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

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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, $\pi_1(S^2 - \{s_1, \ldots, s_n\}, *)$. These results have applications for the theoretical modelling of nematic liquid crystal devices. ***To cite this article: A. Majumdar et al., C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

Résumé

Champs de vecteurs unités tangents : Invariants homotopiques non abelien et énergie de Dirichlet. Soit O un polygone géodésique fermé de S^2. On dit qu'une application de O dans S^2 vérifie des conditions aux limites tangentes si elle associe à chaque côté de O la géodésique qui le contient. Dans le cas où O est un octant de S^2, on calcule l'infimum d'énergie de Dirichlet, $\mathcal{E}(H)$, pour des applications tangentes continues d'un type d'homotopie quelconque H. L'expression de $\mathcal{E}(H)$ utilise un invariant topologique, la longueur nominale, lié au groupe fondamentel (non abélien) de la sphère S^2 à n trous ponctuels, $\pi_1(S^2 - \{s_1, \ldots, s_n\}, *)$. Les réeultats obtenus ont des applications pratiques, notamment dans la modélisation des systèmes contenant de cristaux liquides nématiques. ***Pour citer cet article : A. Majumdar et al., C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

Version française abrégée

On considère un polygone géodésique O, fermé de S^2. On dit qu'une application $\boldsymbol{\nu} : O \to S^2$ vérifie des *conditions aux limits tangents*, si $\boldsymbol{\nu}$ associe à chaque côté de O, la géodésique qui le contient. Soit $\mathcal{C}_T(O, S^2)$ l'espace des applications $\boldsymbol{\nu} : O \to S^2$ qui vérifiant les conditions aux limites tangentes ; on peut partitionner $\mathcal{C}_T(O, S^2)$ en classes d'équivalence d'homotopie H, ensemble d'invariants définés dans [10,8]. Pour une classe d'homotopie donnée, on peut

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considérer l'infimum de l'énergie de Dirichlet notée $\mathcal{E}(H)$. Si O est le premier octant, $\{\mathbf{e} = (e_1, e_2, e_3) \in S^2 \mid e_j \geqslant 0\}$, on obtient une expression explicite de $\mathcal{E}(H)$; cette expression introduit un invariant topologique, la longueur nominale, lié au groupe fondamental (non abélien) de $S^2 - R$, où R est un ensemble de huit points, un de chaque octant de S^2. La démonstration de la minoration de $\mathcal{E}(H)$ utilise une propriété combinatoire des groupes, et la démonstration de la majoration de $\mathcal{E}(H)$ utilise des estimations de l'énergie de Dirichlet pour des applications explicites ; ces applications sont conformes ou non conformes partout, à l'exception d'un sous-ensemble de O d'aire arbitrairement petite.

En théorie d'Oseen–Frank, un cristal liquide nématique dans un domaine polyédrique fermé, $P \subset \mathbb{R}^3$, est décrit par une application dans $\mathbf{n} : P \to S^2$. On utilise, en général, des *conditions aux limites tangentes* pour modéliser de tels systèmes confinés, telles que pour chaque face de P, $\mathbf{n}$ prend des valeurs tangentes à cette face. Pour certaines approximations, l'énergie n est donnée par l'énergie de Dirichlet. Notre formule pour $\mathcal{E}(H)$ fournit la borne supérieure et la borne inférieure de l'infimum de l'énergie de Dirichlet en fonction du type d'homotopie et de la 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 $\boldsymbol{v} : O \to S^2$. A map $\boldsymbol{v} \in \mathcal{C}(O, S^2)$ is said to satisfy *tangent boundary conditions* if $\boldsymbol{v}$ 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 $S^2 \to S^2$ maps are classified up to homotopy by their degree, and the infimum of the Dirichlet energy, $\int_{S^2} |\nabla\phi|^2 \, \mathrm{d}A$, 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,

$$O = \left\{\mathbf{r} = (r_x, r_y, r_z) \in S^2,\ r_j \geqslant 0\right\}, \tag{1}$$

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 $\boldsymbol{v}$ at the vertices of O. Tangent boundary conditions imply that $\boldsymbol{v}(\hat{j}) = e_j \hat{j}$, where $e_j = \pm 1$. The second set of invariants are the *kink numbers*, which are associated with the values of $\boldsymbol{v}$ on the edges of O. Consider, for example, the yz-edge; its image under $\boldsymbol{v}$ 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 $\boldsymbol{v}$, given for differentiable $\boldsymbol{v}$ by:

$$\Omega = -\int_O \boldsymbol{v}^*\omega, \tag{2}$$

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

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

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 $\boldsymbol{v}$ differentiable,

$$w_\sigma = -\sum_{x \in \boldsymbol{v}^{-1}(\mathbf{s}_\sigma)} \operatorname{sgn} \det \boldsymbol{v}'(x) \tag{4}$$

(by convention, we take $w_\sigma \leqslant 0$ for orientation-preserving $\boldsymbol{v}$). 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 $w_\sigma \leqslant 0$ for all σ, *anticonformal* if $w_\sigma \geqslant 0$ 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 $\boldsymbol{v} \in \mathcal{C}_T(O, S^2) \cap W^{1,2}(O, S^2)$ 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:

$$\mathcal{E}(H) = \inf_{\boldsymbol{v} \in H} E(\boldsymbol{v}) = \inf_{\boldsymbol{v} \in H} \int_O |\nabla \boldsymbol{v}|^2 \, \mathrm{d}A. \tag{5}$$

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*

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

where

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

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 nonabelian 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.

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

Proposition 1.2.

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

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 $L_x \geqslant L_y \geqslant L_z$ 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

$$4L_z\mathcal{E}(H) \leqslant \inf_{\mathbf{n}\in H} \int_P |\nabla \mathbf{n}|^2 \, \mathrm{d}V \leqslant 4\sqrt{L_x^2 + L_y^2 + L_z^2}\,\mathcal{E}(H), \tag{10}$$

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 $\boldsymbol{\nu} \in \mathcal{C}_T(O, S^2)$ be differentiable, with boundary map $\partial\boldsymbol{\nu} : \partial O \to S^2$. Let $\mathcal{R}_{\boldsymbol{\nu}}$ denote the set of regular values of $\boldsymbol{\nu}$ (by convention, $\mathcal{R}_{\boldsymbol{\nu}}$ does not include points in the image of $\partial\boldsymbol{\nu}$). By Sard's theorem, $\mathcal{R}_{\boldsymbol{\nu}}$ is of full measure [11]. Let $S = \{\mathbf{s}_0, \mathbf{s}_1, \ldots, \mathbf{s}_n\} \subset \mathcal{R}_{\boldsymbol{\nu}}$ be a set of $(n+1)$-regular values of $\boldsymbol{\nu}$ with $n > 0$. For a given $\mathbf{s}_j \in \mathcal{R}_{\boldsymbol{\nu}}$, we define the algebraic degree, $d_{\boldsymbol{\nu}}(\mathbf{s}_j)$, and its absolute version, $D_{\boldsymbol{\nu}}(\mathbf{s}_j)$, as follows:

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

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

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

The proof of Proposition 1.1 consists of three main steps (refer to [9] for details). Firstly, we show that the quantity $\sum_{j=0}^n D_{\boldsymbol{\nu}}(\mathbf{s}_j)$ has a lower bound in terms of a topological invariant – the minimum *spelling length* over a product of conjugacy classes in the (nonabelian) fundamental group of S^2 with a set of excluded regular values $S = \{\mathbf{s}_0, \mathbf{s}_1, \ldots, \mathbf{s}_n\} \subset \mathcal{R}_{\boldsymbol{\nu}}$, 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 $E(\boldsymbol{\nu})$ has a lower bound in terms of the $D_{\boldsymbol{\nu}}(\mathbf{s}_\sigma)$'s where $\mathbf{s}_\sigma \in \Sigma_\sigma \cap \mathcal{R}_{\boldsymbol{\nu}}$, leading to the 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 $\partial\boldsymbol{\nu}$. Then we can identify $\pi_1(S^2 - S; \mathbf{u})$ with the free group of n generators, $F(c_1, \ldots, c_n)$ [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 $1 \leqslant j \leqslant n$) in which the sum of the exponents of each of the c_j's is equal to -1.

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

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

where $h_j \in F(c_1, \ldots, c_n)$ 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 $g \in F(c_1, \ldots, c_n)$, let $\langle g \rangle$ denote the conjugacy class of g, i.e.

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

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

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

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

The main results are

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

$$V_{P,N} = \big\{[\partial\boldsymbol{\nu}]\big\}\langle c_0\rangle^P\big\langle c_0^{-1}\big\rangle^N \tag{16}$$

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

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

Thus, Proposition 2.1 implies that

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

For our applications, we encounter two different set products depending on whether $k_xk_yk_z < 0$ or otherwise, i.e.

$$V_{P,N} = \big\{c_3^{k_z-1}c_1^{k_x-1}c_2^{k_y-1}\big\}\langle c_3c_1c_2\rangle^P\big\langle (c_3c_1c_2)^{-1}\big\rangle^N, \quad \text{if } k_xk_yk_z < 0$$

and

$$V_{P,N} = \big\{c_3^{k_z-1}c_1^{k_x-1}c_2^{k_y-1}\big\}\langle c_2c_1c_3\rangle^P\big\langle (c_2c_1c_3)^{-1}\big\rangle^N, \quad \text{otherwise.}$$

Then the minimum spelling length in (17) can be explicitly estimated using the following result:

Proposition 2.2. *(See [9].) For $g \in \{A^iB^jC^k\}\langle ABC\rangle^p\langle (ABC)^{-1}\rangle^n \subset F(A,B,C)$ with $i,j,k,n,p \geqslant 0$,*

$$\min_g \Lambda_3(g) \geqslant i+j+k-(p+n)-2. \tag{19}$$

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

$$\min_g \Lambda_3(g) \geqslant i+j+k-(p+n). \tag{20}$$

Finally, we have that

Lemma 2.1. *(See [9].) For any $\boldsymbol{\nu} \in \mathcal{C}_T(O,S^2)\cap W^{1,2}(O,S^2)$ and a set of regular values $\{\mathbf{s}_\sigma\} \in \Sigma_\sigma \cap \mathcal{R}_{\boldsymbol{\nu}}$,*

$$E(\boldsymbol{\nu}) \geqslant \pi \inf_{\{\mathbf{s}_\sigma\}} \sum_\sigma D_{\boldsymbol{\nu}}(\mathbf{s}_\sigma). \tag{21}$$

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 $\boldsymbol{\nu}_\epsilon \in H$ whose Dirichlet energies saturate the upper bound (9) (for conformal and anticonformal homotopy classes, (9) was established in [7]). The maps $\boldsymbol{\nu}_\epsilon \in H$ are conformal or anticonformal except on a set whose area vanishes with ϵ. In terms of complex coordinates on O and S^2, $\boldsymbol{\nu}_\epsilon$ 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, $\boldsymbol{\nu}_\epsilon$ 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, $\boldsymbol{\nu}_\epsilon$ can be constructed to realise the minimum absolute number of preimages consistent with Proposition 1.1.

Lemma 3.1. *(See [9].) For every* $\epsilon > 0$*, there exists a* $\boldsymbol{v}_\epsilon \in H$ *such that*

$$E(\boldsymbol{v}_\epsilon) \leqslant \pi\left(\sum_\sigma |w_\sigma| + \Delta(H)\right) + f(\epsilon),$$

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

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