alternative interpretation of wrapping numbers. We look at an octant of the unit cube and employ spherical polar coordinates (r,θ,ϕ) to describe physical space. The relevant ranges for these parameters are $0\le r\le\frac{3^{1/2}}{2}$, $0\le\theta\le\frac{\pi}{2}$, $0\le\phi\le\frac{\pi}{2}$. Then, consider the general configuration

$$n = (\sin(2m+1)\theta \cos(2n+1)\phi \,, \sin(2m+1)\theta \sin(2n+1)\phi \,, \cos(2m+1)\theta \,)$$

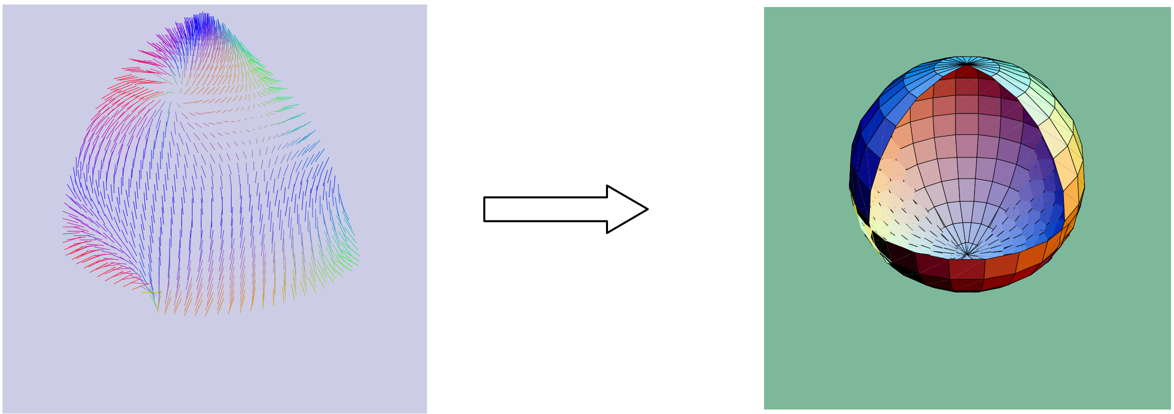
where m, n are given integers. The reference vector is fixed to be $\frac{(1,-1,-1)}{3^{1/2}}$, the corresponding south pole is the diametrically opposite point $\frac{(-1,1,1)}{3^{1/2}}$. (This choice is completely arbitrary. For example, we do not take the south pole to be in the first octant of the target sphere since, ideally, the simplest configuration $m=n=0$ should have wrapping numbers zero and be distinguishable from the remaining configurations.)

m = n = 0



This configuration has wrapping number, $w_{(0,0,0)}$, associated with vertex $(0,0,0)$, zero by convention. The image only occupies an $(1/8)_{\text{th}}$ of the unit sphere as shown above and does not contain our chosen south pole.

m = n = 1



Relative to the preceding diagram, this configuration wraps once around $(0,0,0)$. It is assigned wrapping number +1. The corresponding image covers $(7/8)_{\text{th}}$ of the unit sphere. We conclude that a single point in the interior of t_a is mapped on to the chosen south pole with the positive orientation.

Lastly, we show that the continuity of the vector field imposes a certain sum rule on the wrapping numbers. The boundary of the truncated polyhedron $\partial \widetilde{P}$ can be identified with a unit sphere S^2. Then φ evaluated on $\partial \widetilde{P}$ may be regarded as a map of S^2 into itself – call it Φ, whose degree (roughly speaking the signed number of times the image of Φ covers the target sphere) is readily shown to be the sum of the wrapping numbers associated with all the vertices. However, Φ can be continuously deformed to a trivial constant-valued map of the sphere to itself (just consider φ restricted to a family of surfaces interpolating between $\partial \widetilde{P}$ and a single point in the interior of P). A trivial map has degree zero, necessarily implying that $\sum_{a=1}^{V} w_a = 0$.

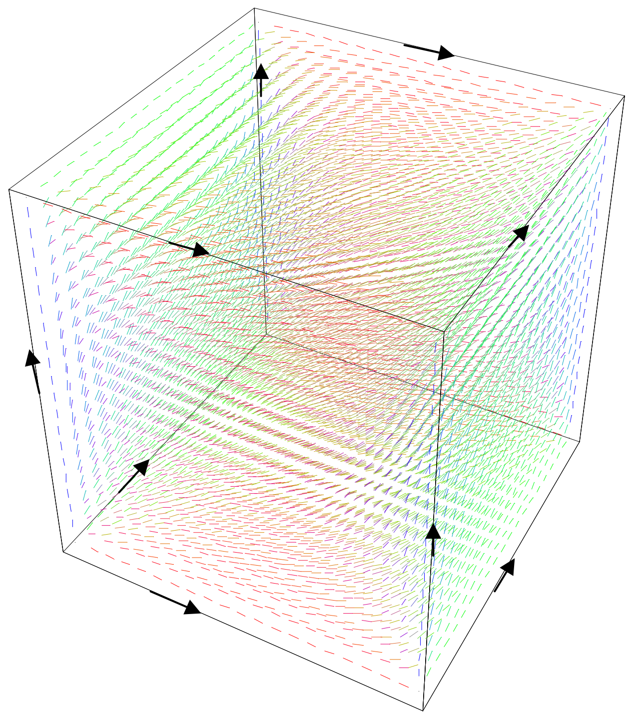
The presence of discontinuities at the vertices eliminates the possibility of any three-dimensional invariants (such as the so-called Hopf number [3]).

SIMPLE EXAMPLE.

As an illustration of our three-dimensional classification scheme, we look at the following configuration contained in the unit cube.

$$n(x,y,z)=\frac{(h(x),h(y),h(z))}{\sqrt{(h^2(x)+h^2(y)+h^2(z))}} \quad 0\le x,y,z\le 1$$

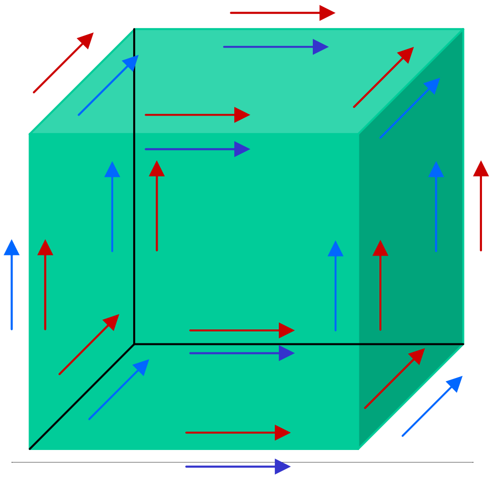
$$h(x)=\begin{cases} x & 0\le x\le \frac{1}{2}-\varepsilon \\ 1-x & \frac{1}{2}+\varepsilon\le x\le 1 \\ \frac{1}{2}-\frac{3}{2\varepsilon}\left(x-\frac{1}{2}\right)^2+\frac{1}{2\varepsilon^3}\left(x-\frac{1}{2}\right)^4 & \frac{1}{2}-\varepsilon\le x\le \frac{1}{2}+\varepsilon \end{cases}$$



The function $h(x)$ ensures that the configuration matches along the planes $x,y,z=(1/2)$ and is continuously differentiable everywhere except at the vertices.

The **associated invariants**.

Each edge e_b is assigned a unit vector $\hat{e}_b$ as indicated below. The chosen convention is to take the vectors $\hat{e}_b$ parallel to the coordinate unit vectors $\hat{x}, \hat{y}$ and $\hat{z}$. The edge sign E_b is +1 for every edge in this set-up since the vector field along e_b is simply $\hat{e}_b$.



The red arrows represent the unit vectors $\hat{e}_b$ whereas the blue arrows denote the actual vector field on the corresponding edges.

The kink and wrapping numbers of this configuration identically vanish. The vector field winds by the minimal amount in the anticlockwise sense while moving between a pair of adjacent edges and its image on any planar surface isolating a given vertex only covers an $(1/8)_{\text{th}}$ of the target sphere.

The **energy.**

We divide our unit cube into octants via the planes $x = \frac{1}{2}$, $y = \frac{1}{2}$, $z = \frac{1}{2}$. The energy density within the cube is assumed to be $|\nabla n|^2$ throughout our study, in agreement with the one-constant approximation. Then one can show that

$$|\nabla n|^2 = \frac{2}{\left(h^2(x) + h^2(y) + h^2(z)\right)}$$

in all eight octants. The symmetry of $h(x)$ ensures that it suffices to compute the energy within any one octant. It should be noted that the interpolatory interval $\frac{1}{2} - \varepsilon \le x \le \frac{1}{2} + \varepsilon$ makes a contribution to the energy of the order of magnitude ε^3. This can be neglected in the limit we are interested in, namely, $\varepsilon \to 0$.

Consider the region of space $0 \le x, y, z \le \frac{1}{2}$ and label it as 'octant 1'. The associated energy density is $|\nabla n|^2 = \frac{2}{\left(x^2 + y^2 + z^2\right)}$. The corresponding energy $\int_{0 \le x,y,z \le \frac{1}{2}} |\nabla n|^2 \, dV$ can be computed exactly using a simple application of the divergence theorem, namely, $\frac{2}{x^2 + y^2 + z^2} = 2\nabla \bullet \left(\frac{(x, y, z)}{x^2 + y^2 + z^2}\right)$. This enables us to express the volume integral in terms of surface integrals over the boundary planes of octant 1.

$$\int\limits_{0\le x,y,z\le \frac{1}{2}} |\nabla n|^2 \, dV = \int\limits_{\{x,y,z=0\}\cup\{x,y,z=\frac{1}{2}\}} 2\,\frac{(x,y,z)}{x^2+y^2+z^2} \bullet d\,S$$

The boundary of octant 1 comprises six planes - $x,y,z=0$ and $x,y,z=\frac{1}{2}$. The surface integrals over the faces $x,y,z=0$ vanish identically. $|\nabla n|^2$ is symmetric in all three variables x,y,z. It immediately follows that $x,y,z=\frac{1}{2}$ make equal contributions to the energy and our result in terms of double integrals is

$$\int\limits_{0\le x,y,z\le \frac{1}{2}} |\nabla n|^2 \, dV = 3\int_0^1\int_0^1 \frac{1}{1+s^2+t^2}\, ds\, dt.$$

It is possible to separate the variables s and t by doing Taylor series expansions of the integrand above. This yields

$$\int_0^1\int_0^1 \frac{1}{1+s^2+t^2}\, ds\, dt = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{(-1)^m}{(2m+1)}\frac{(-1)^n}{(2n+1)}\binom{m+n}{n}.$$

The sum over 'n'can be easily replaced by a hypergeometric function of one variable. This incorporates the binomial coefficient and certainly makes numerical computations far easier and faster. Our final result for the total energy within the unit cube is given below as

$$E = \int\limits_{0\le x,y,z\le 1} |\nabla n|^2 \, dV = 24\sum_{m=0}^{\infty} \frac{(-1)^m}{(2m+1)} F_{2,1}\left(\frac{1}{2}, 1+m, \frac{3}{2}.-1\right) = 15.34...$$

$F_{2,1}(a,b,c,z) = \sum_{k=0}^{\infty} \frac{(a)_k\,(b)_k\,z^k}{(c)_k\,k!}$, $(s)_k = (s)(s+1)...(s+k-1)$. ('s' arbitrary variable)

Our model is similar to the problem studied by Brezis et al in [2]. Using similar methods, it can be shown that the energy, corresponding to all configurations that belong to this particular topological class, is bounded from below by 4π. This will be discussed in greater detail in [5].

THE FUTURE

Our primary aim for the future is to consider various generalizations of the problem presented in this report. We hope to be able to extend our study to periodic arrays of non-convex polyhedral cells placed within the geometry. Periodicity is expected to involve the torus homotopy groups as opposed to the homotopy groups of the sphere studied so far.

Secondly, we intend to model director fields (unit vector fields with opposite orientations identified) instead of vector fields. This would incorporate a transition from S^2, the unit sphere, to RP^2, the projective plane, as our order parameter space.

Further, our set-up only considers tangential boundary conditions so far. Normal boundary conditions also arise in practice and need to be included so that this study is applicable on a much wider scale.

Lastly, singularities and defects should be allowed for. It would be interesting to know how our classification scheme is affected in their presence.

Once the classification scheme is complete, we should have an explicit director field for each topological type. This could be used as an initial condition for numerical minimizing procedures to obtain the actual stable states.

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