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**Tangent unit-vector fields: nonabelian
homotopy invariants and the Dirichlet energy**

by

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Tangent unit-vector fields: nonabelian homotopy invariants and the Dirichlet energy

Partial Differential Equations & Topology

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Abstract

Let O be a closed geodesic polygon in S^2 . Maps from O into S^2 are said to satisfy tangent boundary conditions if the edges of O are mapped into the geodesics which contain them. Taking O to be an octant of S^2 , we evaluate the infimum Dirichlet energy, $\mathcal{E}(H)$, for continuous tangent maps of arbitrary homotopy type H . The expression for $\mathcal{E}(H)$ involves a topological invariant – the spelling length – associated with the (nonabelian) fundamental group of the n -times punctured two-sphere, $\pi_1(S^2 - \{s_1, \dots, s_n\}, *)$. These results have applications for the theoretical modelling of nematic liquid crystal devices.

Résumé: Soit O un polygone géodésique fermé dans S^2 . On dit qu'une application de O dans S^2 satisfait conditions aux limites tangentes si elle associe à chaque côté de O la géodésique qui le contient. Au cas où O serait un octant de S^2 , nous calculons l'infimum d'énergie Dirichlet, $\mathcal{E}(H)$, pour applications tangentes continues avec une type d'homotopie arbitraire, H . L'expression pour $\mathcal{E}(H)$ implique d'utiliser un invariant topologique, le longueur d'orthographe, lié au groupe fondamental (nonabélien) de la 2-sphère percée n fois, $\pi_1(S^2 - \{s_1, \dots, s_n\}, *)$. Ces reultats ont applications pratiques pour la modélisation théorique des dispositifs de cristal liquide nématique.

Version française abrégée : Soit O un polygone géodésique fermé dans S^2 . On dit qu'une application $\nu : O \rightarrow S^2$ satisfait *conditions aux limites tangentes* si ν associe à chaque côté de O la géodésique qui le contient. Soit $\mathcal{C}_T(O, S^2)$ l'espace des applications continues $\nu : O \rightarrow S^2$ qui satisfait conditions aux limites tangentes. L'espace $\mathcal{C}_T(O, S^2)$ peut être partitionné en classes équivalences H sous homotopie; ensembles des invariants classifiants sont qualifiés dans [10, 8]. Pour une classe d'homotopie donnée, on peut considérer l'infimum d'énergie Dirichlet, que nous notons $\mathcal{E}(H)$. Si O est le premier octant $\{e = (e_1, e_2, e_3) \in S^2 \mid e_j \geq 0\}$, nous obtenons une formule explicite pour $\mathcal{E}(H)$. Cette expression implique d'utiliser un invariant topologique, le longueur d'orthographe, lié au groupe fondamental (nonabélien) de $S^2 - R$, où R est un ensemble de huit points, un de chaque octant de S^2 . La démonstration que $\mathcal{E}(H)$ est minoré utilise la théorie combinatoire des groupes et la démonstration que $\mathcal{E}(H)$ est majoré utilise estimats de l'énergie Dirichlet pour applications représentatives explicites. Cettes applications représentatives sont conformes ou nonconformes partout sauf dans un sous-ensemble de O d'aire arbitrairement petite.

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Selon la théorie d'Oseen et Frank, un cristal liquide nématique dans un domaine polyédrique fermé $P \subset \mathbb{R}^3$ est décrit par une application dans S^2 , $\mathbf{n} : P \rightarrow S^2$. On utilise souvent les *conditions aux limites tangentes* pour modéliser tels systèmes confinés tel que, à chaque face de P , \mathbf{n} tient valeurs qui sont tangentes à cette face. Selon certaines approximations, l'énergie libre de n est donnée par l'énergie Dirichlet. Notre formule pour $\mathcal{E}(H)$ fournisse la borne supérieure et la borne inférieure pour l'infimum d'énergie Dirichlet comme fonction de type d'homotopie et de géométrie.

1 Statement of Results

Let O be a closed geodesic polygon in $S^2 \subset \mathbb{R}^3$, and let $\mathcal{C}(O, S^2)$ denote the set of continuous maps $\nu : O \rightarrow S^2$. A map $\nu \in \mathcal{C}(O, S^2)$ is said to satisfy *tangent boundary conditions* if ν maps each edge of O into the geodesic which contains it. Let $\mathcal{C}_T(O, S^2)$ denote the set of maps in $\mathcal{C}(O, S^2)$ which satisfy tangent boundary conditions. Then $\mathcal{C}_T(O, S^2)$ can be partitioned into homotopy classes, for which classifying invariants are described in [10, 8].

We compute the infimum of the Dirichlet energy in each homotopy class of the admissible space $\mathcal{C}_T(O, S^2)$. This is a harmonic map problem. Harmonic map problems are amongst the most celebrated in the calculus of variations [1, 3]. In particular, it is well known that continuous $S^2 \rightarrow S^2$ maps are classified up to homotopy by their degree, and the infimum of the Dirichlet energy, $\int_{S^2} |\nabla \phi|^2 dA$, for maps ϕ of given degree d is equal to $8\pi d$ [3]. However, tangent boundary conditions introduce non-trivial topological features which are not described by existing theory.

We first summarize the relevant results on homotopy classification [10, 8]. We take the domain O to be the positive coordinate octant

$$O = \{\mathbf{r} = (r_x, r_y, r_z) \in S^2, r_j \geq 0\}, \quad (1)$$

with vertices given by the coordinate unit vectors \hat{x} , \hat{y} and \hat{z} . The first set of homotopy invariants are the *edge signs* $e = (e_x, e_y, e_z)$, which are associated with the values of ν at the vertices of O . Tangent boundary conditions imply that $\nu(\hat{j}) = e_j \hat{j}$, where $e_j = \pm 1$. The second set of invariants are the *kink numbers*, which are associated with the values of ν on the edges of O . Consider, for example, the yz -edge; its image under ν is a curve on the yz -coordinate circle with endpoints $e_y \hat{y}$ and $e_z \hat{z}$. The corresponding kink number, denoted k_x , is defined to be the integer-valued winding number of this curve relative to the shortest geodesic between its endpoints. The kink numbers k_y and k_z are defined similarly. The third invariant, the *trapped area* Ω , is defined to be the oriented area of the image of the interior of O under ν , given for ν differentiable by

$$\Omega = - \int_O \nu^* \omega, \quad (2)$$

where ω is the area two-form on S^2 normalised so that $\int_{S^2} \omega = 4\pi$. For given (e, k) , the allowed values of Ω are given by $4\pi m + 2\pi \sum_j k_j - \frac{1}{2}\pi e_x e_y e_z$, where m is an integer. The invariants (e, k, Ω) collectively classify the homotopy classes of $\mathcal{C}_T(O, S^2)$, and all allowed values can be realised.

The homotopy classes can also be characterized by generalised degrees, called *wrapping numbers*, associated with the open coordinate octants of the unit sphere. We label the coordinate octants $\Sigma_\sigma \subset S^2$ by a triple of signs $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ such that

$$\Sigma_\sigma = \{\mathbf{s} = (s_x, s_y, s_z) \in S^2, \sigma_j s_j > 0\}. \quad (3)$$

The corresponding wrapping number w_σ is defined to be a signed count of the number of pre-images of a regular value $\mathbf{s}_\sigma \in \Sigma_\sigma$, taking orientation into account. For ν differentiable,

$$w_\sigma = - \sum_{x \in \nu^{-1}(\mathbf{s}_\sigma)} \text{sgn det } \nu'(x) \quad (4)$$

(by convention, we take $w_\sigma \leq 0$ for orientation-preserving ν). The wrapping numbers can be expressed in terms of the edge signs, kink numbers, and trapped area, and vice versa, so that the wrapping numbers constitute an alternative set of classifying invariants for $\mathcal{C}_T(O, S^2)$.

We introduce some terminology and notation. We say that a homotopy class in $\mathcal{C}_T(O, S^2)$ is *conformal* if $w_\sigma \leq 0$ for all σ , *anticonformal* if $w_\sigma \geq 0$ for all σ , and *nonconformal* otherwise. Also, we say that the octants Σ_σ and $\Sigma_{\sigma'}$ are *adjacent*, denoted $\sigma \sim \sigma'$, if Σ_σ and $\Sigma_{\sigma'}$ have a common edge, or equivalently, if σ and σ' have precisely two components the same.

Given maps $\nu \in \mathcal{C}_T(O, S^2) \cap W^{1,2}(O, S^2)$ and a homotopy class $H \subset \mathcal{C}_T(O, S^2)$, let $\mathcal{E}(H)$ denote the infimum Dirichlet energy in H , defined by

$$\mathcal{E}(H) = \inf_{\nu \in H} E(\nu) = \inf_{\nu \in H} \int_O |\nabla \nu|^2 dA. \quad (5)$$

Our main result is an explicit formula for $\mathcal{E}(H)$.

Theorem 1. *Let H be a homotopy class in $\mathcal{C}_T(O, S^2)$. Then*

$$\mathcal{E}(H) = \pi \left(\sum_{\sigma} |w_\sigma| + \Delta(H) \right), \quad (6)$$

where

$$\Delta(H) = \begin{cases} 0, & H \text{ conformal/anticonformal,} \\ 2 \max \left(0, w_{\sigma_+} - \sum_{\sigma \sim \sigma_+} \Phi(w_\sigma) - \chi, |w_{\sigma_-}| - \sum_{\sigma \sim \sigma_-} \Phi(-w_\sigma) - \chi \right), & H \text{ nonconformal,} \end{cases} \quad (7)$$

Σ_{σ_+} and Σ_{σ_-} are the octants with the largest positive and smallest negative wrapping numbers respectively, $\Phi(x) = \frac{1}{2}(x + |x|)$ and $\chi = 1$ if $k_x k_y k_z < 0$ and is zero otherwise.

The formula (6) follows from a delicate analysis of the minimal number of pre-images for a set of regular values, one in each octant of S^2 . The minimal number of pre-images is captured by a topological invariant, the *spelling length*, associated with the non-abelian fundamental group of S^2 with a set of regular values removed (see Section 2 for details). The minimum spelling length, as can be seen from (6), consists of two contributions - $\sum_{\sigma} |w_\sigma| \pi$, which can be derived from standard degree arguments, and an additional term, $\Delta(H) \pi$, which reflects the fact that the minimal number of pre-images may necessarily exceed the absolute value of the wrapping number (degree) for certain nonconformal homotopy classes.

Theorem 1 follows from two propositions, the first giving a lower bound for $\mathcal{E}(H)$ and the second giving a matching upper bound.

Proposition 1.1.

$$\mathcal{E}(H) \geq \sum_{\sigma} |w_\sigma| \pi + \Delta(H) \pi. \quad (8)$$

Proposition 1.2.

$$\mathcal{E}(H) \leq \sum_{\sigma} |w_\sigma| \pi + \Delta(H) \pi. \quad (9)$$

Our work is motivated by the theoretical modelling of nematic liquid crystals in confined polyhedral geometries. The Oseen-Frank theory describes the configuration of a nematic liquid crystal (i.e., the preferred orientation of the constituent molecules) by a unit-vector field $\mathbf{n}(\mathbf{r})$ [2]. Under certain approximations (*one-constant approximation*), the Oseen-Frank energy reduces to the standard Dirichlet energy [2]. For a right rectangular prism $P \subset \mathbb{R}^3$ with edge lengths $L_x \geq L_y \geq L_z$ and reflection-symmetric tangent unit-vector

fields (a reflection-symmetric unit-vector field is invariant with respect to reflections across the midplanes of the prism), the bounds (8) and (9) directly translate into analytic bounds for the 3D-Dirichlet energy in a given homotopy class $H \subset \mathcal{C}_T(P, S^2)$ i.e. for $\mathbf{n} \in H \cap W^{1,2}(P, S^2)$, we have that

$$4L_z \mathcal{E}(H) \leq \inf_{\mathbf{n} \in H} \int_P |\nabla \mathbf{n}|^2 dV \leq 4\sqrt{L_x^2 + L_y^2 + L_z^2} \mathcal{E}(H), \quad (10)$$

where $\mathcal{E}(H)$ is as stated in (6). These results have implications for the characterization of multistability in prototype bistable liquid crystal devices [4].

2 Lower bound for $\mathcal{E}(H)$

In [6], we established that smooth maps, satisfying tangent boundary conditions, are dense with respect to the Sobolev norm, in the space $\mathcal{C}_T(O, S^2) \cap W^{1,2}(O, S^2)$. Therefore, it suffices to compute the infimum energy $\mathcal{E}(H)$ for differentiable maps. Let $\nu \in \mathcal{C}_T(O, S^2)$ be differentiable, with boundary map $\partial\nu : \partial O \rightarrow S^2$. Let \mathcal{R}_ν denote the set of regular values of ν (by convention, \mathcal{R}_ν does not include points in the image of $\partial\nu$). By Sard's theorem, \mathcal{R}_ν is of full measure [11]. Let $S = \{\mathbf{s}_0, \mathbf{s}_1, \dots, \mathbf{s}_n\} \subset \mathcal{R}_\nu$ be a set of $(n+1)$ -regular values of ν with $n > 0$. For a given $\mathbf{s}_j \in \mathcal{R}_\nu$, we define the algebraic degree, $d_\nu(\mathbf{s}_j)$, and its absolute version, $D_\nu(\mathbf{s}_j)$, as follows -

$$d_\nu(\mathbf{s}_j) = \sum_{x \in \nu^{-1}(\mathbf{s}_j)} \text{sgn det } \nu'(x), \quad (11)$$

$$D_\nu(\mathbf{s}_j) = \sum_{x \in \nu^{-1}(\mathbf{s}_j)} 1. \quad (12)$$

Clearly, $|d_\nu(\mathbf{s}_j)| \leq D_\nu(\mathbf{s}_j)$ and for $\mathbf{s}_\sigma \in \Sigma_\sigma \cap \mathcal{R}_\nu$, $d_\nu(\mathbf{s}_\sigma) = -w_\sigma$ from (4).

The proof of Proposition 1.1 consists of three main steps (refer to [9] for details). Firstly, we show that the quantity $\sum_{j=0}^n D_\nu(\mathbf{s}_j)$ has a lower bound in terms of a topological invariant - the minimum *spelling length* over a product of conjugacy classes in the (non-abelian) fundamental group of S^2 with a set of excluded regular values $S = \{\mathbf{s}_0, \mathbf{s}_1, \dots, \mathbf{s}_n\} \subset \mathcal{R}_\nu$, see Proposition 2.1. Secondly, we compute explicit lower bounds for the minimum spelling length using combinatorial-group-theoretic arguments in Proposition 2.2. Finally, in Lemma 2.1, we show that the Dirichlet energy $E(\nu)$ has a lower bound in terms of the $D_\nu(\mathbf{s}_\sigma)$'s where $\mathbf{s}_\sigma \in \Sigma_\sigma \cap \mathcal{R}_\nu$, leading to an explicit lower bound for $\mathcal{E}(H)$ in Proposition 1.1.

We define the spelling length as follows. Let $\pi_1(S^2 - S; \mathbf{u})$ denote the fundamental group of the $(n+1)$ -times punctured unit sphere, based at $\mathbf{u} \in S^2$, where \mathbf{u} is contained in the image of $\partial\nu$. Then we can identify $\pi_1(S^2 - S; \mathbf{u})$ with the free group of n generators, $F(c_1, \dots, c_n)$ [5]. We take the generator c_j to be the homotopy class $[\delta_j]$ of a loop δ_j in $S^2 - S$ based at \mathbf{u} which encloses \mathbf{s}_j once, separates \mathbf{s}_j from the other \mathbf{s}_k 's and is positively oriented with respect to \mathbf{s}_j . Let δ_0 be a loop in $S^2 - S$ based at \mathbf{u} which encloses \mathbf{s}_0 once, separates \mathbf{s}_0 from the other \mathbf{s}_j 's and is positively oriented with respect to \mathbf{s}_0 . Then $c_0 = [\delta_0]$ may be expressed as a product of positive and negative powers of the c_j 's (with $1 \leq j \leq n$) in which the sum of the exponents of each of the c_j 's is equal to -1 .

Given $g \in F(c_1, \dots, c_n)$, we define a *spelling* to be a factorisation of g into a product of conjugated generators and inverse generators, e.g.

$$g = h_1 c_{i_1}^{\epsilon_1} h_1^{-1} \cdots h_r c_{i_r}^{\epsilon_r} h_r^{-1}, \quad (13)$$

where $h_j \in F(c_1, \dots, c_n)$ and $\epsilon_j = \pm 1$. The number of factors in a spelling of g , i.e. r in (13), is not uniquely determined. We define the *spelling length* of g , denoted $\Lambda_n(g)$, to be the smallest possible number of factors

amongst all spellings of g . Given $g \in F(c_1, \dots, c_n)$, let $\langle g \rangle$ denote the conjugacy class of g , i.e.

$$\langle g \rangle = \{g' \in F(c_1, \dots, c_n) \mid g' = hgh^{-1} \text{ for some } h \in F(c_1, \dots, c_n)\}. \quad (14)$$

Also, given subsets V and W of $F(c_1, \dots, c_n)$, we define their *set product*, denoted VW , to be the subset of $F(c_1, \dots, c_n)$ given by

$$VW = \{vw \mid v \in V, w \in W\}. \quad (15)$$

Let V^n denote n -fold set product of V with itself.

The main results are -

Proposition 2.1. [9] Let $P = \frac{1}{2}(D_\nu(\mathbf{s}_0) + d_\nu(\mathbf{s}_0))$ and $N = \frac{1}{2}(D_\nu(\mathbf{s}_0) - d_\nu(\mathbf{s}_0))$ denote the number of pre-images in $\nu^{-1}(\mathbf{s}_0)$ with positive and negative orientation respectively. Let $\langle c_0 \rangle$ denote the conjugacy class of c_0 in $F(c_1, \dots, c_n)$, and let $V_{P,N} \subset F(c_1, \dots, c_n)$ be the set product given by

$$V_{P,N} = \{[\partial\nu]\}\langle c_0 \rangle^P \langle c_0^{-1} \rangle^N \quad (16)$$

where $[\partial\nu]$ is regarded as an element of $F(c_1, \dots, c_n)$. Then

$$\sum_{j=1}^n D_\mu(s_j) \geq \min_{g \in V_{P,N}} \Lambda_n(g). \quad (17)$$

Thus, Proposition 2.1 implies that

$$\sum_{j=0}^n D_\nu(\mathbf{s}_j) \geq D_\nu(\mathbf{s}_0) + \min_{g \in V_{P,N}} \Lambda_n(g). \quad (18)$$

For our applications, we encounter two different set products depending on whether $k_x k_y k_z < 0$ or otherwise i.e. $V_{P,N} = \{c_3^{k_z-1} c_1^{k_x-1} c_2^{k_y-1}\} \langle c_3 c_1 c_2 \rangle^P \langle (c_3 c_1 c_2)^{-1} \rangle^N$ if $k_x k_y k_z < 0$ and $V_{P,N} = \{c_3^{k_z-1} c_1^{k_x-1} c_2^{k_y-1}\} \langle c_2 c_1 c_3 \rangle^P \langle (c_2 c_1 c_3)^{-1} \rangle^N$ otherwise. Then the minimum spelling length in (17) can be explicitly estimated using the following result.

Proposition 2.2. For $g \in \{A^i B^j C^k\} \langle ABC \rangle^p \langle (ABC)^{-1} \rangle^n \subset F(A, B, C)$ with $i, j, k, n, p \geq 0$,

$$\min_g \Lambda_3(g) \geq i + j + k - (p + n) - 2. \quad (19)$$

For $g \in \{A^i B^j C^k\} \langle CBA \rangle^p \langle (CBA)^{-1} \rangle^n \subset F(A, B, C)$ with $i, j, k, n, p \geq 0$,

$$\min_g \Lambda_3(g) \geq i + j + k - (p + n). \quad (20)$$

Finally, we have that -

Lemma 2.1. For any $\nu \in \mathcal{C}_T(O, S^2) \cap W^{1,2}(O, S^2)$ and a set of regular values $\{\mathbf{s}_\sigma\} \in \Sigma_\sigma \cap \mathcal{R}_\nu$,

$$E(\nu) \geq \pi \inf_{\{\mathbf{s}_\sigma\}} \sum_{\sigma} D_\nu(\mathbf{s}_\sigma). \quad (21)$$

Proposition 1.1 now follows from Lemma 2.1 and Propositions 2.1 and 2.2.

3 Upper bound for $\mathcal{E}(H)$

Let $H \subset \mathcal{C}_T(O, S^2)$ be a nonconformal homotopy class. We prove Proposition 1.2 by constructing a sequence of maps $\nu_\epsilon \in H$ whose Dirichlet energies saturate the upper bound (9) (for conformal and anticonformal homotopy classes, (9) was established in [7]). The maps $\nu_\epsilon \in H$ are conformal or anticonformal except on a set whose area vanishes with ϵ . In terms of complex coordinates on O and S^2 , ν_ϵ is rational away from the vertices of O , with zeros and poles subject to constraints imposed by tangent boundary conditions. Near the vertices of O , ν_ϵ is modified to describe an alternating sequence of rational conformal and anticonformal maps, each of whose image covers a pair of adjacent octants. As is implied by the following, ν_ϵ can be constructed to realise the minimum absolute number of preimages consistent with Proposition 1.1.

Lemma 3.1. [9] *For every $\epsilon > 0$, there exists a $\nu_\epsilon \in H$ such that*

$$E(\nu_\epsilon) \leq \pi \left(\sum_{\sigma} |w_{\sigma}| + \Delta(H) \right) + f(\epsilon)$$

where $f : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ and $f(\epsilon) \rightarrow 0$ as $\epsilon \rightarrow 0$.

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