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CONFORMALLY INVARIANT ENERGIES OF KNOTS

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Abstract Conformally invariant functionals on the space of knots are introduced via extrinsic conformal geometry of knots and integral geometry on the space of spheres. Our functionals are expressed in terms of a complex-valued 2-form, which can be considered as the cross-ratio of a pair of infinitesimal segments of the knot. We show that our functionals detect the unknot as the total curvature does, and that their values explode if a knot degenerates to a singular knot with double points.

Keywords: knot; energy; conformal; cross-ratio; Möbius transformations

AMS 2000 *Mathematics subject classification:* Primary 57M25; 53A30
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Contents

1. Introduction

In 1929, Fenchel [**8**] proved that the total curvature of a closed curve is greater than or equal to 2π. Between 1949 and 1951, Fary [**7**], Fenchel [**9**] and Milnor [**25**] independently proved that the total curvature of a non-trivial knot is greater than 4π. This means that non-triviality of knots imposes a jump on the total curvature functional. For knots in S^3, one has to consider the sum of the length and the total curvature to get such a jump for non-trivial knots (see [**3**, **22**]).

In 1989, the second author introduced the *energy* $E^{(2)}$ of a knot [**27**] as the regularization of modified electrostatic energy of charged knots. This energy $E^{(2)}$ is a functional on the space of knots that explodes if a knot degenerates to a singular knot with double points. In 1994, Freedman *et al*. [**11**] showed that the energy is conformally invariant and that there is a lower bound for the energy of non-trivial knots, which can detect the unknot. Recent results concerning the energy can be found in [**5**].

In this paper we introduce several conformally invariant functionals on the space of knots that satisfy the two properties above, namely, the jump imposed by the non-triviality of knots and the explosion for the singular knots. These functionals can be expressed in terms of the *infinitesimal cross-ratio*, which is a complex-valued 2-form on the configuration space $K \times K \setminus \Delta$ of a knot K defined as follows. Let Σ be a 2-sphere which is tangential to K at both x and y. (We will call such a sphere a twice tangent sphere of K.) Identify Σ with $\mathbb{C} \cup \{\infty\}$. Then the infinitesimal cross-ratio can be obtained as the cross-ratio of x, $x + \mathrm{d}x$, y and $y + \mathrm{d}y$.

This paper is arranged as follows.

In § 2 we introduce the geometry of the space of n-spheres. We realize it as a hypersurface in Minkowski space and give an invariant measure on it. A 4-tuple of points of $\mathbb{R}^3$ or S^3 is contained in a sphere Σ (unique if the four points do not belong to a circle), which allows us to define the cross-ratio of four points.

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In § 3 we make a brief review of the energy $E^{(2)}$, and introduce the cosine formula given by Doyle and Schramm.

In § 4 we show that the integrand of $E^{(2)}$ can be interpreted in terms of the infinitesimal cross-ratio. We show that the real part of this infinitesimal cross-ratio coincides with the pull-back of the canonical symplectic form of the cotangent bundle of S^3. It allows us to deduce the original definition of $E^{(2)}$ from its cosine formula.

In § 5 we define another functional in terms of this infinitesimal cross-ratio and show that it has the jump and the explosion properties.

In § 6 we introduce a *non-trivial sphere* for a knot, which is a sphere that intersects the knot in at least four points. We give a formula of the measure of the set of the non-trivial spheres for a knot (counted with multiplicity), which will be called the *measure of acyclicity*, in terms of the infinitesimal cross-ratio.

In § 7 we then study the position of the knot with respect to a *zone* which is a region bounded by two disjoint 2-spheres. Recall that a zone is characterized up to conformal transformation by one number, which we call the *modulus*. One way to compute it is to send the two boundary spheres by a conformal transformation into concentric position. The modulus is then the logarithm of the ratio of the radii. By showing that zones that are too 'thin' cannot catch the topology of a given non-trivial knot, we prove that the measure of acyclicity has the jump and the explosion properties.

We put an appendix as § 8. In § 8.1 we show that the integrand of $E^{(2)}$ can also be interpreted as the maximal modulus of an infinitesimal zone whose boundary spheres pass through pairs of points $\{x, y\}$ and $\{x + \mathrm{d}x, y + \mathrm{d}y\}$, respectively. In § 8.2 we introduce a conformal geometric generalization of the Gauss integral formula for the linking number. In § 8.3 we express the radius of global curvature, which was introduced by Menger *et al*. [**13**] in terms of the 4-*tuple map* introduced in § 2.

Throughout the paper, for the sake of simplicity, when we consider knots in $\mathbb{R}^3$, we assume that they are parametrized by arc-length unless otherwise mentioned. In what follows, a knot K always means the image of an embedding f from S^1 into $\mathbb{R}^3$ or S^3.

2. The space of spheres and the cross-ratio of four points

2.1. The space of $(n-1)$-spheres in S^n

Definition 2.1.

(1) Define an indefinite quadratic form L on $\mathbb{R}^{n+2}$ and the associated *pseudo inner product* $L(\cdot,\cdot)$,

$$L(x_1,\dots,x_{n+2}) = (x_1)^2 + \cdots + (x_{n+1})^2 - (x_{n+2})^2,$$
$$L(u,v) = u_1v_2 + \cdots + u_{n+1}v_{n+1} - u_{n+2}v_{n+2}.$$

This quadratic form with signature $(n+1, 1)$ is called the *Lorentz quadratic form*. The Euclidean space $\mathbb{R}^{n+2}$ equipped with this pseudo inner product L is called the *Minkowski space* and denoted by $\mathbb{R}^{n+1,1}$.

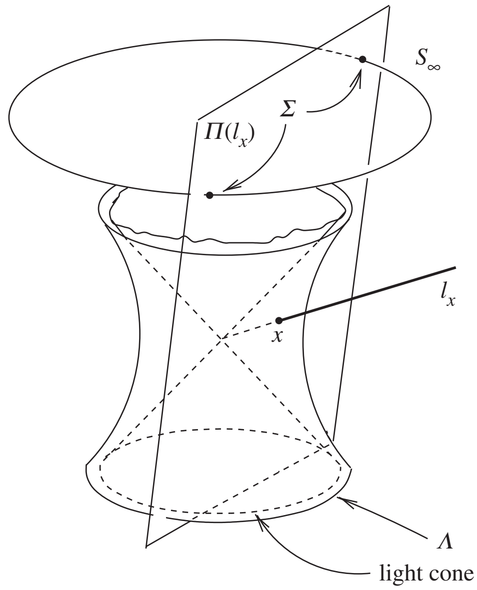

Figure 1. S^n_∞ and the correspondence between Λ and $\mathcal{S}$.

(2) The set $\mathcal{G} = O(n+1,1)$ of linear isomorphism of $\mathbb{R}^{n+2}$ which preserves this pseudo inner product L is called the (*full homogeneous*) *Lorentz group*. We also call it the *conformal group* for short.

(3) A vector v in $\mathbb{R}^{n+2}$ is called *space-like* if $L(v) > 0$, *light-like* if $L(v) = 0$ and *time-like* if $L(v) < 0$. A line is called space-like (or time-like) if it contains a space-like (or, respectively, time-like) vector. The isotropy cone $\{v \in \mathbb{R}^{n+2} \mid L(v) = 0\}$ of L is called the *light cone*.

(4) The points at infinity of the light cone in the upper half space $\{x_{n+2} > 0\}$ form an n-dimensional sphere. Let it be denoted by S^n_∞. Since it can be considered as the set of lines through the origin in the light cone, it is identified with the intersection S^n_1 of the upper half-light cone and the hyperplane $\{x_{n+2} = 1\}$, which is given by $S^n_1 = \{(x_1, \dots, x_{n+1}) \mid (x_1)^2 + \cdots + (x_{n+1})^2 - 1 = 0\}$.

(5) An element of the Lorentz group $\mathcal{G}$ acts on S^n_∞ as a *conformal transformation* which is a composition of reflections in $(n-1)$-spheres in S^n_∞. The set of conformal transformations of $S^n_\infty \cong \mathbb{R}^n \cup \{\infty\}$ is called the *conformal group* and is also denoted by $\mathcal{G}$.

Claim 2.2. *Let $\mathcal{S}$ denote the set of oriented $(n-1)$-spheres in S^n and let $\Lambda = \{x \in \mathbb{R}^{n+2} \mid L(x) = 1\}$ be the hyperbolic quadric hypersurface of one sheet.* (*This Λ is called de Sitter space.*) *Then there is a canonical bijection between $\mathcal{S}$ and Λ.*

Proof. (See Figure 1.) A point x in Λ determines an oriented half line $l_x = \overrightarrow{Ox}$ from the origin. Let $\Pi(l_x)$ be the oriented hyperplane passing through the origin that is

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orthogonal to l_x with respect to the Lorentz quadratic form L. Since l_x is space-like, $\Pi(l_x)$ intersects the light cone transversely and therefore $\Pi(l_x)$ intersects S^3_∞ in an oriented sphere $\Sigma = \Sigma_{\Pi(l_x)}$. The map $\Lambda \ni x \mapsto \Sigma_{\Pi(l_x)} \in \mathcal{S}$ defines the bijection from Λ to $\mathcal{S}$. □

This bijection can be considered as a modern version of pentaspherical coordinates in [**6**]. Let us identify Λ with $\mathcal{S}$ through this bijection.

Let S_1 and S_2 be oriented 2-spheres. Considered as points in Λ, S_1 and S_2 satisfy

$$S_1 \cap S_2 \neq \phi \quad \text{if and only if } |L(S_1, S_2)| \leqslant 1, \tag{2.1}$$

$$S_1 \cap S_2 = \phi \quad \text{if and only if } |L(S_1, S_2)| > 1. \tag{2.2}$$

Two spheres S_1 and S_2 are said to be *nested* if $S_1 \cap S_2 = \emptyset$ and *intersecting* if $S_1 \cap S_2 \neq \emptyset$ and $S_1 \neq S_2$.

Dimension-2 planes through the origin intersect the quadric $\Lambda \subset \mathbb{R}^{n+2}$ in curves. These curves are geodesics in the sense that they are critical (but not minimal) points of the length function which assigns the length $\int_a^b \sqrt{|L(c'(t))|}\,\mathrm{d}t$ to any given arc $c : [a, b] \to \Lambda$. There are three cases.

(1a) When all the vectors of the plane P are space-like, its intersection with Λ is connected and closed. Any tangent vector to this intersection is space-like. The corresponding set of spheres is a *pencil* of spheres with a common $(n-2)$-sphere $\Gamma = P^\perp \cap S^n_\infty$ (here, $P^\perp$ means the subspace L-orthogonal to P, that is, $P^\perp = \{w \mid L(v, w) = 0\ \forall v \in P\}$) (Figure 2, top).

In (2.1), the length of one of the arcs joining S_1 to S_2 in the pencil is the angle θ_0 between the two spheres. This angle satisfies $L(S_1, S_2) = \cos(\theta_0)$.

(1b) When the plane is tangent to the light cone, the intersection is again two non-compact curves, but the pencil is made of spheres all tangent at the point $P \cap S^n_\infty$.

(2) When the plane contains a time-like vector, the intersection consists of two non-compact curves. The pencil of spheres has limit (or Poncelet) points which are $P \cap S^n_\infty$; it is called a *Poncelet pencil* (Figure 2, bottom).

In (2.2), we can get an interesting invariant of the annulus bounded by S_1 and S_2 from the number $|L(S_1, S_2)|$ (see Remark 7.2): the length t_0 of the arc of the pencil joining S_1 to S_2 satisfies $|L(S_1, S_2)| = \cosh(t_0)$.

Working in $\Lambda \subset \mathbb{R}^4$, we get the 'usual' theory of pencils of circles. We will be mainly interested in $\Lambda \subset \mathbb{R}^5$, which is the set of oriented 2-spheres in S^3. We do not study the case when $n > 3$.

Remark 2.3. Let $v_1, v_2, \ldots, v_{n+1}$ be $n+1$ vectors in $T_x\Lambda$. The volume of the parallelepiped constructed on these vectors is

$$|\det(x, v_1, v_2, \ldots, v_{n+1})| = \sqrt{-\det(L(v_i, v_j))}.$$

This result is a corollary of the Lemma 2.6.

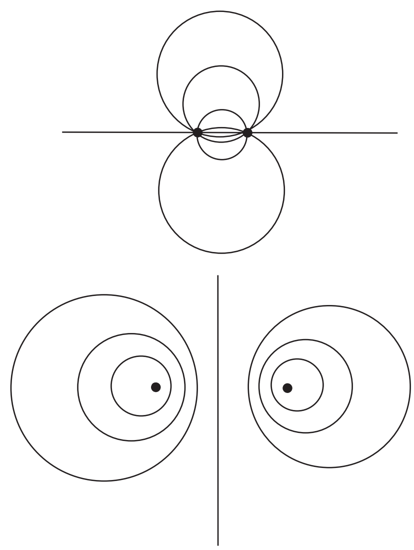

Figure 2. A pencil with a base circle and a Poncelet pencil.

Let $\Delta = \{x \in \mathbb{R}^{n+2} \mid L(x) = -1,\ x_{n+2} > 0\}$ be the upper half of the hyperbolic quadric hypersurface of two sheets. The restriction of the quadratic form L to each tangent space of Δ is positive definite. Then Δ is a model for the $(n+1)$-dimensional hyperbolic space $\mathbb{H} = \mathbb{H}^{n+1}$. Each sphere Σ in S^n is the 'boundary at infinity' of a totally geodesic subspace h of $\mathbb{H}$. The restriction of the full homogeneous Lorentz group $\mathcal{G} = O(n+1,1)$ to $\mathbb{H}$ is the group of isometries of the hyperbolic space $\mathbb{H}$.

A choice of a point z in $\mathbb{H}$ determines a metric on the sphere S^n at infinity of $\mathbb{H}$ by the projection on S^n of the metric of $T_z(\mathbb{H})$ using the geodesic rays which starts from z. Another choice of the point z determines another conformally equivalent metric on the sphere S^n. Although the sphere does not admit a measure which is invariant under the action of the conformal group $\mathcal{G}$, the set $\mathcal{S} \cong \Lambda$ of spheres in S^n do. Namely, Λ is endowed with a $\mathcal{G}$-invariant measure $\mathrm{d}\Sigma$. We define $\mathrm{d}\Sigma$ in several ways in what follows.

(1) The Lebesgue measure $|\mathrm{d}x_1 \wedge \cdots \wedge \mathrm{d}x_{n+2}|$ is invariant under the action of $\mathcal{G}$. The measure $\mathrm{d}\Sigma$ is given by $\mathrm{d}\Sigma = |\iota_x(\mathrm{d}x_1 \wedge \cdots \wedge \mathrm{d}x_{n+2})|$ at each point $x \in \Lambda$.

(2) This measure is given by the volume $(n+1)$-form

$$\omega_\Lambda = \frac{\sum_{i=1}^{n+2} (-1)^i x_i \,\mathrm{d}x_1 \wedge \cdots \widehat{\wedge\, \mathrm{d}x_i} \wedge \cdots \wedge \mathrm{d}x_{n+2}}{\{(x_1)^2 + \cdots + (x_{n+1})^2 - (x_{n+2})^2\}^{(n+2)/2}}$$

of Λ associated with the Lorentz form L, where $\widehat{\wedge \mathrm{d}x_i}$ means that $\wedge \mathrm{d}x_i$ is removed. Then ω_Λ is invariant under the action of $\mathcal{G}_+ = SO(n+1,1)$. We remark that ω_Λ is expressed as

$$\omega_{\Lambda_+} = \frac{1}{x_{n+2}}\, \mathrm{d}x_1 \wedge \cdots \wedge \mathrm{d}x_{n+1}$$

on $\Lambda_+ = \{(x_1, \ldots, x_{n+2}) \in \Lambda \mid x_{n+2} > 0\}$ if we take $(x_1, \ldots, x_{n+1})$ as its local coordinates.

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(3) This measure can also be regarded as a measure on the set of totally geodesic hyperplanes of the hyperbolic space $\mathbb{H}$ which is invariant by the action of the hyperbolic isometries [**30**].

(4) Let us now project the sphere S^n stereographically on an affine space $\mathbb{R}^n$ with Euclidean coordinates $(x_1, x_2, \ldots, x_n)$. There, a sphere Σ is given by its centre $(x_1, x_2, \ldots, x_n)$ and radius r. The measure $\mathrm{d}\Sigma$ is expressed by

$$\mathrm{d}\Sigma = \frac{1}{r^{n+1}} |\mathrm{d}x_1 \wedge \mathrm{d}x_2 \wedge \cdots \wedge \mathrm{d}x_n \wedge \mathrm{d}r|.$$

The quadric Λ is unbounded and the total measure of Λ is infinite. The measure of the set of spheres intersecting a given arc of any size is infinite. Since the set of spheres with geodesical radius larger than r is compact in Λ, its volume is finite.

Remark 2.4. In what follows, we assume that circles and spheres include lines and planes respectively as we work in conformal geometry.

2.2. The 4-tuple map and the cross-ratio of four points

In this subsection we define the cross-ratio of ordered four points in S^3 or $\mathbb{R}^3$ by means of the oriented 2-sphere that passes through them, which is determined uniquely unless the four points are concircular.

The *configuration space* $\mathrm{Conf}_n(X)$ of a space X is given by

$$\begin{aligned}\mathrm{Conf}_n(X) &= \{(x_1, \ldots, x_n) \in X^n \mid x_i \neq x_j \text{ if } i \neq j\} \\ &= X \times \cdots \times X \setminus \Delta,\end{aligned}$$

where Δ is called the *big diagonal set*. Let $\mathcal{C}c(S^3)$ be the subset of $\mathrm{Conf}_4(S^3)$ consisting of concircular points.

In what follows, we define a map Σ from $\mathrm{Conf}_4(S^3) \setminus \mathcal{C}c(S^3)$ to the set of oriented 2-spheres, $\mathcal{S} \cong \Lambda$, which assigns to ordered 4-points (x, y, z, w) the oriented 2-sphere $\Sigma(x, y, z, w)$ that passes through them.

Definition 2.5. The $(4,1)$-*exterior product* $v^1 \wedge \cdots \wedge v^4$ of ordered 4-vectors $v^i = (v^i_1, \ldots, v^i_5)$ in $\mathbb{R}^5$ $(i = 1, 2, 3, 4)$ is the uniquely determined vector u that satisfies

$$L(u, w) = \det(v^1, v^2, v^3, v^4, w) \in \mathbb{R} \quad \forall w \in \mathbb{R}^5.$$

Then it is given by

$$v^1 \wedge \cdots \wedge v^4 = (\tilde{\nu}_1, \tilde{\nu}_2, \tilde{\nu}_3, \tilde{\nu}_4, -\tilde{\nu}_5),$$

with

$$\tilde{\nu}_j = (-1)^{j+1} \begin{vmatrix} v^1_1 & \cdots & \hat{v}^1_j & \cdots & v^1_5 \\ \vdots & & \vdots & & \vdots \\ v^4_1 & \cdots & \hat{v}^4_j & \cdots & v^4_5 \end{vmatrix},$$

where a hat means that the jth column is removed.

We remark that this is a generalization of the vector product of two vectors in $\mathbb{R}^3$.

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Lemma 2.6.

(1) *$v^1 \wedge v^2 \wedge v^3 \wedge v^4 \neq 0$ if and only if v^1, v^2, v^3, v^4 are linearly independent.*

(2) *$L(v^1 \wedge v^2 \wedge v^3 \wedge v^4, v^j) = 0$ for $j = 1, 2, 3, 4$, namely, $v^1 \wedge v^2 \wedge v^3 \wedge v^4$ is L-orthogonal to $\mathrm{span}\langle v^1, v^2, v^3, v^4\rangle$.*

(3) *The norm of $v^1 \wedge v^2 \wedge v^3 \wedge v^4$ is equal to the absolute value of the volume of the parallelepiped spanned by v^1, v^2, v^3 and v^4 associated with the Lorentz quadratic form L,*

$$\sqrt{|L(v^1 \wedge v^2 \wedge v^3 \wedge v^4)|} = \sqrt{|\det(L(v^i, v^j))|}.$$

Proof. (3) The last equality is a consequence of a formula in linear algebra,

$$\det(L(v^i, v^j)) = \det\left\{\begin{pmatrix} v_1^1 & \cdots & v_5^1 \\ \vdots & & \vdots \\ v_1^4 & \cdots & v_5^4 \end{pmatrix}\begin{pmatrix} v_1^1 & \cdots & v_1^4 \\ \vdots & & \vdots \\ v_4^1 & \cdots & v_4^4 \\ -v_5^1 & \cdots & -v_5^4 \end{pmatrix}\right\}$$
$$= -\tilde{\nu}_1^2 - \tilde{\nu}_2^2 - \tilde{\nu}_3^2 - \tilde{\nu}_4^2 + \tilde{\nu}_5^2.$$

□

Claim 2.7.

(1) *Let $u = (u_1, \ldots, u_5)$ and $v = (v_1, \ldots, v_5)$ be linearly independent light-like vectors with $u_5, v_5 > 0$. Then $L(u, v) < 0$.*

Therefore, any pair of linearly independent light-like vectors cannot be L-orthogonal.

(2) *Let $u = (u_1, \ldots, u_5)$ be a non-zero light-like vector. Then the hyperplane $u^\perp$ is tangent to the light-cone along the generatrix $\mathbb{R} \cdot u$.*

(3) *If $u = (u_1, \ldots, u_5)$ is a non-zero time-like vector, then the hyperplane $u^\perp$ is space-like.*

Corollary 2.8. *Suppose v^1, v^2, v^3, v^4 are linearly independent.*

(1) *If $v^1 \wedge v^2 \wedge v^3 \wedge v^4$ is time-like, then all of v^1, v^2, v^3, v^4 are space-like.*

(2) *$v^1 \wedge v^2 \wedge v^3 \wedge v^4$ is light-like if and only if $\mathrm{span}\langle v^1, v^2, v^3, v^4\rangle$ is the tangent space of the light cone at $v^1 \wedge v^2 \wedge v^3 \wedge v^4$.*

Let us identify the 3-sphere S^3 with the intersection S^3_1 of the light-cone $\{L = 0\}$ and the hyperplane in $\mathbb{R}^5$ defined by $\{(x_1, \ldots, x_5) \mid x_5 = 1\}$. Let $x^i = (x^i_1, x^i_2, x^i_3, x^i_4) \in S^3$ $(i = 1, 2, 3, 4)$ and $\tilde{x}^i = (x^i_1, x^i_2, x^i_3, x^i_4, 1) \in S^3_1 \subset \mathbb{R}^5$. Then the $\tilde{x}^i$ are linearly dependent if and only if the x^i are concircular.

Since an oriented 2-sphere $\Sigma(x^1, x^2, x^3, x^4)$ that passes through $\{x^1, x^2, x^3, x^4\}$ is obtained as the intersection of S^3_1 and an oriented hyperplane in $\mathbb{R}^5$ that passes through x^1, x^2, x^3, x^4 and the origin, we obtain the following result.

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Proposition 2.9. *Define the '4-tuple map' of the 3-sphere by*

$$\Sigma : \mathrm{Conf}_4(S^3) \setminus \mathcal{C}c(S^3) \ni (x^1, x^2, x^3, x^4) \mapsto \frac{\tilde{x}^1 \wedge \tilde{x}^2 \wedge \tilde{x}^3 \wedge \tilde{x}^4}{\sqrt{L(\tilde{x}^1 \wedge \tilde{x}^2 \wedge \tilde{x}^3 \wedge \tilde{x}^4)}} \in \Lambda \cong \mathcal{S}.$$

Then $\Sigma(x^1, x^2, x^3, x^4)$ *is the oriented* 2*-sphere that passes through* $\{x^1, x^2, x^3, x^4\}$.

Assume that the complex plane $\mathbb{C}$ has the standard orientation.

Definition 2.10. Let $(x^1, x^2, x^3, x^4) \in \mathrm{Conf}_4(S^3)$. Let $p : \Sigma(x^1, x^2, x^3, x^4) \to \mathbb{C}$ be any stereographic projection that preserves the orientation, where, when x^1, x^2, x^3 and x^4 are concircular, we can choose any oriented 2-sphere that passes through them as $\Sigma(x^1, x^2, x^3, x^4)$.

The *cross-ratio of ordered four points* (x^1, x^2, x^3, x^4) is defined as the cross-ratio

$$(p(\tilde{x}^2), p(\tilde{x}^3); p(\tilde{x}^1), p(\tilde{x}^4)) = \frac{p(\tilde{x}^2) - p(\tilde{x}^1)}{p(\tilde{x}^2) - p(\tilde{x}^4)} : \frac{p(\tilde{x}^3) - p(\tilde{x}^1)}{p(\tilde{x}^3) - p(\tilde{x}^4)}. \tag{2.3}$$

We denote it by $(x^2, x^3; x^1, x^4)$. When x^1, x^2, x^3 and x^4 are concircular, their cross-ratio is real and independent of the choice of $\Sigma(x^1, x^2, x^3, x^4)$.

The 4*-tuple map* Σ *of* $\mathbb{R}^3$ and the *cross-ratio of four points in* $\mathbb{R}^3$ are defined through an orientation-preserving stereographic projection: $S : S^3 \to \mathbb{R}^3$. When x^1, x^2, x^3 and x^4 are concircular in $\mathbb{R}^3$, we define $\Sigma(x^1, x^2, x^3, x^4)$ to be any oriented sphere that passes through them.

Lemma 2.11. *The image of* $\mathrm{Conf}_4(S^3) \setminus \mathcal{C}c(S^3)$ *by the cross-ratio map of formula (2.3) is contained in a component of* $\mathbb{C} \setminus \mathbb{R}$.

Proof. The set $\Delta \subset (S^3)^4$ is of codimension 3, the set $\mathcal{C}c(S^3)$ is of codimension 2 in $\mathrm{Conf}_4(S^3)$ and the cross-ratio map is continuous on the arcwise connected set $\mathrm{Conf}_4(S^3) \setminus \mathcal{C}c(S^3)$. □

3. Review of r^{-2}-modified potential energy

3.1. What is an energy functional for knots?

In the following three sections we study knots in $\mathbb{R}^3$. By an *open knot* we mean an embedding $\tilde{f}$ from a line into $\mathbb{R}^3$ or its image $\tilde{K} = \tilde{f}(\mathbb{R})$ that approaches asymptotically a straight line at both ends. We assume that knots are of class C^2.

The *energy of knots* was proposed by Fukuhara [**12**] and Sakuma [**29**], motivated by the following problem: define a suitable functional on the space of knots, which we call '*energy*', and define a good-looking '*canonical knot*' for each isotopy class as one of the embeddings that attain the minimum value of this 'energy' within its isotopy class.

For this purpose, we try to deform a given embedding along the negative gradient flow of the 'energy' until it comes to a critical point without changing its knot type. Hence the crossing changes should be avoided.

Thus we are led to the notion of the *energy functional for knots*, which is a functional that explodes if a knot degenerates to an immersion with double points. More precisely, we have the following.

Definition 3.1. A functional e on the space of knots is an *energy functional for knots* if, for any real numbers b and δ with $0 < \delta \leqslant \frac{1}{2}$, there exists a positive constant $C = C(b, \delta)$ that satisfies the following condition: if a knot f with length $l(f)$ contains a pair of points x and y which satisfy that the shorter arc-length between them is equal to $\delta l(f)$ and that $|x - y| \leqslant Cl(f)$, then $e(f) \geqslant b$.

We call a functional an *energy functional in the weak sense* when it satisfies the same condition as above if the knot f satisfies an additional geometric condition; for example, if the curvature of f is bounded above by a constant.

3.2. The regularization of r^{-2}-modified potential energy, $E^{(2)}$

One of the most natural and naive candidates for an energy functional for knots would be the electrostatic energy of charged knots.

The first attempt to consider the electrostatic energy of charged knots was carried out in the finite-dimensional category by Fukuhara [**12**]. He considered the space of the polygonal knots whose vertices are charged, and studied their *modified* electrostatic energy under the assumption that Coulomb's repelling force between a pair of point charges of distance r is proportional to r^{-m} $(m = 3, 4, 5, \dots)$.

The first example of an energy functional for smooth knots was defined by the second author in [**27**]. (Details can be found in [**28**]. Related topics can be found in [**1**].)

Let $K = f(S^1)$ with $f : S^1 = [0,1]/(0 \sim 1) \to \mathbb{R}^3$ be a knot of class C^2 that is parametrized by the arc-length. Suppose that the knot is uniformly electrically charged. In order to obtain an energy functional for knots, we have to make the non-realistic assumption that Coulomb's repelling force between a pair of point charges of distance r is proportional to $r^{-(\alpha+1)}$, and hence the potential is proportional to $r^{-\alpha}$, where $\alpha \geqslant 2$. Put $\alpha = 2$ in what follows. Then its 'r^{-2}*-modified potential energy*' is given by

$$\iint_{K\times K} \frac{\mathrm{d}x\,\mathrm{d}y}{|x-y|^2},$$

which blows up at the diagonal set Δ for any knot. We normalize this blowing-up in the following way.

Let $\delta_K(x, y)$ denote the shorter arc-length between x and y along the knot K. Define the 'r^{-2}*-modified* ε*-self avoiding voltage*' at a point x, $V_\varepsilon^{(2)}(K; x)$, and the '$r^{-2}$*-modified* ε*-off-diagonal potential energy*', $E_\varepsilon^{(2)}(K)$, by

$$V_\varepsilon^{(2)}(K;x) = \int_{y\in K,\, \delta_K(x,y)\geqslant\varepsilon} \frac{\mathrm{d}y}{|x-y|^2},$$

$$E_\varepsilon^{(2)}(K) = \int_K V_\varepsilon^{(2)}(K;x)\,\mathrm{d}x = \iint_{K\times K,\, \delta_K(x,y)\geqslant\varepsilon} \frac{\mathrm{d}x\,\mathrm{d}y}{|x-y|^2}.$$

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Then the order of the blowing-up of $V_\varepsilon^{(2)}(K;x)$ and $E_\varepsilon^{(2)}(K)$, as ε goes down to 0, is independent of the knot K and the point x. Therefore, we have the limits

$$\left.\begin{aligned} V^{(2)}(K;x) &= \lim_{\varepsilon\to 0}\left(\int_{y\in K,\,\delta_K(x,y)\geqslant\varepsilon}\frac{\mathrm{d}y}{|x-y|^2}-\frac{2}{\varepsilon}\right)+4,\\ E^{(2)}(K) &= \lim_{\varepsilon\to 0}\left(\iint_{K\times K,\,\delta_K(x,y)\geqslant\varepsilon}\frac{\mathrm{d}x\,\mathrm{d}y}{|x-y|^2}-\frac{2}{\varepsilon}\right)+4.\end{aligned}\right\} \tag{3.1}$$

Then $E^{(2)}(K)$ is equal to

$$E^{(2)}(K)=\iint_{K\times K}\left(\frac{1}{|x-y|^2}-\frac{1}{\delta_K(x,y)^2}\right)\mathrm{d}x\,\mathrm{d}y.$$

We remark that the integrand converges near the diagonal set for knots of class C^4. This expression* works for open knots and (open) knots that are not necessarily parametrized by arc-length.

Then $E^{(2)}$ is an energy functional for knots. In fact, we can take a constant $C(b)$, which is independent of δ, as $C(b,\delta)$ in Definition 3.1.

Freedman *et al*. showed that $E^{(2)}$ is conformally invariant in [**11**]. After their proof, Doyle and Schramm obtained a new formula for $E^{(2)}$ from a geometric interpretation, which implies a simpler proof. We introduce their formula in the next subsection.

Remark 3.2. If the power '2' in the formula of $E^{(2)}$ is replaced by α, with $\alpha\geqslant 1$, then $E^{(\alpha)}$ can be defined similarly if $\alpha<3$. $E^{(\alpha)}$ thus defined is an energy functional for knots if and only if $\alpha\geqslant 2$ and is conformally invariant if and only if $\alpha=2$.

The jump of $E^{(2)}$ for non-trivial knots is shown as follows.

Freedman and He defined the *average crossing number* $\mathrm{ac}(K)$ of a knot as the average of the numbers of the crossing points of the projected knot diagrams, where the average is taken over all the directions of the projection (see [**10**]).

Then Freedman *et al*. showed that $E^{(2)}$ bounds the average crossing number from above (see [**11**]), which implies the infimum of the value of $E^{(2)}$ for non-trivial knots, because the average crossing number of a non-trivial knot is greater than or equal to 3.

3.3. The cosine formula for $E^{(2)}$

In this subsection we introduce the cosine formula for $E^{(2)}$ discovered by Doyle and Schramm (see [**2**]).

Let us first recall a couple of formulae in the conformal geometry. Let T be a conformal transformation of $\mathbb{R}^3\cup\{\infty\}$. Put

$$|T'(p)|=|\det\,\mathrm{d}T(p)|^{1/6}$$

* The idea of using the arc-length as the subtracting counter term to cancel the blowing up of the integral at the diagonal set was introduced by Nakauchi [**26**].

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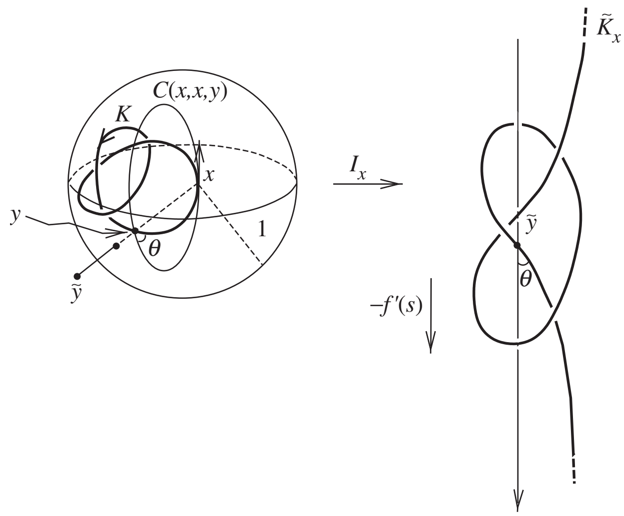

Figure 3. The inverted open knot $\tilde{K}_x$ and the angle θ.

for $p \in \mathbb{R}^3$. In particular, if T is a reflection in a sphere of radius r with centre 0, then $|T'(p)| = r/|p|$. Then

$$|T(p) - T(q)| = |T'(p)|\,|T'(q)|\,|p-q|$$

for $p, q \in \mathbb{R}^3$ and

$$|(T \circ f)'(s)| = |T'(f(s))|^2 |f'(s)|$$

for $f : S^1$ or $\mathbb{R} \to \mathbb{R}^3$.

Let I_x be the reflection with respect to the sphere with centre $x = f(s)$ and radius 1 (Figure 3), $\tilde{K}_x = I_x(K)$, $\tilde{y} = I_x(y)$, $x_\pm(\varepsilon) = f(s \pm \varepsilon)$ and $\tilde{x}_\pm(\varepsilon) = I_x(x_\pm(\varepsilon))$ for $0 < \varepsilon \ll 1$. We call $\tilde{K}_x$ the *inverted open knot* of K at x.

Then

$$|I_x'(y)| = \frac{1}{|x-y|}$$

and

$$|\mathrm{d}\tilde{y}| = |\mathrm{d}(I_x(y))| = |I_x{}'(y)|^2 |\mathrm{d}y| = \frac{|\mathrm{d}y|}{|x-y|^2}.$$

For us, $\mathrm{d}x$ and $\mathrm{d}y$ are infinitesimal arcs on $K \subset \mathbb{R}^3$ or S^3, and $|\mathrm{d}x|$, $|\mathrm{d}y|$ their lengths. We may, later, when the context is clear, also use $\mathrm{d}x$ and $\mathrm{d}y$ as two one-forms on $K \times K \setminus \Delta$.

Therefore,

$$V_\varepsilon^{(2)}(K;x) = \int_{y \in K,\, \delta(x,y) \geqslant \varepsilon} \frac{\mathrm{d}y}{|x-y|^2} = \int_{\tilde{x}_+(\varepsilon)}^{\tilde{x}_-(\varepsilon)} |\mathrm{d}\tilde{y}|$$

is the arc-length between $\tilde{x}_+(\varepsilon)$ and $\tilde{x}_-(\varepsilon)$ along the inverted knot $\tilde{K}_x$.

Let $\bar{t} = f'(s)$ be the unit tangent vector, $n = f''(s)/|f''(s)|$ the unit principal normal vector and $k = |f''(s)|$ the curvature of K at x. Put $n = 0$ when $|f''(s)| = 0$. Then

$$x_{\pm}(\varepsilon) = x \pm \varepsilon\bar{t} + \tfrac{1}{2}\varepsilon^2 kn + O(\varepsilon^3),$$

which implies

$$\tilde{x}_{\pm}(\varepsilon) = x \pm \frac{1}{\varepsilon}\bar{t} + \tfrac{1}{2}kn + O(\varepsilon).$$

Hence

$$|\tilde{x}_+(\varepsilon) - \tilde{x}_-(\varepsilon)| = \frac{2}{\varepsilon} + O(\varepsilon).$$

Therefore,

$$\int_{y\in K,\delta(x,y)\geqslant\varepsilon} \frac{\mathrm{d}y}{|x-y|^2} - \frac{2}{\varepsilon} = \int_{\tilde{x}_+(\varepsilon)}^{\tilde{x}_-(\varepsilon)} |\mathrm{d}\tilde{y}| - |\tilde{x}_+(\varepsilon) - \tilde{x}_-(\varepsilon)| + O(\varepsilon)$$

is equal to the difference of the arc-length along $\tilde{K}_x$ and the distance between $\tilde{x}_+(\varepsilon)$ and $\tilde{x}_-(\varepsilon)$ up to $O(\varepsilon)$. (This was called the *'wasted length'* of the inverted open knot.)

Definition 3.3. Let $C(x, x, y)$ denote the circle* tangent to a knot K at x that passes through y with the natural orientation derived from that of K at point x, and let θ $(0 \leqslant \theta \leqslant \pi)$ be the angle between $C(x, x, y)$ and $C(y, y, x)$ at x or at y.

We call $\theta = \theta_K(x, y)$ the *conformal angle.*

Put $\tilde{C}(\infty, \infty, \tilde{y}) = I_x(C(x, x, y))$. Then $\tilde{C}(\infty, \infty, \tilde{y})$ is the line that passes through $\tilde{y}$ and has the tangent vector $-f'(s)$ (Figure 3). The line passing through $\tilde{x}_+(\varepsilon)$ and $\tilde{x}_-(\varepsilon)$ approaches parallel to the line $\tilde{C}(\infty, \infty, \tilde{y})$ as ε goes down to 0. Since I_x is a conformal map, the angle between the line $\tilde{C}(\infty, \infty, \tilde{y})$ and the tangent line of $\tilde{K}_x$ at $\tilde{y}$ is equal to θ. Therefore,

$$\begin{aligned} V^{(2)}(K; x) - 4 &= \lim_{\varepsilon\to 0}\left(\int_{y\in K,\,\delta(x,y)\geqslant\varepsilon} \frac{\mathrm{d}y}{|x-y|^2} - \frac{2}{\varepsilon}\right) \\ &= \lim_{\varepsilon\to 0}\int_{\tilde{x}_+(\varepsilon)}^{\tilde{x}_-(\varepsilon)} \mathrm{d}\tilde{y}\,(1-\cos\theta) \\ &= \lim_{\varepsilon\to 0}\int_{y\in K} \frac{(1-\cos\theta)\,\mathrm{d}y}{|x-y|^2}. \end{aligned}$$

Hence

$$E^{(2)}(K) = \iint_{K\times K} \frac{1-\cos\theta}{|x-y|^2}\,\mathrm{d}x\,\mathrm{d}y + 4, \tag{3.2}$$

which is called the *cosine formula* for $E^{(2)}$ by Doyle and Schramm.

* In general, $C(x, y, z)$ will denote the uniquely determined circle that passes through x, y and z after the notation of [**13**].

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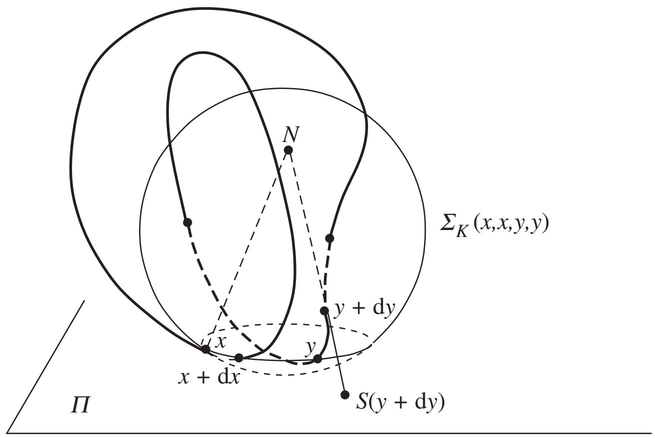

Figure 4. The twice tangent sphere and the infinitesimal cross-ratio. Stereographic projection: $x = S(x)$; $x + \mathrm{d}x = S(x + \mathrm{d}x)$; $y = S(y)$.

4. The infinitesimal cross-ratio

In this section we introduce an infinitesimal interpretation of the 2-form

$$\frac{\mathrm{d}x\,\mathrm{d}y}{|x-y|^2}$$

in the integrand of $E^{(2)}$ in terms of the cross-ratio.

4.1. The infinitesimal cross-ratio as a 'bilocal' function

In what follows in this section, we use the following notation:

$$K = f(S^1), \quad x = f(s), \quad x + \mathrm{d}x = f(s + \mathrm{d}s), \quad y = f(t) \quad \text{and} \quad y + \mathrm{d}y = f(t + \mathrm{d}t).$$

As stated in § 2.2, we can define the cross-ratio $(x + \mathrm{d}x, y; x, y + \mathrm{d}y)$ of the ordered four points x, $x + \mathrm{d}x$, y, $y + \mathrm{d}y$ via the oriented 2-sphere $\Sigma(x, x + \mathrm{d}x, y, y + \mathrm{d}y)$ that passes through them, which is uniquely defined unless the four points are concircular.

Definition 4.1. A *twice tangent sphere* $\Sigma_K(x, x, y, y)$ is an oriented 2-sphere that is tangent to the knot K at the points x, y obtained as the limit of the sphere $\Sigma(x, x + \mathrm{d}x, y, y + \mathrm{d}y)$ as $\mathrm{d}x$ and $\mathrm{d}y$ go to 0.

It is uniquely determined unless $f(s)$, $f'(s)$, $f(t)$, and $f'(t)$ are concircular. We will give a formula for the twice tangent spheres in the next subsection.

Let $\Pi = \Pi_x(y)$ be the plane that contains $C(x, x, y)$, with an identification with the complex plane $\mathbb{C}$, and let

$$S : \Sigma_K(x, x, y, y) \to \Pi_x(y) \cup \{\infty\} \cong \mathbb{C} \cup \{\infty\}$$

be the orientation-preserving stereographic projection (Figure 4). When $f(s)$, $f'(s)$, $f(t)$ and $f'(t)$ are concircular, we can take Π with any orientation as Σ_K. Let $\tilde{x} = S(x)$,

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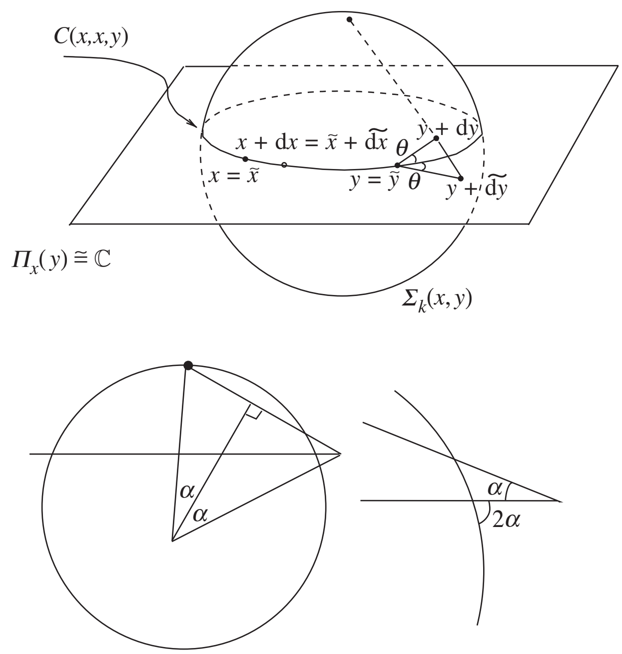

Figure 5. The twice tangent sphere, stereographic projection and computation of the infinitesimal cross-ratio.

$\tilde{x} + \widetilde{\mathrm{d}x} = S(x + \mathrm{d}x)$, $\tilde{y} = S(y)$ and $\tilde{y} + \widetilde{\mathrm{d}y} = S(y + \mathrm{d}y)$ denote the corresponding complex numbers. Then the cross ratio $(x + \mathrm{d}x, y; x, y + \mathrm{d}y)$ is given by*

$$\frac{(\tilde{x} + \widetilde{\mathrm{d}x}) - \tilde{x}}{(\tilde{x} + \widetilde{\mathrm{d}x}) - (\tilde{y} + \widetilde{\mathrm{d}y})} : \frac{\tilde{y} - \tilde{x}}{\tilde{y} - (\tilde{y} + \widetilde{\mathrm{d}y})} \sim \frac{\widetilde{\mathrm{d}x}\widetilde{\mathrm{d}y}}{(\tilde{x} - \tilde{y})^2}.$$

Let $v_x(y)$ be the unit tangent vector of $C(x, x, y)$ at y.

Definition 4.2. We call $v_x(y)$ the *unit tangent vector at x conformally translated to y*.

Let $\theta_K(x, y)$ $(-\pi \leqslant \theta_K(x, y) \leqslant \pi)$ be the angle from $v_x(y)$ to $f'(t)$, where the sign of $\theta_K(x, y)$ is given according to the orientation of $\Sigma_K(x, y)$. Then $|\theta_K(x, y)|$ is equal to the angle θ between $C(x, x, y)$ and $C(y, y, x)$ in the cosine formula. As x, $x + \mathrm{d}x$ and y are in $\Sigma_K(x, x, y, y) \cap \Pi$, they are invariant by p.

Since $|\widetilde{\mathrm{d}y}| = |\mathrm{d}y|$, as illustrated in Figure 5, which considers the case when the argument of the cross-ratio is negative, the cross-ratio $(x + \mathrm{d}x, y; x, y + \mathrm{d}y)$ has the absolute value

$$\frac{|\mathrm{d}x|\,|\mathrm{d}y|}{|x - y|^2}$$

and the argument $\theta_K(x, y)$.

* R. Kusner already mentioned such an infinitesimal cross-ratio in a joint AMS–SMM meeting in Oaxaca, Mexico, in the autumn of 1997 and in a talk on quadrupoles in Illinois (1998).

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Definition 4.3. We call $(x+\mathrm{d}x, y; x, y+\mathrm{d}y)$ the *infinitesimal cross-ratio* of $\mathrm{d}x$ and $\mathrm{d}y$ and denote it by Ω_{CR}.

Unlike local invariants defined in [**4**], the infinitesimal cross-ratio can be defined by local data up to the first derivatives at a pair of points on a curve. This is why we call it a bilocal function.

A stereographic projection from a sphere is a restriction of a conformal transformation of $\mathbb{R}^3 \cup \{\infty\}$. Hence the infinitesimal cross-ratio (or its is complex conjugate class) is the unique invariant of $\mathrm{d}x$ and $\mathrm{d}y$ under the action of the orientation-preserving conformal group $\mathcal{G}_+$ (or, respectively, the action of the conformal group $\mathcal{G}$).

Since the absolute value of the 2-form

$$\frac{|\mathrm{d}x|\,|\mathrm{d}y|}{|x-y|^2}$$

on $K \times K \setminus \Delta$ is the absolute value of Ω_{CR} and the angle θ $(0 \leqslant \theta \leqslant \pi)$ is the absolute value of the argument of Ω_{CR}, the cosine formula (3.2) implies that

$$E^{(2)}(K) = \iint_{K\times K\setminus\Delta} \{|\Omega_{\mathrm{CR}}| - \mathrm{Re}\,\Omega_{\mathrm{CR}}\} + 4. \tag{4.1}$$

Therefore, it is conformally invariant.

We close this subsection with the following claim, which we will use later.

Claim 4.4. *The argument of cross-ratio of a knot K is identically 0 if and only if K is the standard circle.*

Proof. Fix a point $x \in K$ and consider the inverted open knot at x, $\tilde{K}_x$. Since $\theta(x,y) = 0$ for any $y \in K$, the tangent vector of $\tilde{K}_x$ at $\tilde{y}$ is equal to $-f'(s)$ for any $\tilde{y} \in \tilde{K}_x$. Therefore, $\tilde{K}_x$ is the straight line, which means that K is the standard circle. □

4.2. The 4-tuple map for a knot and the twice tangent spheres

In this subsection we define a map that assigns the oriented 2-sphere that passes through a given 4-tuples of points on a knot, and then a map that assigns the twice tangent sphere.

Definition 4.5. The *open concircular point set $\mathcal{C}c(K)$ of a knot K* is given by $\mathcal{C}c(K) = (f^4)^{-1}(\mathcal{C}c(S^3))$, where $f^4 = f \times f \times f \times f : \mathrm{Conf}_4(S^1) \to \mathrm{Conf}_4(S^3)$ is the natural map.

Suppose K is a non-trivial knot. Kuperberg showed that K contains four points that are collinear (see [**17**]). As a corollary, $\mathcal{C}c(K)$ is not empty.

Question 4.6. *Is $\mathcal{C}c(K)$ not empty for any trivial knot K?*

Moreover, we will show later that $\mathcal{C}c(K)$ is generically of dimension 2. This is indicated by the following observation.

Let $K_p = I_{\Sigma_p}(K)$ be the inverted closed knot with respect to a sphere with centre $p \in \mathbb{R}^3 \setminus K$. Then Kuperberg's theorem implies that there is a line L_p satisfying that

$L_p \cap K_p$, and hence $I_p(L_p) \cap K$, contains four points. This means that, for any point $p \in \mathbb{R}^3 \setminus K$, there is a circle C_p that intersects K in at least four points. This implies that, by considering the normal plane to C_p at p, the set of such circles, and hence $\mathcal{C}c(K)$, has dimension 2.

Assume that

$$f(t_i) = (f_1(t_i), f_2(t_i), f_3(t_i), f_4(t_i), 1) \in S^3_1 = \{L = 0\} \cap \{x_5 = 1\} \subset \mathbb{R}^5$$

for $i = 1, 2, 3, 4$. Put

$$\nu_f = \nu_f(t_1, t_2, t_3, t_4) = (\nu_1, \dots, \nu_5) = f(t_1) \wedge f(t_2) \wedge f(t_3) \wedge f(t_4).$$

We remark that $\nu_5(t_1, t_2, t_3, t_4) = 0$ if and only if the $f(t_i)$ are linearly dependent as vectors in $\mathbb{R}^5$, which means that the $f(t_i)$ are concircular as vectors in $S^3_1 \cong S^3$.

Definition 4.7. The 4-*tuple map* ψ_K *for a knot* K is a map that assigns the oriented 2-sphere that passes through $f(t_i)$ $(i = 1, 2, 3, 4)$ to a 4-tuple $(t_1, t_2, t_3, t_4) \in \mathrm{Conf}_4(S^1) \setminus \mathcal{C}c(K)$, which is given by

$$\begin{aligned}\psi_K = \Sigma \circ f^4 : \mathrm{Conf}_4(S^1) \setminus \mathcal{C}c(K) \ni (t_1, t_2, t_3, t_4) \\ \mapsto \frac{\nu_f}{\sqrt{L(\nu_f)}} = \frac{f(t_1) \wedge f(t_2) \wedge f(t_3) \wedge f(t_4)}{\sqrt{L(f(t_1) \wedge f(t_2) \wedge f(t_3) \wedge f(t_4))}} \in \Lambda \cong \mathcal{S}.\end{aligned}$$

Claim 4.8. *The open concircular point set* $\mathcal{C}c(K)$ *is of dimension greater than or equal to* 2 *if it is not an empty set, especially if* K *is a non-trivial knot.*

Proof. Assume that $(t_1, t_2, t_3, t_4) \in \mathcal{C}c(K) \in \mathrm{Conf}_4$. Then, considered as vectors in $\mathbb{R}^5$, $f(t_1)$, $f(t_2)$, $f(t_3)$ and $f(t_4)$ are linearly dependent, but three of them, say, $f(t_1)$, $f(t_2)$ and $f(t_3)$, are linearly independent. Suppose

$$f(t_4) = af(t_1) + bf(t_2) + cf(t_3).$$

Then

$$\begin{aligned}\frac{\partial \nu_f}{\partial t_1} &= -af(t_1) \wedge f(t_2) \wedge f(t_3) \wedge f'(t_1), \\ \frac{\partial \nu_f}{\partial t_2} &= -bf(t_1) \wedge f(t_2) \wedge f(t_3) \wedge f'(t_2), \\ \frac{\partial \nu_f}{\partial t_3} &= -cf(t_1) \wedge f(t_2) \wedge f(t_3) \wedge f'(t_3), \\ \frac{\partial \nu_f}{\partial t_4} &= f(t_1) \wedge f(t_2) \wedge f(t_3) \wedge f'(t_4).\end{aligned}$$

Since $f(t_1)$, $f(t_2)$ and $f(t_3)$ are linearly independent,

$$\mathrm{span}\left\langle \frac{\partial \nu_f}{\partial t_1}, \frac{\partial \nu_f}{\partial t_2}, \frac{\partial \nu_f}{\partial t_3}, \frac{\partial \nu_f}{\partial t_4} \right\rangle$$

has dimension at most 2. Therefore, the kernel of $\mathrm{d}\nu_f$, which is equal to the tangent space of $\mathcal{C}c(K)$, has dimension at least 2. □

Let us consider the behaviour of ψ_K when t_2 and t_4 approach t_1 and t_3, respectively. Then Taylor's expansion formula implies

$$\begin{aligned} f(t_1) \wedge f(t_2) \wedge f(t_3) \wedge f(t_4) \\ = (t_2 - t_1)(t_4 - t_3) f(t_1) \wedge f(t_1') \wedge f(t_3) \wedge f'(t_3) + \text{higher-order terms.} \end{aligned}$$

Put

$$\nu_f^{(2,2)}(t_1, t_3) = f(t_1) \wedge f(t_1') \wedge f(t_3) \wedge f'(t_3).$$

Then $\nu_f^{(2,2)}(t_1, t_3) = 0$ if and only if $f(t_1)$, $f(t_1')$, $f(t_3)$ and $f'(t_3)$ are linearly dependent as vectors in $\mathbb{R}^5$, which occurs if and only if $f'(t_3)$ can be expressed as a linear combination of $f(t_1) - f(t_3)$ and $f(t_1')$. This is equivalent to the condition that $f'(t_3)$, considered as a tangent vector at $f(t_3) \in S_1^3$, lies in the circle that can be obtained as the intersection of S_1^3 and the three-dimensional vector subspace spanned by $f(t_1) - f(t_3)$ and $f(t_1')$. Therefore, $\nu_f^{(2,2)}(t_1, t_3) = 0$ if and only if $f(t_1)$, $f'(t_1)$, $f(t_3)$ and $f'(t_3)$ are concircular.

Put

$$\mathcal{C}c^{(2,2)}(K) = \{(s, t) \in S^1 \times S^1 \setminus \Delta \mid f(t_1),\ f'(t_1),\ f(t_3) \text{ and } f'(t_3) \text{ are concircular}\}.$$

Generically, $\mathcal{C}c^{(2,2)}(K)$ is of dimension 0, since $(x, y) = (f(s), f(t))$ belongs to $\mathcal{C}c^{(2,2)}(K)$ if and only if $f'(t)$ coincides with $v_x(y)$, the unit tangent vector at x conformally translated to y. We remark that $\mathcal{C}c^{(2,2)}(K)$ has dimension 1 when K is a (p, q)-torus knot, which is an orbit of an S^1-action defined by

$$S^1 \ni \mathrm{e}^{2\pi \mathrm{i}t} \mapsto (\mathbb{C}^2 \supset S^3 \ni (z, w) \mapsto (\mathrm{e}^{2\pi \mathrm{i}pt} z, \mathrm{e}^{2\pi \mathrm{i}qt} w) \in S^3 \subset \mathbb{C}^2).$$

Definition 4.9. The *twice tangent sphere map* $\psi_K^{(2,2)}$ for a knot K, which assigns the twice tangent sphere $\Sigma_K(f(s), f(s), f(t), f(t))$ to $(s, t) \in \mathrm{Conf}_2(S^1) \setminus \mathcal{C}c^{(2,2)}(K)$, is given by

$$\begin{aligned} \psi_K^{(2,2)} : \mathrm{Conf}_2(S^1) \setminus \mathcal{C}c^{(2,2)}(K) \ni (s, t) \\ \mapsto \frac{\nu_f^{(2,2)}(s, t)}{\sqrt{L(\nu_f^{(2,2)}(s, t))}} = \frac{f(s) \wedge f'(s) \wedge f(t) \wedge f'(t)}{\sqrt{L(f(s) \wedge f'(s) \wedge f(t) \wedge f'(t))}} \in \Lambda \cong \mathcal{S}. \end{aligned}$$

Conjecture 4.10. *If K is non-trivial, then the twice tangent sphere map $\psi_K^{(2,2)}$ is not injective, namely, there is a sphere Σ that is tangent to K at three points or more.*

When t approaches s, the twice tangent sphere approaches an *osculating sphere* that is the 2-sphere which is the most tangent to K at $f(s)$. It contains the osculating circle and is tangent to K in the fourth order. Taylor's expansion formula implies

$$\nu_f^{(2,2)}(s, t) = \tfrac{1}{12}(t - s)^4 f(s) \wedge f'(s) \wedge f''(s) \wedge f'''(s) + \text{higher-order terms.}$$

Put

$$\nu_f^{(4)}(s) = f(s) \wedge f'(s) \wedge f''(s) \wedge f'''(s).$$

Suppose that $\nu_f^{(4)}(s) \neq 0$. Lemma 2.7 (3) shows that $\nu_f^{(4)}(s)$ is not a time-like vector. If it is a light-like vector, then Lemma 2.7 (2) implies that $\nu_f^{(4)}(s) = kf(s)$ for some $k \in \mathbb{R}$. Since $L(f(t), f(t)) = 0$ for any $t \in S^1$,

$$L(f(t), f''(t)) = -L(f'(t), f'(t)) = \sum_{i=1}^{4} (f_i'(t))^2 \neq 0 \quad \text{for any } t \in S^1.$$

On the other hand, as $L(\nu_f, f''(s)) = 0$, we have $k = 0$, which is a contradiction.* Therefore, when $\nu_f^{(4)}(s) \neq 0$, the osculating sphere at $f(s)$ is given by $\nu_f^{(4)}(s)/\sqrt{(\nu_f^{(4)}(s))}$.

4.3. The real part as the canonical symplectic form on T^*S^3

In this subsection we show that the real part of the infinitesimal cross-ratio can be interpreted as the pull-back of the canonical symplectic form on the cotangent bundle T^*S^3 of the 3-sphere. This interpretation allows us to deduce the original definition (3.1) from the cosine formula in terms of the infinitesimal cross-ratio (4.1).

4.3.1. *The pull-back of the symplectic form to $S^n \times S^n \setminus \Delta$*

Recall that a cotangent bundle $\pi : T^*M \to M$ of a manifold M^n admits the canonical symplectic form ω_0 given by

$$\omega_0 = \sum \mathrm{d}p_i \wedge \mathrm{d}q_i,$$

where $(p_1, \dots, p_n)$ is a local coordinate of M and $(q_1, \dots, q_n)$ is the local coordinate of T^*M defined by

$$T_x^*M \ni v^* = \sum q_i \, \mathrm{d}p_i. \tag{4.2}$$

We remark that ω_0 is an exact 2-form with $\omega_0 = \mathrm{d}(-\sum q_i \, \mathrm{d}p_i)$.

Lemma 4.11.

(1) *There is a canonical bijection*

$$\psi_n : S^n \times S^n \setminus \Delta \to T^*S^n.$$

(2) *Let $(x_1, \dots, x_{n+1})$ be a system of local coordinates of*

$$U_{n+1}^+ = \{(x_1, \dots, x_{n+1}) \in S^n \subset \mathbb{R}^{n+1} \mid x_{n+1} > 0\}.$$

It determines the associated system of local coordinates of $\pi^{-1}(U_{n+1}^+) \subset T^*S^n$ by (4.2). The canonical bijection $\psi_n : S^n \times S^n \setminus \Delta \to T^*S^n$ is expressed with respect to these systems of local coordinates as

$$\begin{aligned}\psi_n(x(x_1, \dots, x_{n+1}), y(y_1, \dots, y_{n+1}))\\ = \left(x_1, \dots, x_n, \frac{y_1 - (y_{n+1}/x_{n+1})x_1}{1 - x \cdot y}, \dots, \frac{y_n - (y_{n+1}/x_{n+1})x_n}{1 - x \cdot y}\right)\end{aligned}$$

on $U_{n+1}^+ \times S^n \setminus \Delta$, where $x \cdot y$ denotes the inner product.

* We assumed that $|f'(t)|$ never vanishes.

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Proof. (1) Let Π_x be the n-dimensional hyperplane in $\mathbb{R}^{n+1}$ passing through the origin that is perpendicular to $x \in S^n$, and $p_x : S^n \setminus \{x\} \to \Pi_x$ be the stereographic projection. We identify Π_x with $T_x S^n$. Take an orthonormal basis $\{v_1, \ldots, v_n\}$ of $\Pi_x \cong T_x S^n$. Suppose $y \in S^n \setminus \{x\}$ is expressed as

$$y = \tilde{y}_1 v_1 + \cdots + \tilde{y}_n v_n + \tilde{y}_{n+1} x$$

with respect to the orthonormal basis $\{v_1, \ldots, v_n, x\}$ of $\mathbb{R}^{n+1}$. Then

$$p_x(y) = \frac{\tilde{y}_1}{1-\tilde{y}_{n+1}} v_1 + \cdots + \frac{\tilde{y}_n}{1-\tilde{y}_{n+1}} v_n.$$

Put

$$\psi_x(y) = \frac{\tilde{y}_1}{1-\tilde{y}_{n+1}} v_1^* + \cdots + \frac{\tilde{y}_n}{1-\tilde{y}_{n+1}} v_n^* \in T_x^* S^n, \tag{4.3}$$

where $\{v_i^*\}$ is the dual basis of $T_x^* S^n$. Then the map $\psi_x : S^n \setminus \{x\} \to T_x^* S^n$ does not depend on the choice of the orthonormal basis $\{v_i\}$ of $\Pi_x \cong T_x S^n$. Thus the map

$$\psi_n : S^n \times S^n \setminus \Delta \ni (x, y) \mapsto (x, \psi_x(y)) \in T^* S^n$$

makes the canonical bijection. □

Lemma 4.12. *The pull-back $\omega = \psi_n^* \omega_0$ of the canonical symplectic form ω_0 of $T^* S^n$ by $\psi_n : S^n \times S^n \setminus \Delta \to T^* S^n$ is given by*

$$\begin{aligned}\omega &= \mathrm{d}\left(-\frac{\sum_{i=1}^{n+1} y_i \,\mathrm{d}x_i}{1 - x \cdot y}\right) \\ &= \mathrm{d}\left(\frac{\sum_{i=1}^{n+1} x_i \,\mathrm{d}y_i}{1 - x \cdot y}\right) \\ &= \frac{\sum_{i=1}^{n+1} \mathrm{d}x_i \wedge \mathrm{d}y_i}{1 - x \cdot y} + \frac{(\sum_{i=1}^{n+1} y_i \,\mathrm{d}x_i) \wedge (\sum_{i=1}^{n+1} x_i \,\mathrm{d}y_i)}{(1 - x \cdot y)^2}.\end{aligned}$$

Proof. As $\omega_0 = -\mathrm{d} \sum q_i \,\mathrm{d}p_i$,

$$\psi_n^* \omega_0 = -\mathrm{d} \sum_{i=1}^{n} \frac{y_i - (y_{n+1}/x_{n+1}) x_i}{1 - x \cdot y} \,\mathrm{d}x_i$$

on $U_{n+1}^+ \times S^n \setminus \Delta$ by Lemma 4.11 (2). Since $-\sum_{i=1}^{n} x_i \,\mathrm{d}x_i = x_{n+1} \,\mathrm{d}x_{n+1}$ on S^n, it implies the formula. □

Lemma 4.13. *Let $S : S^n \setminus \{(0, \ldots, 0, 1)\} \to \mathbb{R}^n$ be the stereographic projection. Put*

$$P_n = S^{-1} \times S^{-1} : \mathbb{R}^n \times \mathbb{R}^n \setminus \Delta \to S^n \times S^n \setminus \Delta.$$

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Then the pull-back $\omega_{\mathbb{R}^n} = P_n{}^*\omega = P_n{}^*\psi_n{}^*\omega_0$ *is given by*

$$\begin{aligned}\omega_{\mathbb{R}^n} &= 2\mathrm{d}\left(\frac{\sum(x_i-y_i)\,\mathrm{d}y_i}{|x-y|^2}\right)\\ &= 2\mathrm{d}\left(\frac{\sum(x_i-y_i)\,\mathrm{d}x_i}{|x-y|^2}\right)\\ &= 2\left(\frac{\sum \mathrm{d}x_i\wedge\mathrm{d}y_i}{|x-y|^2} - 2\frac{(\sum(x_i-y_i)\,\mathrm{d}x_i)\wedge(\sum(x_j-y_j)\,\mathrm{d}y_j)}{|x-y|^4}\right).\end{aligned}$$

Proof. Suppose that

$$P_n(x(x_1,\dots,x_n),y(y_1,\dots,y_n)) = (X(X_1,\dots,X_{n+1}),Y(Y_1,\dots,Y_{n+1})).$$

Then

$$P_n^*\left(\frac{\sum_{i=1}^{n+1}X_i\,\mathrm{d}Y_i}{1-X\cdot Y}\right) = 2\frac{\sum_{i=1}^{n}(x_i-y_i)\,\mathrm{d}y_i}{|x-y|^2} + \mathrm{d}\log(|y|^2+1).$$

Therefore,

$$P_n^*\omega = P_n{}^*\mathrm{d}\left(\frac{\sum_{i=1}^{n+1}X_i\,\mathrm{d}Y_i}{1-X\cdot Y}\right) = 2\mathrm{d}\left(\frac{\sum_{i=1}^{n}(x_i-y_i)\,\mathrm{d}y_i}{|x-y|^2}\right).$$

□

Proposition 4.14. *The 2-form* $\omega_{\mathbb{R}^n}$ *is invariant under the diagonal action of the conformal group* $\mathcal{G}$ *on* $\mathbb{R}^n\times\mathbb{R}^n\setminus\Delta$ *defined by*

$$g\cdot(x,y) = (g\cdot x, g\cdot y),$$

where $g\in\mathcal{M}$ *and* $(x,y)\in\mathbb{R}^n\times\mathbb{R}^n\setminus\Delta$.*

Proof. It is obvious that $\omega_{\mathbb{R}^n}$ is invariant under the diagonal action of multiplication by scalars $(x,y)\mapsto(cx,cy)$ and of addition of vectors $(x,y)\mapsto(x+a,y+a)$. The previous lemma implies that $\omega_{\mathbb{R}^n}$ is invariant under the diagonal action of the orthogonal group $O(n)$.

Therefore, it suffices to show the invariance under the diagonal action $I\times I$ of the inversion I with respect to the $(n-1)$-sphere with radius 1 whose centre is the origin.

Suppose

$$(I\times I)(x(x_1,\dots,x_n),y(y_1,\dots,y_n)) = (X(X_1,\dots,X_n),Y(Y_1,\dots,Y_n)).$$

Then

$$(I\times I)^*\left(\frac{\sum(X_i-Y_i)\,\mathrm{d}Y_i}{|X-Y|^2}\right) = \left(\frac{\sum(x_i-y_i)\,\mathrm{d}y_i}{|x-y|^2}\right) + \tfrac{1}{2}\mathrm{d}\log(|y|^2).$$

Therefore,

$$(I\times I)^*\omega_{\mathbb{R}^n} = (I\times I)^*2\mathrm{d}\left(\frac{\sum(X_i-Y_i)\,\mathrm{d}Y_i}{|X-Y|^2}\right) = 2\mathrm{d}\left(\frac{\sum(x_i-y_i)\,\mathrm{d}y_i}{|x-y|^2}\right) = \omega_{\mathbb{R}^n}.$$

We give another proof of the invariance.

* See 'Note added in proof' preceding the references.

Let Σ_1 be the n-sphere in $\mathbb{R}^{n+1}$ with centre 0 and radius 1, and let $\Sigma_{\sqrt{2}}$ be the n-sphere in $\mathbb{R}^{n+1}$ with centre $(0,\ldots,0,1)$ and radius $\sqrt{2}$. Let I_Σ be the inversions of $\mathbb{R}^{n+1}\cup\{\infty\}$ in an n-sphere Σ in $\mathbb{R}^{n+1}$.

Then

$$S^{-1}(I(x)) = I_{\Sigma_{\sqrt{2}}}(I_{\Sigma_1}(x)) = I_{I_{\Sigma_{\sqrt{2}}}(\Sigma_1)}(I_{\Sigma_{\sqrt{2}}}(x)) = I_{\mathbb{R}^n}(S^{-1}(x))$$

for $x \in \mathbb{R}^n$. Therefore,

$$P_n \circ (I \times I) = (I_{\mathbb{R}^n} \times I_{\mathbb{R}^n}) \circ P_n : \mathbb{R}^n \times \mathbb{R}^n \setminus \Delta \to S^n \times S^n \setminus \Delta.$$

As

$$\psi_n \circ (I_{\mathbb{R}^n} \times I_{\mathbb{R}^n}) = \psi_n : S^n \times S^n \setminus \Delta \to T^*S^n,$$

we get the conclusion,

$$(I\times I)^*\omega_{\mathbb{R}^n} = (I\times I)^* {P_n}^* {\psi_n}^* \omega_0 = (\psi_n \circ P_n \circ (I\times I))^*\omega_0 = (\psi_n \circ P_n)^*\omega_0 = \omega_{\mathbb{R}^n}.$$

□

Lemma 4.15. *Let*

$$\lambda = \frac{\mathrm{d}w \wedge \mathrm{d}z}{(w-z)^2}, \quad (w,z) \in \mathbb{C}\times\mathbb{C}\setminus\Delta,$$

be the 2-form on $\mathbb{C}\times\mathbb{C}\setminus\Delta \cong \mathbb{R}^2\times\mathbb{R}^2\setminus\Delta$ obtained as the infinitesimal cross-ratio of dw *and* dz*. Then the following hold.*

(1) *Both* $\operatorname{Re}\lambda$ *and* $\operatorname{Im}\lambda$ *are exact 2-forms.*

(2) $\operatorname{Re}\lambda$ (*or* $\operatorname{Im}\lambda$) *is invariant* (*or invariant up to sign, respectively*) *under the diagonal action of the conformal group** *on* $\mathbb{R}^2\times\mathbb{R}^2\setminus\Delta$.

Proof. As for the real part, since the next lemma implies $\operatorname{Re}\lambda = -\frac{1}{2}\omega_{\mathbb{R}^2}$, Proposition 4.14 shows that $\operatorname{Re}\lambda$ satisfies the desired properties.

As for the imaginary part, direct calculation shows

$$\operatorname{Im}\lambda = -2\frac{(x_1-y_1)(x_2-y_2)(\mathrm{d}x_1\wedge\mathrm{d}y_1 - \mathrm{d}x_2\wedge\mathrm{d}y_2)}{\{(x_1-y_1)^2+(x_2-y_2)^2\}^2} + \frac{\{(x_1-y_1)^2-(x_2-y_2)^2\}(\mathrm{d}x_1\wedge\mathrm{d}y_2 + \mathrm{d}x_2\wedge\mathrm{d}y_1)}{\{(x_1-y_1)^2+(x_2-y_2)^2\}^2}.$$

(1) If we put

$$\rho = \frac{(x_1-y_1)\,\mathrm{d}x_2 - (x_2-y_2)\,\mathrm{d}x_1}{(x_1-y_1)^2+(x_2-y_2)^2},$$

then $\operatorname{Im}\lambda = -\mathrm{d}\rho$.

* By 'conformal group' we mean the group of transformations generated by the transformations $z \mapsto (az+b)/(cz+d)$ and $z \mapsto \bar{z}$ acting on the Riemann sphere $\mathbb{C}\cup\infty$ (or the restriction of elements of this group to $\mathbb{R}^2\setminus\{$the point where it is not defined, if necessary$\}$).

(2) Let I be the inversion with respect to the circle with radius 1 whose centre is the origin. Then

$$(I \times I)^* \rho = -\rho + \mathrm{d} \arctan\left(\frac{x_2}{x_1}\right),$$

which implies the invariance as in the proof of Proposition 4.14.

We remark that the lemma can be proved by a direct calculation with either complex or real coordinates. □

Lemma 4.16 (folklore). *The real part of the infinitesimal cross-ratio 2-form is equal to minus one-half of the pull-back of the canonical symplectic form of the cotangent bundle* T^*S^2,

$$\mathrm{Re}\left(\frac{\mathrm{d}w \wedge \mathrm{d}z}{(w-z)^2}\right) = -\tfrac{1}{2}\omega_{\mathbb{R}^2} = -\tfrac{1}{2}{P_2}^* {\psi_2}^* \omega_0.$$

Proof. The left-hand side is equal to

$$\begin{aligned}
&\frac{\{(x_1-y_1)^2-(x_2-y_2)^2\}(\mathrm{d}x_1 \wedge \mathrm{d}y_1 - \mathrm{d}x_2 \wedge \mathrm{d}y_2)}{\{(x_1-y_1)^2+(x_2-y_2)^2\}^2} \\
&\quad + 2\frac{(x_1-y_1)(x_2-y_2)(\mathrm{d}x_1 \wedge \mathrm{d}y_2 + \mathrm{d}x_2 \wedge \mathrm{d}y_1)}{\{(x_1-y_1)^2+(x_2-y_2)^2\}^2} \\
&\qquad = -\frac{\mathrm{d}x_1 \wedge \mathrm{d}y_1 + \mathrm{d}x_2 \wedge \mathrm{d}y_2}{(x_1-y_1)^2+(x_2-y_2)^2} \\
&\qquad\quad + 2\frac{\{(x_1-y_1)\,\mathrm{d}x_1 + (x_2-y_2)\,\mathrm{d}x_2\} \wedge \{(x_1-y_1)\,\mathrm{d}y_1 + (x_2-y_2)\,\mathrm{d}y_2\}}{\{(x_1-y_1)^2+(x_2-y_2)^2\}^2},
\end{aligned}$$

which is equal to the right-hand side. □

4.3.2. *From cosine formula to the original definition of* $E^{(2)}$

Now let us recall the definition of the infinitesimal cross-ratio. Let

$$(x_0, y_0) = (f(s_0), f(t_0)) \in K \times K \setminus \Delta.$$

Then there is an oriented twice tangent sphere $\varSigma_K(x_0, x_0, y_0, y_0)$, which is given by $\psi_K^{(2,2)}(s_0, t_0)$ when $(s_0, t_0) \in \mathrm{Conf}_2(S^1) \setminus \mathcal{C}c^{(2,2)}(K)$, and otherwise by any oriented 2-sphere that contains the circle $C(x_0, x_0, y_0)$. Let T_0 be a conformal transformation of $\mathbb{R}^3 \cup \{\infty\}$ that maps $\varSigma_K(x_0, x_0, y_0, y_0)$ to $\mathbb{R}^2 \times \{0\} \subset \mathbb{R}^3$, preserving the orientations. Let

$$\frac{\mathrm{d}w \wedge \mathrm{d}z}{(w-z)^2}$$

be a complex-valued 2-form on

$$\mathbb{R}^3 \times \mathbb{R}^3 \setminus \Delta \cong \{((w, x_3), (z, y_3)) \in (\mathbb{C} \times \mathbb{R}) \times (\mathbb{C} \times \mathbb{R}) \setminus \Delta\}.$$

Then, as a 2-form, the infinitesimal cross-ratio $\varOmega_{\mathrm{CR}}$ satisfies

$$\varOmega_{\mathrm{CR}}(x_0, y_0) = (T_0 \times T_0)^* \left(\frac{\mathrm{d}w \wedge \mathrm{d}z}{(w-z)^2}\right)(x_0, y_0).$$

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Lemma 4.17. *Let $K = f(S^1)$ be a knot. Then the real part of the infinitesimal cross-ratio Ω_{CR} defined in Definition 4.3 is equal to minus one-half of the pull-back of the canonical symplectic form of the cotangent bundle T^*S^3,*

$$\cos\theta \frac{\mathrm{d}x\,\mathrm{d}y}{|x-y|^2} = \mathrm{Re}\,\Omega_{\mathrm{CR}} = -\tfrac{1}{2}\omega_{\mathbb{R}^3}|_{K\times K\setminus\Delta} = -\tfrac{1}{2}(\iota_K \times \iota_K)^* P_3{}^* \psi_3{}^* \omega_0,$$

where $\iota_K : K \to \mathbb{R}^3$ is the inclusion map.

Proof. We show that their pull-backs $(f\times f)^*\,\mathrm{Re}\,\Omega_{\mathrm{CR}}$ and $-\frac{1}{2}(f\times f)^*\omega_{\mathbb{R}^3}$ coincide at any given $(s_0,t_0) \in S^1\times S^1 \setminus \Delta$.

Proposition 4.14 implies

$$-\tfrac{1}{2}(f\times f)^*\omega_{\mathbb{R}^3} = -\tfrac{1}{2}((T_0\circ f)\times(T_0\circ f))^*\omega_{\mathbb{R}^3}.$$

On the other hand, since

$$((T_0\circ f)^*\,\mathrm{d}x_3)(s_0,t_0) = \left(\frac{\mathrm{d}}{\mathrm{d}s}(T_0\circ f)_3\right)(s_0) = 0,$$
$$((T_0\circ f)^*\,\mathrm{d}y_3)(s_0,t_0) = \left(\frac{\mathrm{d}}{\mathrm{d}t}(T_0\circ f)_3\right)(t_0) = 0,$$

we have

$$\begin{aligned}
&-\tfrac{1}{2}((T_0\circ f)\times(T_0\circ f))^*\omega_{\mathbb{R}^3}(s_0,t_0)\\
&\quad= ((T_0\circ f)\times(T_0\circ f))^*\\
&\qquad\times\left(-\frac{\sum_{i=1}^3 \mathrm{d}x_i\wedge \mathrm{d}y_i}{|x-y|^2} + 2\frac{(\sum_{i=1}^3 (x_i-y_i)\wedge \mathrm{d}x_i)\wedge(\sum_{i=1}^3 (x_i-y_i)\wedge \mathrm{d}y_i)}{|x-y|^4}\right)(s_0,t_0)\\
&\quad= ((T_0\circ f)\times(T_0\circ f))^*\\
&\qquad\times\left(-\frac{\sum_{i=1}^2 \mathrm{d}x_i\wedge \mathrm{d}y_i}{|x-y|^2} + 2\frac{(\sum_{i=1}^2 (x_i-y_i)\wedge \mathrm{d}x_i)\wedge(\sum_{i=1}^2 (x_i-y_i)\wedge \mathrm{d}y_i)}{|x-y|^4}\right)(s_0,t_0)\\
&\quad= (f\times f)^*(T_0\times T_0)^*\,\mathrm{Re}\left(\frac{\mathrm{d}w\wedge \mathrm{d}z}{(w-z)^2}\right)(s_0,t_0)\\
&\quad= (f\times f)^*\,\mathrm{Re}\,\Omega_{\mathrm{CR}}(s_0,t_0).
\end{aligned}$$

□

For $0 < \varepsilon \ll 1$, put

$$N(\varepsilon) = \{(s,t)\in S^1\times S^1 \mid \varepsilon \leqslant |s-t| \leqslant 1-\varepsilon\},$$

where $S^1 = [0,1]/(0\sim 1)$, and assume that $N(\varepsilon)$ has a natural orientation as a subspace of the torus. Then its boundary $\partial N(\varepsilon)$ consists of two closed curves L_+ and L_- with opposite orientations, where

$$L_\pm = \{(s,t)\in S^1\times S^1 \mid t-s = \pm\varepsilon \pmod{\mathbb{Z}}\}.$$

Then

$$E^{(2)}(K) = \iint_{S^1\times S^1\setminus\Delta} (f\times f)^*\left(\frac{\mathrm{d}x\,\mathrm{d}y}{|x-y|^2} - \operatorname{Re}\Omega_{\mathrm{CR}}\right) + 4$$
$$= \lim_{\varepsilon\to 0}\iint_{N(\varepsilon)}\left(\frac{\mathrm{d}s\,\mathrm{d}t}{|f(s)-f(t)|^2} - (f\times f)^*\operatorname{Re}\Omega_{\mathrm{CR}}\right) + 4.$$

On the other hand, as

$$-(f\times f)^*\operatorname{Re}\Omega_{\mathrm{CR}} = \tfrac{1}{2}(f\times f)^*\omega_{\mathbb{R}^3} = \mathrm{d}(f\times f)^*\left(\frac{\sum(x_i-y_i)\,\mathrm{d}y_i}{|x-y|^2}\right),$$

by Lemmas 4.17 and 4.13, there holds

$$E^{(2)}(K) = \lim_{\varepsilon\to 0}\left\{E^{(2)}_{\varepsilon}(K) + \int_{L_+\cup L_-}(f\times f)^*\left(\frac{\sum(x_i-y_i)\,\mathrm{d}y_i}{|x-y|^2}\right)\right\} + 4$$

by Stokes's theorem. As

$$(f(s)-f(t), f'(t)) = (s-t) + O(|s-t|^3),$$

we have

$$\int_{L_+\cup L_-}(f\times f)^*\left(\frac{\sum(x_i-y_i)\,\mathrm{d}y_i}{|x-y|^2}\right) = \int_{L_+\cup L_-}\frac{(f(s)-f(t), f'(t))}{|f(s)-f(t)|^2}\,\mathrm{d}t$$
$$= \int_0^1 \frac{-\varepsilon + O(\varepsilon^3)}{\varepsilon^2 + O(\varepsilon^4)}\,\mathrm{d}t + \int_1^0 \frac{\varepsilon + O(\varepsilon^3)}{\varepsilon^2 + O(\varepsilon^4)}\,\mathrm{d}t$$
$$= -\frac{2}{\varepsilon} + O(\varepsilon).$$

Therefore, we restored the original definition (3.1),

$$E^{(2)}(K) = \lim_{\varepsilon\to 0}\left(E^{(2)}_{\varepsilon}(K) - \frac{2}{\varepsilon}\right) + 4.$$

5. The (absolute) imaginary cross-ratio energy, $E_{|\sin\theta|}$

In the previous section we introduced the infinitesimal cross-ratio Ω_{CR}, which is the unique conformal invariant of a pair of infinitesimal curve segments $\mathrm{d}x$ and $\mathrm{d}y$, and showed that $E^{(2)}$ can be expressed in terms of the absolute value and the real part of it. On the other hand, one can use the imaginary part of Ω_{CR}.

5.1. The projection of the inverted open knot

Definition 5.1. The *absolute imaginary cross-ratio energy* or the *conformal* $|\sin\theta|$ *energy*, $E_{|\sin\theta|}$, is defined by

$$E_{|\sin\theta|}(K) = \iint_{K\times K\setminus\Delta}|\operatorname{Im}\Omega_{\mathrm{CR}}| = \iint_{K\times K\setminus\Delta}\frac{|\sin\theta|\,\mathrm{d}x\,\mathrm{d}y}{|x-y|^2}.$$

$E_{|\sin\theta|}$ is well defined since the argument of cross-ratio, θ, is of the same order as $|x-y|^2$ near the diagonal set by the following lemma.

The interest of the $E_{|\sin\theta|}$ energy has already been noticed by Kusner and Sullivan [**18**, § 4].

Remark 5.2. Lemma 2.11 shows that the sign of $\sin\theta$ is constant; the absolute value allows us to forget it.

Lemma 5.3. *If a knot is of class C^4, the conformal angle $\theta_K(x,y)$ satisfies*

$$\theta_K(x,y) = \tfrac{1}{6}\sqrt{k^2\tau^2 + k'^2}|x-y|^2 + O(|x-y|^3)$$

near the diagonal set, where $k = |f''|$ is the curvature and τ is the torsion of the knot at x.

Proof. Let us first remark that the unit tangent vector at x conformally translated to y, $v_x(y)$, is expressed as

$$v_x(y) = 2\left(f'(s), \frac{f(t)-f(s)}{|f(t)-f(s)|}\right) \cdot \frac{f(t)-f(s)}{|f(t)-f(s)|} - f'(s),$$

since $v_x(y)$ is symmetric to $f'(s)$ with respect to $f(t)-f(s)$.

Assume that a knot f is of class C^4 and parametrized by the arc-length. Put $s=0$ and take the Frenet frame at x. Then, by Bouquet's formula, $f(t)$ is expressed as

$$f_1(t) = t - \tfrac{1}{6}k^2t^3 + \cdots, \qquad f_2(t) = \tfrac{1}{2}kt^2 + \tfrac{1}{6}k't^3 + \cdots, \qquad f_3(t) = \tfrac{1}{6}k\tau t^3 + \cdots.$$

Then, as $f'(0) = (0,0,1)$, the unit tangent vector at x conformally translated to y is given by

$$\begin{aligned} v_x(y) &= \frac{({f_1}^2(t) - {f_2}^2(t) - {f_3}^2(t), 2f_1(t)f_2(t), 2f_1(t)f_3(t))}{|f(t)|^2} \\ &= \frac{(t^2 - \frac{7}{12}k^2t^4 + O(t^5), kt^3 + \frac{1}{3}k't^4 + O(t^5), \frac{1}{3}k\tau t^4 + O(t^5))}{t^2(1 - \frac{1}{12}k^2t^2 + O(t^3))}. \end{aligned}$$

On the other hand,

$$\frac{f'(t)}{|f'(t)|} = \frac{(1 - \frac{1}{2}k^2t^2 + O(t^3), kt + \frac{1}{2}k't^2 + O(t^3), \frac{1}{2}k\tau t^2 + O(t^3))}{1 + O(t^3)}.$$

Hence

$$\begin{aligned} |\sin\theta| &= \left|\frac{f'(t)}{|f'(t)|} \times v_x(y)\right| \\ &= \frac{|(O(t^5), \frac{1}{6}k\tau t^4 + O(t^5), -\frac{1}{6}k't^4 + O(t^5))|}{t^2(1 - \frac{1}{12}k^2t^2 + O(t^3))(1 + O(t^3))} \\ &= \tfrac{1}{6}\sqrt{k^2\tau^2 + k'^2}\,t^2 + O(t^3). \end{aligned}$$

□

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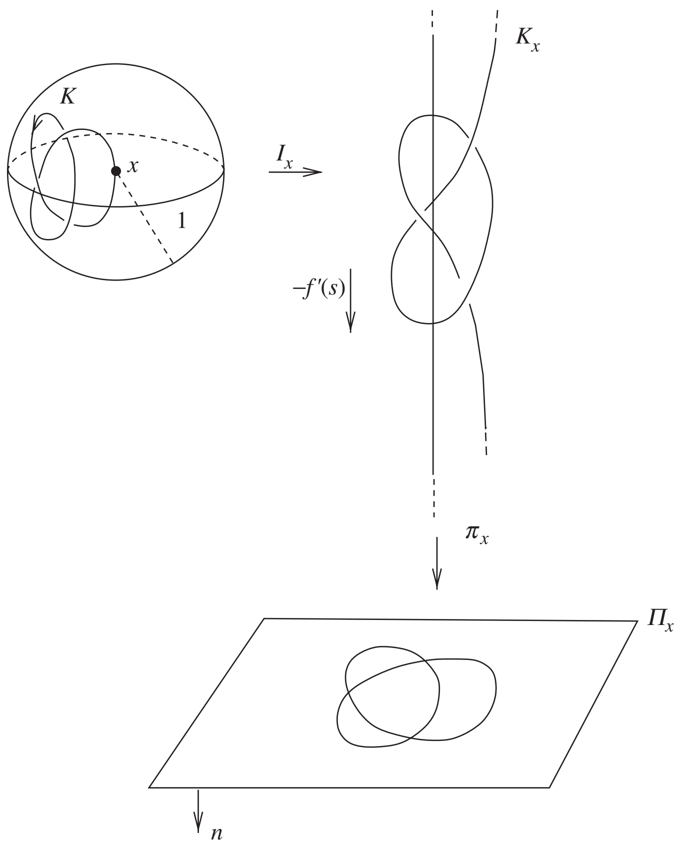

Figure 6. The projection of the inverted open knot.

Let us give a geometric interpretation of $E_{|\sin\theta|}$ using the inverted open knots. Put

$$V_{|\sin\theta|}(K;x) = \int_K \frac{|\sin\theta|\,\mathrm{d}y}{|x-y|^2}.$$

Let I_x, $\tilde{K}_x = I_x(K)$ and $\tilde{y} = I_x(y)$ be as in § 3.3. Let Π_x be the normal plane to K at x, $n = -f'(s)$ the normal vector to Π_x and $\pi_x : \mathbb{R}^3 \to \Pi_x$ the orthogonal projection (Figure 6). Since $I_{x*}(v_x(y)) = n$, the absolute value of the argument of cross-ratio $\theta_K(x,y)$ is equal to the angle between n and the tangent vector to $\tilde{K}_x$ at $\tilde{y}$. Hence

$$V_{|\sin\theta|}(K;x) = \int_K \frac{|\sin\theta|\,\mathrm{d}y}{|x-y|^2} = \int_{\tilde{K}_x} |\sin\theta|\,|\mathrm{d}\tilde{y}|$$

is the length of the projection $\pi_x(\tilde{K}_x) \subset \Pi_x$.

Thus the imaginary cross-ratio energy is equal to the *total length of the projection of the inverted open knots*,

$$E_{|\sin\theta|}(K) = \int_K \mathrm{length}(\pi_x(I_x(K)))\,\mathrm{d}x.$$

5.2. The properties of $E_{|\sin\theta|}$

We show first that $E_{|\sin\theta|}$ can detect the unknot.

Example 5.4. Let $K_\circ$ be the standard planar circle. Then $\theta_{K_\circ}(x,y)=0$ for any (x,y). Therefore, $E_{|\sin\theta|}(K_\circ)=0$.

We remark that Claim 4.4 implies that $E_{|\sin\theta|}(K)=0$ if and only if $K=K_\circ$.

Theorem 5.5 (cf. [23]). *The imaginary cross-ratio energy bounds the average crossing number from above, namely,*

$$E_{|\sin\theta|}(K)\geqslant 4\pi\,\mathrm{ac}(K),$$

for any knot K.

Corollary 5.6. *If K is a non-trivial knot, then $E_{|\sin\theta|}(K)\geqslant 12\pi$.*

Proof. Assume that a knot is parametrized by the arc-length. Put

$$u=f'(s),\quad v=f'(t),\quad w=\frac{f(t)-f(s)}{|f(t)-f(s)|}\quad\text{and}\quad \tilde{u}=v_{f(s)}(f(t)).$$

Recall that $\tilde{u}=2(u,w)w-u$, and that the conformal angle θ is the angle between $\tilde{u}$ and v.

Suppose that $\theta\neq 0,\pi$. Then the tangent plane $T_{f(t)}\Sigma$ at $f(t)$ to the twice tangent sphere $\Sigma=\Sigma_K(f(s),f(t))$ is spanned by $\tilde{u}$ and v. Let $\psi=\psi(s,t)$ be the angle between the chord joining $f(t)$ and $f(s)$ and the tangent plane $T_{f(t)}\Sigma$.

Then the numerator of the integrand of the average crossing number (which is the absolute value of the integrand in Gauss formula) is

$$|(u\times v,w)|=|(\tilde{u}\times v,w)|=|\sin\psi|\,|\sin\theta|.$$

Therefore,

$$\mathrm{ac}(K)=\frac{1}{4\pi}\iint_{S^1\times S^1}\frac{|\sin\psi(s,t)|\,|\sin\theta(f(s),f(t))|}{|f(s)-f(t)|^2}\,\mathrm{d}s\,\mathrm{d}t\leqslant\frac{1}{4\pi}E_{|\sin\theta|}(K).$$

When $\theta=0$ or π, then $|(u\times v,w)|=\sin\theta=0$. □

Next we show that $E_{|\sin\theta|}$ is an energy functional for knots in the weak sense.

Theorem 5.7. *For any real numbers b, δ ($0<\delta\leqslant\frac{1}{2}$) and κ_0, there exists a positive constant $C=C(b,\delta,\kappa_0)$ such that, if a knot K with length $l(K)$ whose curvature is not greater than κ_0 has a pair of points x, y on it that satisfy $\delta_K(x,y)=\delta l(K)$ and that $|x-y|\leqslant Cl(K)$, then $E_{|\sin\theta|}(K)\geqslant b$.*

Proof. Fix δ and κ_0 ($\kappa_0\geqslant 2\pi$), and let $0<d\leqslant\delta$. Put

$$\begin{aligned}\mathcal{K}(d)&=\mathcal{K}_{\delta,\kappa_0}(d)\\&=\left\{K:\text{a knot}\;\middle|\;\begin{array}{l}\text{the length of }K\text{ is }1;\\ \text{the curvature of }K\text{ is not greater than }\kappa_0;\\ \exists x,y\in K\text{ such that (i) the shorter arc-length}\\ \text{between }x\text{ and }y\text{ is }\delta,\text{ and (ii) }|x-y|\leqslant d\end{array}\right\}.\end{aligned}$$

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We show that

$$\lim_{d\to+0}\Bigl(\inf_{K\in\mathcal{K}(d)} E_{|\sin\theta|}(K)\Bigr)=\infty.$$

Lemma 5.8. *Let*

$$d_0=\min\left\{\tfrac{1}{100},\tfrac{1}{5}\delta^2,\left(\frac{1}{2}\left(-1+\sqrt{1+\frac{1}{50\kappa_0}}\right)\right)^2\right\}.$$

Let $d\leqslant d_0$. Suppose that $K=f(S^1)\in\mathcal{K}(d)$ is parametrized by arc-length and satisfies $|f(0)-f(\delta)|=d$. If $5d\leqslant t\leqslant\sqrt{d}$, then at least one of

$$V_{|\sin\theta|}(K;f(\pm t)),\ V_{|\sin\theta|}(K;f(\delta\pm t))$$

is greater than $1/(100(d+t))$.

We show that lemma implies theorem. Since $10d\leqslant\sqrt{d}<\frac{1}{2}\delta$,

$$f([-\sqrt{d},-5d])\sqcup f([5d,\sqrt{d}])\sqcup f([\delta+5d,\delta+\sqrt{d}])\sqcup f([\delta-\sqrt{d},\delta-5d])$$

is a disjoint union of curve segments of K, where S^1 is regarded as $\mathbb{R}$ modulo $\mathbb{Z}$. Since $V_{|\sin\theta|}(K;y)\geqslant 0$ for any $y\in K$,

$$\begin{aligned}E_{|\sin\theta|}(K)&\geqslant\int_{5d}^{\sqrt{d}}\{V_{|\sin\theta|}(K;f(-t))+V_{|\sin\theta|}(K;f(t))\\&\qquad+V_{|\sin\theta|}(K;f(\delta-t))+V_{|\sin\theta|}(K;f(\delta+t))\}\,\mathrm{d}t\\&\geqslant\int_{5d}^{\sqrt{d}}\frac{1}{100}\cdot\frac{1}{d+t}\,\mathrm{d}t\\&=\frac{1}{100}\left\{\log\left(1+\frac{1}{\sqrt{d}}\right)-\log 6\right\},\end{aligned}$$

which explodes as d goes down to 0, which completes the proof of Theorem 5.7. □

Proof of Lemma 5.8. Assume there is a t with $5d\leqslant t\leqslant\sqrt{d}$ such that

$$V_{|\sin\theta|}(K;f(\pm t)),V_{|\sin\theta|}(K;f(\delta\pm t))\leqslant\frac{1}{100}\cdot\frac{1}{d+t}.$$

Put $x_\pm=f(\pm t)$. Let $R_t=1/|f''(t)|$ be the radius of curvature at x_+, and $C(x_+,x_+,x_+)$, I_{x_+} be the inversion as in § 3.3, $\tilde{K}_{x_+}=I_{x_+}(K)$, the plane $\varPi_{x_+}$ and the projection π_{x_+} be as in Figure 6. Define x'_+ by (Figure 7, top)

$$C(x_+,x_+,x_+)\cap\varPi_{x_+}=\{x_+,x'_+\}.$$

Let $\hat{x}_+=I_{x_+}(x'_+)$. Then

$$\lim_{K\setminus\{x_+\}\ni y\to x_+}\pi_{x_+}(I_{x_+}(y))=\hat{x}_+.$$

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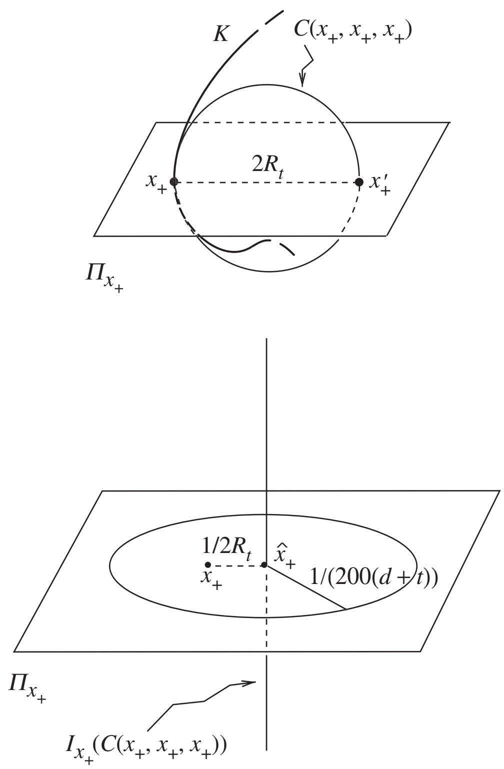

Figure 7. The osculating circle, x_+, x'_+ and $\hat{x}_+$.

Since

$$V_{|\sin\theta|}(K;x_+) = \text{length}(\pi_{x_+}(\tilde{K}_{x_+})) \leqslant \frac{1}{100}\cdot\frac{1}{d+t},$$

$\pi_{x_+}(\tilde{K}_{x_+})$ lies inside the circle on Π_{x_+} with centre $\hat{x}_+$ and radius $1/(200(d+t))$ (Figure 7, bottom). Since

$$\sqrt{d} \leqslant \frac{1}{2}\left(-1+\sqrt{1+\frac{1}{50\kappa_0}}\right),$$

there holds

$$|x_+ - \hat{x}_+| = \frac{1}{2R_t} \leqslant \tfrac{1}{2}\kappa_0 \leqslant \frac{1}{2}\cdot\frac{1}{200}\cdot\frac{1}{d+\sqrt{d}} \leqslant \frac{1}{400}\cdot\frac{1}{d+t}.$$

Thus $\pi_{x_+}(\tilde{K}_{x_+})$ lies inside the circle Γ on Π_{x_+} with centre x_+ and radius $3/(400(d+t))$. This means that $\tilde{K}_{x_+}$ lies inside the cylinder $D^2\times\mathbb{R}$, where $\partial D^2 = \Gamma$ and the direction of $\mathbb{R}$ is $f'(t)$. If we apply the inversion I_{x_+} again, this implies that K lies outside the '*degenerate** *open solid torus*' N_t whose meridian disc has radius $\frac{1}{3}(200(d+t))$, as illustrated in Figure 8.

* By a '*degenerate solid torus*' we mean a torus of revolution of a circle around a tangent line.

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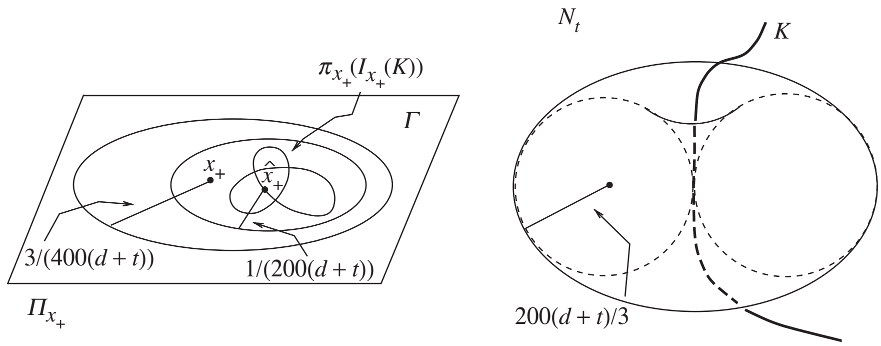

Figure 8. The circle Γ and the degenerate solid torus.

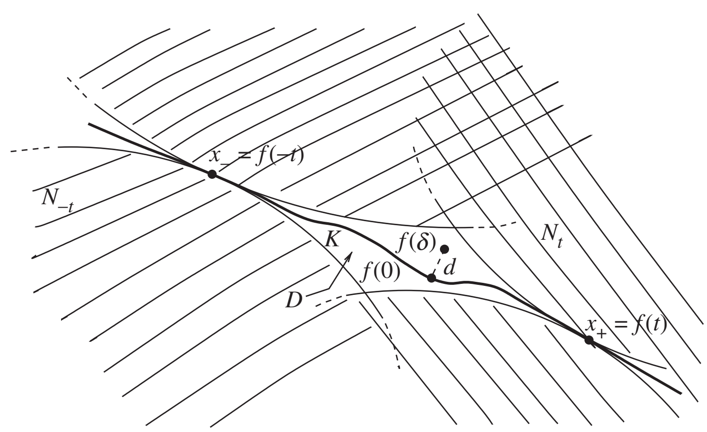

Figure 9. The domain D illustrated as a two-dimensional figure.

The same argument applies to $-t$ to conclude that K lies outside the 'degenerate open solid torus' N_{-t}. Since

$$|f(t) - f(-t)| \leqslant 2t \ll \tfrac{400}{3}(d+t),$$

$f([-t,t])$ is contained in a region D bounded by N_t and N_{-t}, as illustrated in Figure 9.*

Sublemma 5.9. *$f(\delta)$ is contained in D.*

We show that Sublemma 5.9 implies Lemma 5.8. If $f(\delta)$ is contained in D, then the knot K must have double points at x_+ and x_-, which is a contradiction. (End of the proof of Lemma 5.8.)

Proof of Sublemma 5.9. Since $|f(0) - f(\delta)| = d$, which is much smaller than the radius $\frac{1}{3}(400(d+t))$ of the meridian discs of the degenerate solid tori N_t and N_{-t}, it suffices to show that

$$|f(0) - f(\pm t)| > d$$

* D is the bounded component of $\mathbb{R}^3 \setminus (N_t \cup N_{-t})$.

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to prove the sublemma. First we remark that

$$t \leqslant \sqrt{d} \leqslant \frac{1}{2}\left(-1+\sqrt{1+\frac{1}{50\kappa_0}}\right) < \frac{1}{200\kappa_0}.$$

For $0 < s \leqslant t$,

$$\frac{\mathrm{d}}{\mathrm{d}s}(f'(0), f'(s)) = (f'(0), f''(s)) \leqslant \kappa_0,$$

and hence

$$(f'(0), f'(s)) \leqslant 1 - \kappa_0 s.$$

As $s \leqslant 1/\kappa_0$, we have

$$|f(0) - f(t)| \geqslant \int_0^t (1-\kappa_0 s)\,\mathrm{d}s = t(1 - \tfrac{1}{2}\kappa_0 t) > d.$$

□

6. Measure of non-trivial spheres

Strangely enough, four-dimensional subsets of Λ appeared first in the study of foliations [**20**]. Here we will associate such sets of spheres to knots.

6.1. Spheres of dimension 0

We will start with spheres of dimension 0 in S^1, and study their positions with respect to a 'torus' T made of four distinct points.

Notice that, if the conformal images of four points under $S^1 \to \mathbb{R}^1 \cup \{\infty\}$ are $-R, -1, 1, R$, the cross ratio is R. We will use this remark later to give an interpretation of the modulus of a ring or of the zone between two non-intersecting spheres.

An oriented sphere σ disjoint from T bounds an interval I. We will say that σ is non-trivial if I contains two points of T (Figure 10). Roughly speaking, spheres which are small enough are trivial.

Proposition 6.1. *The 'torus' T that minimizes the measure of the set of the non-trivial spheres is the 'torus' made of the four vertices of a square* (*or its image by the conformal group of the circle*).

The domain Z of $\mathcal{S} = \{$pairs of points of $S^1\}$ formed by the non-trivial spheres is bounded by segments of light rays formed by the spheres containing one of the four points of T (Figure 11).

As the only conformal invariant of a set of four points is their cross-ratio, the measure $m(Z)$ is a function of this cross-ratio.

Proof. The proof of the proposition is a computation. Using the stereographic projection of S^1 on $\mathbb{R}$, the measure on $\mathcal{S}$ is $(2/(y-x)^2)|\mathrm{d}x \wedge \mathrm{d}y|$. Without loss of generality, we can suppose that the four points of the 'torus' T are $\{\infty, 0, 1, z\}$, where $z > 1$. We will

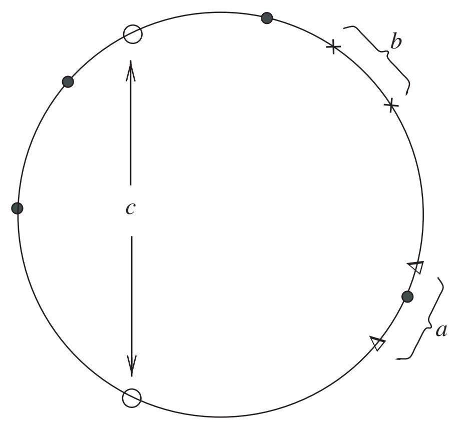

Figure 10. A non-trivial (c), and two trivial (a, b) 0-spheres.

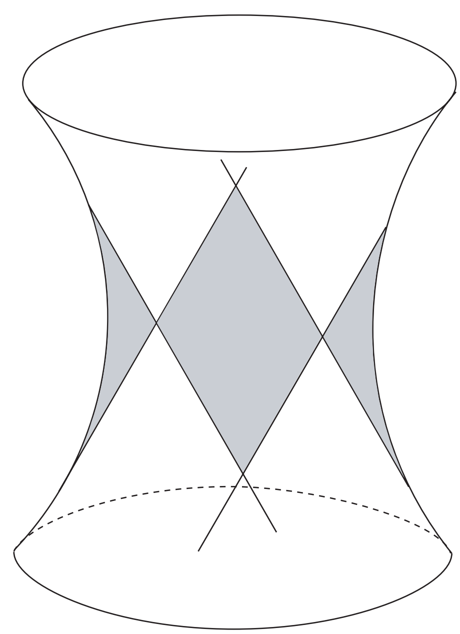

Figure 11. The set of the non-trivial 0-spheres.

compute the measure of ‘half’ of the points of Z, that is, $Z_z = \{\infty < x < 0;\ 1 < y < z\}$. The other cases are analogous. One has

$$m(Z_z) = m(\{\infty < x < 0;\ 1 < y < z\}) + m(\{0 < x < 1;\ z < y < \infty\}).$$

Then

$$m(\{\infty < x < 0;\ 1 < y < z\}) = \int_{1<y<z} \int_{-\infty<x<0} \frac{2}{(y-x)^2} |\mathrm{d}x \wedge \mathrm{d}y| = 2\log(z).$$

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In the same way, we compute

$$m(\{0 < x < 1;\ z < y < \infty\}) = 2\log(z) - 2\log(z-1).$$

The minimum of $m(Z_z)$ is achieved for $z = 2$, when we have $m(Z_2) = 4\log(2)$. This corresponds to the 'square' 'torus' $T = \{e^{ik\pi/2}\}$. □

6.2. Non-trivial spheres in $\mathcal{S}$, tangent spheres and twice tangent spheres

Observe first that a circle is intersected by a sphere in at most two points if the sphere does not contain the circle. Generically, a sphere can intersect a knot K in zero, two or any even number of points.

We remark that the volume of the set of spheres that intersect a given knot K is infinite for any knot K. In order to have a finite-valued functional, we should get rid of the contribution of the set of 'small spheres', which intersect K in at most two points.

Definition 6.2. An oriented 2-sphere Σ is called a *non-trivial sphere* for a knot K if Σ intersects K in at least four points, where the number of the intersection points in $K \cap \Sigma$ is counted with multiplicity. An oriented 2-sphere Σ with $\Sigma = \partial D^3$ is called a *non-trivial sphere in the strict sense* for a knot K if $\operatorname{Int} D^3 \cap K$ contains at least two connected components of $K \setminus \Sigma$.

Let $\overline{NT}(K) \subset \Lambda$ (or, respectively, $NT(K) \subset \Lambda$) denote the set of the non-trivial spheres (or, respectively, the non-trivial spheres in the strict sense).

If we fix a metric on the ambient sphere S^3, then, for a constant α depending on the curve K, spheres of geodesical radius smaller than α can intersect K in at most two points. This implies that the set $\overline{NT}(K)$ of non-trivial spheres is bounded in $\mathcal{S}$. It therefore has a finite volume.

Definition 6.3. Let $mnts_1(K)$ denote the volume of the set $\overline{NT}(K)$ of non-trivial spheres for a knot K.

The subset $\overline{NT}(K) \subset \mathcal{S}$ is, when K is not a circle, a four-dimensional region whose boundary consists of spheres which are tangent to the knot K. This boundary is not smooth. In particular, it has 'corners', which are the transverse intersections of two folds of the set of the tangent spheres. Therefore, the 'corner' of $\partial\overline{NT}(K)$ consists of spheres which are tangent to the knot in two distinct points, that is, the twice tangent spheres. The closure of the boundary $\partial\overline{NT}(K)$ and the closure of its corner may have other singularities.

Definition 6.4. Let $TWT(K)$ denote the set of the twice tangent spheres and $atwt(K)$ its area.

Remark 6.5. Then the set $TWT(K)$ of the twice tangent spheres forms a surface of space type. Namely, the restriction of the Lorentz form to the tangent space at each regular point of this surface is positive definite. Therefore, its area $atwt(K)$ is a positive number, which is a conformal invariant of the knot K.

Remark 6.6. Unlike $E^{(2)}$ or $E_{|\sin\theta|}$, $atwt(K)$ cannot be expressed as an integral over T^2 of a function of the infinitesimal cross-ratio $\Omega_{\rm CR}$ which does not contain its derivatives. This is because the local contribution of a neighbourhood of a pair of points on K to $atwt(K)$ depends on the curvature, whereas $\Omega_{\rm CR}$ itself is independent of f''.

Question 6.7. *Can $atwt(K)$ be expressed in terms of the infinitesimal cross-ratio and its derivatives,*

$$\frac{e^{i\theta}}{|f(s)-f(t)|^2}, \quad \frac{\partial}{\partial s}\left(\frac{e^{i\theta}}{|f(s)-f(t)|^2}\right), \quad \textit{etc.?}$$

Remark 6.8. The area $atwt(K)$ is not an energy functional for knots.

It is enough to check that the contribution to $atwt(K_n)$ of two orthogonal segments of length 1, $I_n \subset K_n$ of middle point p_n and $J_n \subset K_n$ of middle point q_n, such that $d(I_n, J_n) = d(p_n, q_n) = 1/n$ does not blow up when n goes to ∞. This contribution is bounded by the area of the spheres tangent to two orthogonal lines distant of 1.

6.3. The volume of the set of the non-trivial spheres

The measure $mnts_1(K)$ of the set of the non-trivial spheres is not expressed as a 'bilocal integral' like $E^{(2)}$ or $E_{|\sin\theta|}$, since it does not take into account the number of intersection points of K with spheres. In order to get such an integral, we have to count each sphere Σ with multiplicity, which is a number of pairs of points in $\Sigma \cap K$ where the algebraic intersection number has the same sign.

Definition 6.9. The *measure of acyclicity $mnts(K)$* is defined by

$$mnts(K) = \int_{NT(K)} \binom{n}{2}\, d\Sigma, \quad \text{where } n = n_K(\Sigma) = \tfrac{1}{2}(\sharp(\Sigma \cap K)),$$

where the number of the intersection points $\sharp(\Sigma \cap K)$ is counted with multiplicity, and $d\Sigma$ denotes the $\mathcal{G}$-invariant measure of Λ.

Another related functional of interest is the *measure of the image of the* 4*-tuple map for a knot with multiplicity*, which is given by

$$mnts^{(4)}(K) = \int_{\mathrm{Conf}_4(S^1)\setminus \mathcal{C}c(K)} \psi_K^* \omega_\Lambda = \int_{NT(K)} \binom{2n}{4}\, d\Sigma,$$

where ω_Λ is $\mathcal{G}_+$-invariant volume 4-form of Λ. This definition of $mnts^{(4)}$ is based on the suggestion by Cantanella to the second author when he gave a talk on $mnts(K)$. It cannot be expressed as a 'bilocal integral'.

Claim 6.10. *These three functionals, $mnts_1$, $mnts$ and $mnts^{(4)}$, are conformally invariant.*

Proof. Let $g \in \mathcal{G}$ be a conformal transformation. Then g maps a non-trivial sphere Σ of K to a non-trivial sphere $g \cdot \Sigma$ of $g \cdot K$ preserving the number of the intersection points. Therefore, $g(NT(K)) = NT(g \cdot K)$ and $n_K(\Sigma) = n_{g\cdot K}(g \cdot \Sigma)$. Since the measure $d\Sigma$ is $\mathcal{G}$-invariant, i.e. $d\Sigma = d(g \cdot \Sigma)$, we have $mnts(g \cdot K) = mnts(K)$, etc. □

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As we mentioned before, the measure $mnts_1(K)$ of the set $\overline{NT}(K)$ of the non-trivial spheres is finite for any smooth knot K, since $NT(K)$ is bounded in Λ. On the other hand, it is not easy to control the number of the intersection points of K and a sphere Σ. We will show later at the end of the next subsection that the measure of acyclicity is finite for a smooth knot using Proposition 6.13.

Question 6.11. *Is $mnts^{(4)}$ finite for any smooth knot?*

We conjecture that, for any smooth knot K, there exists a natural number n such that the measure of the set of spheres that intersect K in at least n points is 0, and hence the answer to the above question is affirmative.

Remark 6.12. These three functionals, $mnts_1$, $mnts$ and $mnts^{(4)}$, are different. There holds $mnts_1(K) \leqslant mnts(K) \leqslant mnts^{(4)}(K)$ because $1 \leqslant \binom{n}{2} \leqslant \binom{2n}{4}$ when $n \geqslant 2$.

6.4. The measure of acyclicity in terms of the infinitesimal cross-ratio

Assume that K is oriented. Let $p \in K \cap \Sigma$ be a transversal intersection point. We say that *Σ intersects K at p positively* if the orientation of K is '*outward*' at p with respect to the orientation of Σ, namely, if the algebraic intersection number $K \cdot \Sigma$ is equal to $+1$ at p. We call p a *positive intersection point*. Then the measure of acyclicity satisfies

$$mnts(K) = \int_{NT(K)} \binom{n'}{2} \omega,$$

where n' is the number of positive intersection points of K and Σ. We remark that the above definition does not depend on the choice of the orientation of a knot K.

Let $|NT_K^{(4)}(x, x'; y, y')|$ denote the volume of the set of the non-trivial spheres for K which intersect xx' and yy' positively, where xx' denotes the curve segment of K between x and x' with the natural orientation derived from that of K. Put

$$|NT_K^{(4)}(\mathrm{d}x, \mathrm{d}y)| = |NT_K^{(4)}(x, x + \mathrm{d}x; y, y + \mathrm{d}y)|.$$

Let

$$|nt_K^{(4)}(x, y)| = \lim_{|x-x'|,|y-y'| \to 0} \frac{|NT_K^{(4)}(x, x'; y, y')|}{|x - x'|\,|y - y'|}.$$

Then the measure of acyclicity of K is equal to

$$\begin{aligned} mnts(K) &= \lim_{\max|x_i - x_{i+1}| \to 0} \sum_{i<j} |NT_K^{(4)}(x_i, x_{i+1}, x_j, x_{j+1})| \\ &= \frac{1}{2} \iint_{K \times K \setminus \Delta} |nt_K^{(4)}(x, y)| \,\mathrm{d}x\,\mathrm{d}y. \end{aligned}$$

Proposition 6.13. *The measure of acyclicity is expressed as*

$$mnts(K) = \tfrac{1}{4}\pi \iint_{K \times K} (\sin\theta - \theta\cos\theta) \frac{\mathrm{d}x\,\mathrm{d}y}{|x - y|^2},$$

where θ is the argument of cross-ratio.

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The proof consists of the following two lemmas.

Lemma 6.14. *There holds the dimension reduction formula*

$$|NT_K^{(4)}(\mathrm{d}x,\mathrm{d}y)| = \tfrac{1}{2}\pi|NT_K^{(3)}(\mathrm{d}x,\mathrm{d}y)|,$$

where $NT_K^{(3)}(\mathrm{d}x,\mathrm{d}y)$ *denotes the set of the non-trivial circles of the twice tangent sphere* $\Sigma_K(x,x,y,y)$ *which intersect both* $\mathrm{d}x$ *and* $\mathrm{d}y$ *positively. We denote the volume of this set by* $|NT_K^{(3)}(\mathrm{d}x,\mathrm{d}y)|$.

Proof. Since $|NT_K^{(4)}(\mathrm{d}x,\mathrm{d}y)|$ is conformally invariant, we may assume that x, $x+\mathrm{d}x$, y and $y+\mathrm{d}y$ are in $\mathbb{R}^2=\{(X,Y,0)\}\subset\mathbb{R}^3$ by a stereographic projection from the twice tangent sphere. Suppose the set of the non-trivial spheres or circles is parametrized by

$$\begin{aligned} &CTR^{(3)}(\mathrm{d}x,\mathrm{d}y)\\ &\qquad=\{(X,Y,r)\in\mathbb{R}^3_+ \mid \exists C\in NT_K^{(3)}(\mathrm{d}x,\mathrm{d}y) \text{ with centre } (X,Y) \text{ and radius } r\}\end{aligned}$$

and

$$\begin{aligned} &CTR^{(4)}(\mathrm{d}x,\mathrm{d}y)\\ &\qquad=\{(X,Y,Z,r)\in\mathbb{R}^4_+ \mid \exists \Sigma\in NT_K^{(4)}(\mathrm{d}x,\mathrm{d}y) \text{ with centre } (X,Y,Z) \text{ and radius } r\}\\ &\qquad\cong\{(X,Y,Z,\sqrt{r^2+Z^2}) \mid (X,Y,r)\in CTR^{(3)}(\mathrm{d}x,\mathrm{d}y),\ Z\in\mathbb{R}\}.\end{aligned}$$

Then

$$\begin{aligned} |NT_K^{(4)}(\mathrm{d}x,\mathrm{d}y)| &= \int_{CTR^{(4)}(\mathrm{d}x,\mathrm{d}y)} \frac{1}{r^4}\,\mathrm{d}X\,\mathrm{d}Y\,\mathrm{d}Z\,\mathrm{d}r\\ &= \int_{CTR^{(3)}(\mathrm{d}x,\mathrm{d}y)} \biggl(\int_{-\infty}^{\infty} \frac{1}{(r^2+Z^2)^2}\,\mathrm{d}Z\biggr)\,\mathrm{d}X\,\mathrm{d}Y\,\mathrm{d}r\\ &= \tfrac{1}{2}\pi \int_{CTR^{(3)}(\mathrm{d}x,\mathrm{d}y)} \frac{1}{r^3}\,\mathrm{d}X\,\mathrm{d}Y\,\mathrm{d}r\\ &= \tfrac{1}{2}\pi|NT_K^{(3)}(\mathrm{d}x,\mathrm{d}y)|.\end{aligned}$$

□

In what follows, we calculate $|NT_K^{(3)}(\mathrm{d}x,\mathrm{d}y)|$ in the case when θ satisfies $0\leqslant\theta\leqslant\frac{1}{2}\pi$. Similar calculation works for $\frac{1}{2}\pi\leqslant\theta\leqslant\pi$.

We may assume that

$$x=\infty,\quad x+\mathrm{d}x=(0,0),\quad y=(1,0)\quad\text{and}\quad y+\mathrm{d}y=(1+a,b)\quad(b\geqslant 0),$$

by a suitable orientation-preserving conformal transformation. Then, as the cross-ratio is preserved,

$$a=\cos\theta\frac{|\mathrm{d}x|\,|\mathrm{d}y|}{|x-y|^2},\qquad b=\sin\theta\frac{|\mathrm{d}x|\,|\mathrm{d}y|}{|x-y|^2}.$$

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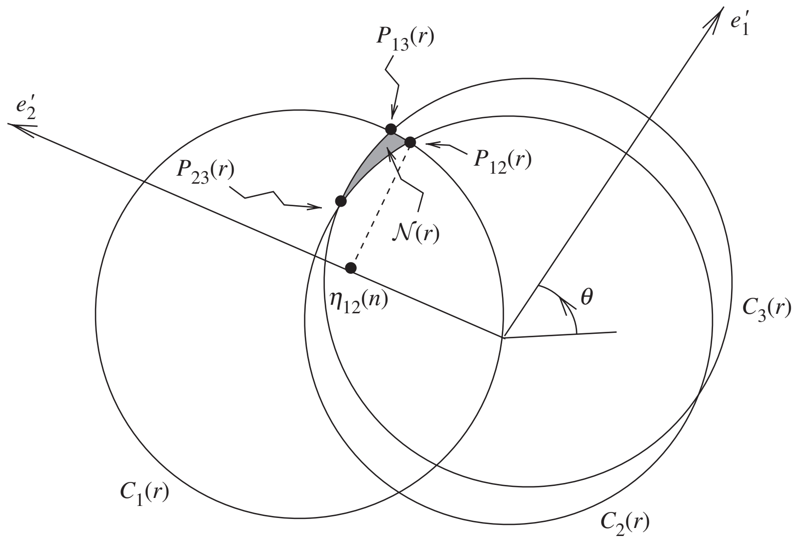

Figure 12. $\mathcal{N}(r)$ and $P_{ij}(r)$.

Then $CTR^{(3)}(\mathrm{d}x, \mathrm{d}y)$ is given by

$$CTR^{(3)}(\mathrm{d}x, \mathrm{d}y) = \{(X, Y, r) \in \mathbb{R}^3_+ \mid X^2 + Y^2 < r^2,\ (X-1)^2 + Y^2 > r^2,\\ (X-(1+a))^2 + (Y-b)^2 < r^2\}.$$

Let $\mathcal{N}(r_0)$ be the intersection of $CTR^{(3)}(\mathrm{d}x, \mathrm{d}y)$ and the level plane defined by $\{r = r_0\}$. Then

$$|NT_K^{(3)}(\mathrm{d}x, \mathrm{d}y)| = \int_0^\infty \frac{1}{r^3} \operatorname{area}(\mathcal{N}(r))\,\mathrm{d}r.$$

Let $C_i(r)$ be circles defined by

$$C_1(r) = \{(X, Y) \mid X^2 + Y^2 = r^2\},$$
$$C_2(r) = \{(X, Y) \mid (X-1)^2 + Y^2 = r^2\},$$
$$C_3(r) = \{(X, Y) \mid (X-(1+a))^2 + (Y-b)^2 = r^2\}.$$

Let $P_{ij}(r) = (X_{ij}(r), Y_{ij}(r))$ $(i \neq j)$ be one of the two intersection points of $C_i(r) \cap C_j(r)$ (we choose the one with the bigger y-coordinate, as shown in Figure 12),

$$P_{12}(r) = \left(\tfrac{1}{2}, \sqrt{r^2 - \tfrac{1}{4}}\right),$$

$$P_{13}(r) = \left(\tfrac{1}{2}(1+a) - b\sqrt{\frac{r^2}{(1+a)^2 + b^2} - \frac{1}{4}}, \tfrac{1}{2}b + (1+a)\sqrt{\frac{r^2}{(1+a)^2 + b^2} - \frac{1}{4}}\right),$$

$$P_{23}(r) = \left(1 + \tfrac{1}{2}a - \frac{b}{\sqrt{a^2+b^2}}\sqrt{r^2 - \tfrac{1}{4}(a^2+b^2)}, \tfrac{1}{2}b + \frac{a}{\sqrt{a^2+b^2}}\sqrt{r^2 - \tfrac{1}{4}(a^2+b^2)}\right).$$

Let $(\xi_{ij}(r), \eta_{ij}(r))$ be the coordinate of $P_{ij}(r)$ with respect to the frame $((1,0), e_1', e_2')$, where $e_1' = (\cos\theta, \sin\theta)$ and $e_2' = (-\sin\theta, \cos\theta)$.

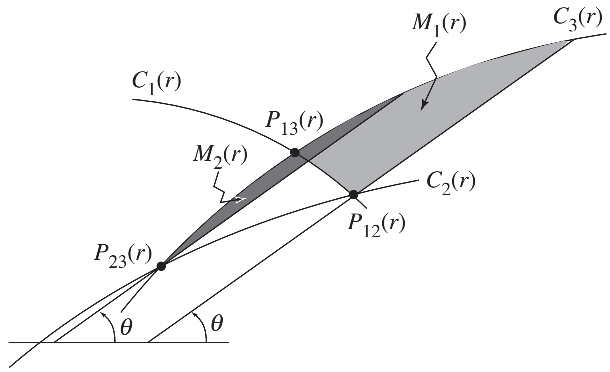

Figure 13. The regions $M_1(r)$ and $M_2(r)$.

Lemma 6.15. *There holds*

$$\begin{aligned}|NT_K^{(3)}(\mathrm{d}x, \mathrm{d}y)| &= \int_{1/2\sin\theta}^{\infty} \frac{1}{r^3} \cdot \sqrt{a^2+b^2}(\eta_{23}(r) - \eta_{12}(r))\,\mathrm{d}r + o\big(\sqrt{a^2+b^2}\,\big) \\ &= \left(\int_{1/2\sin\theta}^{\infty} \frac{\eta_{23}(r)-\eta_{12}(r)}{r^3}\,\mathrm{d}r\right)\frac{|\mathrm{d}x|\,|\mathrm{d}y|}{|x-y|^2} + o\left(\frac{|\mathrm{d}x|\,|\mathrm{d}y|}{|x-y|^2}\right).\end{aligned}$$

Proof. We first remark that $\mathcal{N}(r)$ is not empty if and only if $X_{12}(r) \geqslant X_{23}(r)$, which is equivalent to $1 - r\sin\theta \leqslant \frac{1}{2}$ when $a, b \ll 1$.

The second equality is a consequence of

$$\sqrt{a^2+b^2} = \frac{|\mathrm{d}x|\,|\mathrm{d}y|}{|x-y|^2}.$$

Let $\mathcal{P}(r) \subset \mathbb{R}^2$ be a subset which is swept by the arc in $C_2(r)$ between $P_{23}(r)$ and $P_{12}(r)$ when it moves parallel by $\sqrt{a^2+b^2}$ in the direction e_1'. Let $M_1(r)$ be a curved triangle bounded by $C_1(r)$, $C_3(r)$ and the half-line starting from $P_{12}(r)$ in the direction e_1', and let $M_2(r)$ be a subset bounded by $C_3(r)$ and the half-line starting from $P_{23}(r)$ in the direction e_1' as in Figure 13.

Then $\mathcal{N}(r) = (\mathcal{P}(r) \cup M_2(r)) \setminus M_1(r)$. We have only to show that

$$\int_{1/2\sin\theta}^{\infty} \frac{1}{r^3} \cdot \mathrm{area}(M_i(r))\,\mathrm{d}r = o\big(\sqrt{a^2+b^2}\,\big) \quad (i = 1, 2). \tag{6.1}$$

Since $\mathrm{area}(M_2(r)) \leqslant a^2 + b^2$, Equation (6.1) holds for $i = 2$. On the other hand,

$$\begin{aligned}\mathrm{area}(M_1(r)) &= \tfrac{1}{2}\sqrt{a^2+b^2}(\eta_{13}(r) - \eta_{12}(r)) + o\big(\sqrt{a^2+b^2}\,\big) \\ &= \tfrac{1}{2}\sqrt{a^2+b^2}\{\sin\theta\cdot(X_{12}(r) - X_{13}(r)) - \cos\theta\cdot(Y_{12}(r) - Y_{13}(r))\} \\ &\qquad + o\big(\sqrt{a^2+b^2}\,\big).\end{aligned}$$

Since

$$X_{12}(r) - X_{13}(r) = \sqrt{a^2+b^2}\left(-\tfrac{1}{2}\cos\theta + \sin\theta\sqrt{\frac{r^2}{(1+a)^2+b^2} - \frac{1}{4}}\right),$$

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we have

$$\begin{aligned}\int_{1/2\sin\theta}^{\infty} \frac{1}{r^3}\cdot\frac{1}{2}\sqrt{a^2+b^2}\cdot\sin\theta\cdot(X_{12}(r)-X_{13}(r))\,\mathrm{d}r \\ \leqslant \tfrac{1}{2}\sin\theta(a^2+b^2)\int_{1/2\sin\theta}^{\infty}\left(-\frac{\cos\theta}{2r^3}+\frac{\sin\theta}{r^2}\right)\mathrm{d}r \\ = O(a^2+b^2).\end{aligned}$$

On the other hand, since

$$\begin{aligned}Y_{13}(r)-Y_{12}(r) &= \tfrac{1}{2}b + a\sqrt{\frac{r^2}{(1+a)^2+b^2}-\frac{1}{4}}+\sqrt{\frac{r^2}{(1+a)^2+b^2}-\frac{1}{4}}-\sqrt{r^2-\tfrac{1}{4}} \\ &= \tfrac{1}{2}b + a\sqrt{\frac{r^2}{(1+a)^2+b^2}-\frac{1}{4}}-\frac{(2a+a^2+b^2)/((1+a)^2+b^2)r^2}{\sqrt{r^2-\frac{1}{4}}+\sqrt{r^2/((1+a)^2+b^2)-\frac{1}{4}}},\end{aligned}$$

we have

$$\begin{aligned}\int_{1/2\sin\theta}^{\infty}\frac{1}{r^3}\cdot\frac{1}{2}\sqrt{a^2+b^2}\cdot\cos\theta\cdot(Y_{13}(r)-Y_{12}(r))\,\mathrm{d}r \\ \leqslant \tfrac{1}{2}\cos\theta(a^2+b^2)\int_{1/2\sin\theta}^{\infty}\left(\frac{\sin\theta}{2r^3}+\frac{\cos\theta}{r^2}+\frac{\cos\theta}{r\sqrt{r^2-\frac{1}{4}}}\right)\mathrm{d}r + o\big(\sqrt{a^2+b^2}\,\big).\end{aligned}$$

As

$$\sqrt{r^2-\tfrac{1}{4}} \geqslant r\cos\theta \quad \text{when } r \geqslant 1/2\sin\theta,$$

the right-hand side satisfies

$$\leqslant \tfrac{1}{2}\cos\theta(a^2+b^2)\int_{1/2\sin\theta}^{\infty}\left(\frac{\sin\theta}{2r^3}+\frac{1+\cos\theta}{r^2}\right)\mathrm{d}r + o\big(\sqrt{a^2+b^2}\,\big) = O(a^2+b^2).$$

This completes the proof of Lemma 6.15. □

Proof of Proposition 6.13. Since

$$\begin{aligned}\eta_{23}(r)-\eta_{12}(r) &= \sin\theta(X_{12}(r)-X_{23}(r))-\cos\theta(Y_{12}(r)-Y_{23}(r)) \\ &= \sqrt{r^2-\tfrac{1}{4}(a^2+b^2)}-\tfrac{1}{2}\sin\theta-\cos\theta\sqrt{r^2-\tfrac{1}{4}},\end{aligned}$$

we have

$$\begin{aligned}\int_{1/2\sin\theta}^{\infty}&\frac{\eta_{23}(r)-\eta_{12}(r)}{r^3}\,\mathrm{d}r \\ &= \int_{1/2\sin\theta}^{\infty}\frac{1}{r^3}\left(r-\tfrac{1}{2}\sin\theta-\cos\theta\sqrt{r^2-\tfrac{1}{4}}\right)\mathrm{d}r + o\big(\sqrt{a^2+b^2}\,\big) \\ &= 2\int_0^{\sin\theta}(1-u\sin\theta-\cos\theta\sqrt{1-u^2})\,\mathrm{d}u + o\big(\sqrt{a^2+b^2}\,\big) \quad \left(u=\frac{1}{2r}\right) \\ &= \sin\theta-\theta\cos\theta+o\big(\sqrt{a^2+b^2}\,\big),\end{aligned}$$

which, combined with Lemma 6.15, completes the proof of Proposition 6.13. □

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Lemma 5.3 implies that the integrand $(\sin\theta - \theta\cos\theta)/|x-y|^2$ of the measure of acyclicity is 0 at the diagonal set. Therefore, the measure of acyclicity is finite for any knot of class C^4. Lemma 5.3 also implies that $E^{(2)}$, $E_{|\sin\theta|}$ and *mnts* are independent.

We remark that Claim 4.4 implies that the measure of acyclicity of K, and hence $mnts^{(4)}(K)$, is equal to 0 if and only if K is the standard circle.

7. Non-trivial zones

7.1. Non-trivial zones and their moduli

A circle is generically intersected by a sphere in zero or two points. It is a necessary and sufficient condition for a knot to be the circle. A curve which is not a circle should therefore admit spheres intersecting it transversally in at least four points. Thickening such a non-trivial sphere, we get a region bounded by two disjoint spheres which is crossed by at least four strands.

Definition 7.1.

(1) A *zone* Z is a region of S^3 or $\mathbb{R}^3$ diffeomorphic to $S^2 \times [0,1]$ bounded by two disjoint spheres.

(2) Let Z be a zone with $\partial Z = S_1 \cup S_2$ and $T : \mathbb{R}^3$ (or S^3) $\to \mathbb{R}^3$ (or $\mathbb{R}^3 \cup \{\infty\}$, respectively) be a conformal transformation which maps the two boundary spheres of Z into a concentric position (Figure 14). Then the *modulus* $\rho(Z) > 0$ of the zone Z is $\rho(Z) = |\log R_1/R_2|$, where R_1 and R_2 are the radii of the two concentric boundary spheres of $T(Z)$.

(3) Instead of using a particular conformal transformation T, one can use the *Lorentzian modulus* $\lambda(Z) = |L(S_1, S_2)|$ of a zone Z with $\partial Z = S_1 \cup S_2$, where S_1 and S_2 are considered* as points in Λ.

Remark 7.2. A zone Z is uniquely determined by its modulus up to a motion by a conformal transformation.

Remark 7.3. The modulus $\rho(Z)$ is an increasing function of the Lorentzian modulus $\lambda(Z)$ with

$$\rho = \log(\lambda + \sqrt{\lambda^2 - 1}) \quad \text{and} \quad \lambda = \cosh\rho. \tag{7.1}$$

In fact, one can assume, after a conformal transformation, that S_1 is an equator 2-sphere of S^3 and S_2 is a parallel 2-sphere to S_1. Then the Poncelet pencil in Λ generated by S_1 and S_2, which is a hyperbola in the 2-plane in $\mathbb{R}^5$ generated by S_1 and S_2, can be parametrized by $(\cosh t, \sinh t)$, where $t = 0$ corresponds to S_1. The restriction of L to this Poncelet pencil is a quadratic form of type $(1,1)$. Let t_0 be the parameter for S_2. Then $\rho(Z) = t_0$, whereas $\lambda(Z) = \cosh t_0$.

It can also be computed from the cross ratio of the four points intersections of the two spheres with a circle containing the two base points of the pencil generated by the two spheres.

* S_1 and $-S_2$ are endowed with the orientation as the boundary of Z.

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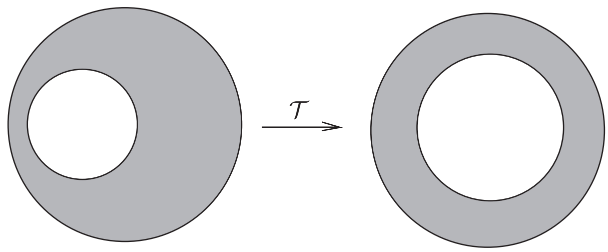

Figure 14. A zone and its concentric representative.

Remark 7.4. If the zones Z_1 and Z_2 satisfy $Z_1 \subset Z_2$, one has $\rho(Z_2) \geqslant \rho(Z_1)$.

Definition 7.5. Let K be a knot and Z a zone with $\partial Z = S_1 \cup S_2$.

(1) A *strand* is an arc of K that is contained in the zone Z and whose end points are on ∂Z. A *small strand* (*of* K *in* Z) is a closure of a connected component of the intersection of the interior of Z with K whose two end points lie on the same boundary sphere of Z. A *degenerate small strand* is a closed connected component of the intersection of K with ∂Z.

(2) A *cross-strand* is a strand of K with one end point contained in S_1 and another in S_2. A *minimal cross-strand* is a cross-strand whose intersection with the interior of Z is connected. If a cross-strand has a common end point with a small strand, one can connect them to obtain a longer cross-strand.

(3) A zone will be called *non-trivial* for a knot K if its intersection with K contains at least four closed cross-strands of the knot K with disjoint interiors (Figure 15).

The existence of spheres intersecting a curve in at least four points transversally implies the existence of non-trivial zones. In particular, such non-trivial zones exist for a non-trivial knot K.

Definition 7.6. The *modulus* ρ *of a knot* K is the supremum of the modulus of a non-trivial zone for K,

$$\rho = \sup_{A\text{: non-trivial zone}} \rho(A).$$

Definition 7.7. A non-trivial zone for a knot K is called *maximal* if it has the maximum modulus among the set of non-trivial zones for K.

Remark 7.8. There exists a maximal non-trivial zone for any non-trivial knot K since the set of pairs of boundary spheres of non-trivial zones is a non-empty compact subset of $\Lambda \times \Lambda$, as a 'small' sphere intersects the knot in at most two points.

Let us now look for properties of maximal non-trivial zones.

Proposition 7.9. *Let Z be a maximal non-trivial zone for K with $\partial Z = S_1 \cup S_2$. Applying a suitable conformal transformation, we can suppose that S_1 and S_2 are spheres of $\mathbb{R}^3$ centred at the origin. Then K is contained in Z.*

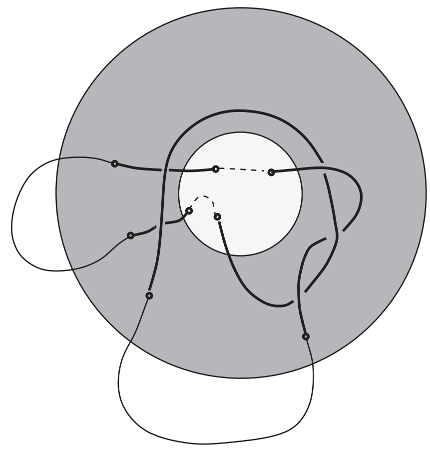

Figure 15. Non-trivial zone.

Proposition 7.10. *Under the same assumptions as above, we have the following.*

(1) $K \cap S_1$ *(or* $K \cap S_2$*) consists of two points where* K *is tangent to* S_1 *(or* S_2*, respectively).*

(2) *The two tangent points of* $K \cap S_1$ *(or* $K \cap S_2$*) are antipodal.*

Let us first prove Proposition 7.9.

Proof. The knot K is a finite union of open minimal cross-strands, $m_1, \ldots, m_n$, and arcs or points $c_1, \ldots, c_n$, $K = m_1 \cup c_1 \cup m_2 \cup c_2 \cup \cdots \cup m_n \cup c_n$ in cyclic order on K. Each arc c_i meets either S_1 or S_2, but cannot meet both.

Suppose that one of these arcs, say, c_1, meets S_1 and exits Z (Figure 16). At least two other points or arcs c_n and c_2 meet S_2. As $n \geqslant 4$, two different arcs, m_3 and m_n $(n \geqslant 4)$ exist. The difference $K \setminus (m_n \cup c_n \cup m_1 \cup c_1 \cup m_2 \cup c_2 \cup m_3)$ is a closed arc containing (at least) a point $A \in S_1$. Moving S_1 in the pencil of spheres tangent to S_1 at A, we can enlarge the zone Z keeping minimal strands containing m_1 and m_2. □

Corollary 7.11. *If a non-trivial zone* Z *with* $\partial Z = S_1 \cup S_2$ *is maximal, then the points* c_i *or both endpoints of the arcs* c_i *are alternatively contained in* S_1 *and in* S_2*. Therefore, at least two are contained in or touch each of spheres* S_1 *and* S_2

To prove Proposition 7.10, we will show that, if we can find on the sphere S_1 two points $x_1 \in c_i$, $x_3 \in c_j$ belonging to two different arcs $c_i \neq c_j$ which are not antipodal, or in the sphere S_2 two points $x_2 \in c_k$, $x_4 \in c_l$ belongings to two different arcs $c_k \neq c_l$ which are not antipodal, then the zone Z is not maximal. The numeration of the four points can be chosen such that they are in cyclic order on K.

7.2. The modulus of four points

For a moment, let us consider only the four points x_1, x_2, x_3, x_4 and forget the rest of the knot.

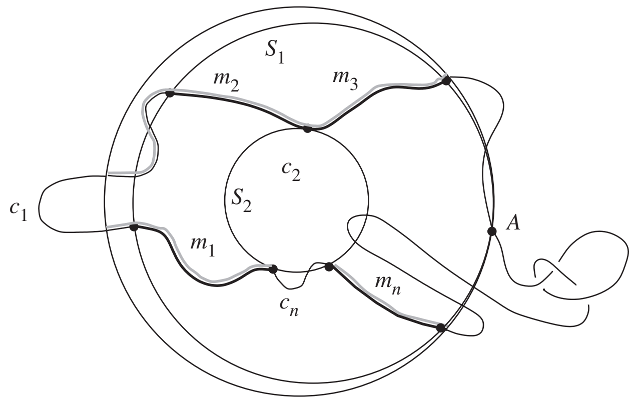

Figure 16. Increasing the modulus of the zone Z.

Definition 7.12. Let x_1, x_2, x_3 and x_4 be ordered four points in $\mathbb{R}^3$ (or S^3).

(1) A zone Z with $\partial Z = S_1 \cup S_2$ is called to be *separating* if x_1 and x_3 are contained in one of the connected component of $\mathbb{R}^3 \setminus \operatorname{Int} Z$ (or $S^3 \setminus \operatorname{Int} Z$) and x_2 and x_4 in the other component.

(2) The *maximal modulus* $\rho(x_1, x_2, x_3, x_4)$ *of the ordered four points* (x_1, x_2, x_3, x_4) is the supremum of the moduli $\rho(Z)$ of separating zones Z with $\partial Z = S_1 \cup S_2$ (when $S_1 = S_2$, $\rho = 0$).

(3) A separating zone that attains the maximal modulus will be called the *maximal separating zone of the four point*.

(4) We can also consider $L(S_1, S_2)$, where $\partial Z = S_1 \cup S_2$, and define $\mu_{\mathrm{L}}(x_1, x_2, x_3, x_4)$ to be the value of $L(S_1, S_2)$ for a maximal separating zone (when $S_1 = S_2$, $\mu_{\mathrm{L}} = 1$).

We remark that if Z is a maximal separating zone of the four points, then one of its boundary sphere should contain both x_1 and x_3, and the other x_2 and x_4 (Figure 17).

Lemma 7.13.

(1) *There is no separating zone, i.e.* $\rho = 0$*;* $\mu_{\mathrm{L}} = 1$ *if and only if the* x_i *are concircular in such a way that* x_1 *and* x_3 *are not adjacent, i.e. when the cross-ratio* $(x_2, x_3; x_1, x_4)$ *is a real number between* 0 *and* 1*.*

(2) *Let* Z *be a maximal separating zone for* (x_1, x_2, x_3, x_4) *with* $\partial Z = S_1 \cup S_2$*. Suppose we transform the picture by a conformal map so that the images of* S_1 *and* S_2 *are concentric. Then, in the new picture,* x_1 *and* x_3 *are antipodal in one of the boundary spheres of* Z*, and* x_2 *and* x_4 *are antipodal in the other boundary sphere.*

(3) *When separating zones exist, the maximal separating zone* Z *is unique.*

Remark 7.14. The condition of being antipodal does not seem to be conformally invariant.

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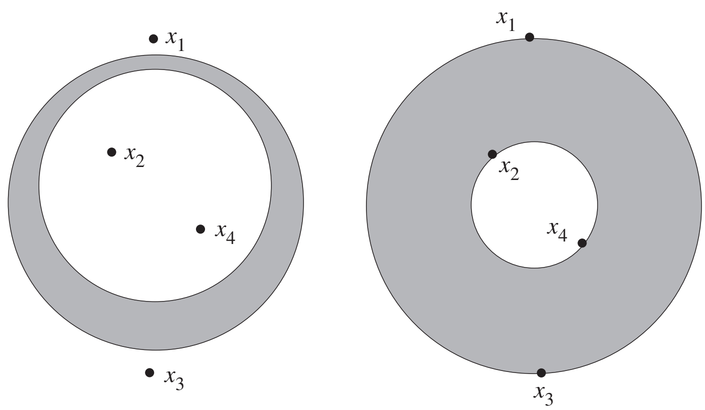

Figure 17. Maximal modulus for four points.

The condition can be rephrased as follows. The two points x_1 and x_3 have to belong to a circle containing the two limit points of the pencil generated by the two boundary spheres of the zone; the two points x_2 and x_4 satisfy a similar condition (the circle containing x_2 and x_4 belong to the same pencil as the circle containing x_1 and x_3). The conformal transformation such that the images of S_1 and S_2 are concentric has to send the limit points of the pencil generated by the two boundary spheres of the zone to 0 and ∞; circles through the limit points become lines through the origin.

Remark 7.15. The proof of statement (3) will be given in the appendix.

Remark 7.16. Statements (2) and (3) of the lemma also hold when the four points are concircular and (x_1, x_3) are consecutive (and also (x_2, x_4)).

The proof is the consequence of the following sublemma.*

Sublemma 7.17. *Let $\mathcal{P}$ be a Poncelet pencil of spheres; it is the intersection of Λ with a plane P. Let $\mathcal{B}$ be the two-dimensional linear family of spheres $\mathcal{B} = B \cap \Lambda$, where $B = P^\perp$. At a point $\sigma \in \mathcal{P}$, the 3-plane orthogonal to $\mathcal{P}$ is generated by the vectors tangent at σ to the pencils of spheres with base circle a circle of the form $(\sigma^\perp \cap S_\infty) \cap (b^\perp \cap S_\infty)$ $(b \in \mathcal{B})$.*

Proof of Sublemma 7.17. The intersection $\mathcal{B} = B \cap \Lambda$ is the set of spheres containing the two limit points of the Poncelet pencil $\mathcal{P}$. Let $F = B \oplus \mathbb{R} \cdot \sigma$. The tangent vectors to $F \cap \Lambda$ are in $F \cap T_\sigma \Lambda = F \cap \sigma^\perp = B$. Therefore, the tangent space at σ to $F \cap \Lambda$ is an affine 3-space parallel to B. Hence it is orthogonal to $\mathcal{P}$.

The tangent at σ to $\mathcal{P}$ is time-like. The vector space generated by σ and a point $b \in \mathcal{B}$ is space-like. It intersects Λ in a closed geodesic. The tangent line at σ to this geodesic is parallel to b. This closed geodesic is a pencil of spheres with base circle $(\sigma^\perp \cap S^3_\infty) \cap (b^\perp \cap S^3_\infty)$ (see Figure 18). □

* We state other proofs in § 8.1.

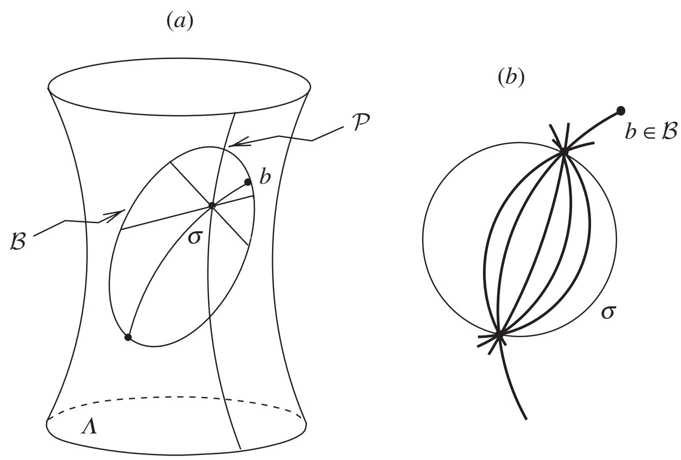

Figure 18. The 3-plane in $T_\sigma\Lambda$ orthogonal at σ to $T_\sigma\mathcal{P}$.

Proof of Lemma 7.13. The last sublemma implies the lemma, since, if two points contained in S_1 are not antipodal, there exists a non-geodesic circle γ containing them.

Let us call $\mathcal{B}_\gamma$ the pencil with base circle γ. Consider the Poncelet pencil $\mathcal{P}$ generated by S_1 and S_2. The Lorentz modulus λ of the region bounded by the disjoint spheres S_2 and $\sigma \in \mathcal{P}$ is just $|L(S_2, \sigma)|$. Let us call this function $\varphi(\sigma)$. The connected component of its level hypersurface through S_1 is therefore the hypersurface of equation $L(S_2, \tau) = L(S_2, S_1)$. Its (affine) tangent plane at S_1 has the equation $L(S_2, v - S_1) = 0$. The set of tangent vectors to this level hypersurface is $B = P^\perp$ (where P is the plane such that $\mathcal{P} = P \cap \Lambda$).

Before finishing the proof, we transform the picture by a conformal map sending the limit points of $\mathcal{P}$ to 0 and ∞. Therefore, the spheres S_1 and S_2 are concentric.

Spheres $b \in \mathcal{B}$ (notation of the sublemma) appear as planes through the origin. Therefore, the base circle of the pencil generated by S_1 and b is a geodesic circle on S_1.

To say that a vector $w \in T_{S_1}\Lambda$ is not orthogonal to $\mathcal{P}$ is equivalent to saying that the vector w is tangent at S_1 to a pencil with base circle which is not a geodesic circle of S_1.

Therefore, for w a vector tangent to $\mathcal{B}_\gamma$ at S_1, we have $L(S_2, w) \neq 0$. This implies that the derivative of the Lorentzian modulus λ of the region between S_2 and a sphere $\tau \in \mathcal{B}$ is not zero in S_1, allowing to increase the modulus of the zone keeping the four points x_1, x_2, x_3 and x_4 in the boundary spheres.

What we did for the Lorentzian modulus λ is enough to prove the same result for the modulus ρ, as the correspondence between λ and ρ is a diffeomorphism (see formula (7.1)). □

7.3. Knots of small moduli

The goal of this section is to prove the following result.

Theorem 7.18. *There exists a constant $a > 0$ such that, if a knot K is a non-trivial knot, then its modulus is larger than a.*

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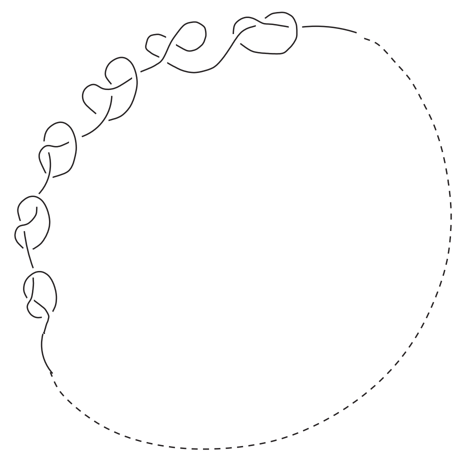

Figure 19. Knitted curve.

Let us start with a curve K of modulus ρ. Let us consider a stereographic projection to $\mathbb{R}^3$ such that the two boundary spheres of a maximal zone Z are concentric, with centre the origin. We may imagine a very thin knitted curve (Figure 19) contained in a zone of small modulus. In order to prove that the knot is trivial, we need to use the condition that the maximal modulus is very small to control the knot at all scales.

We remark that the modulus $\rho(K)$ of a knot K is larger than the maximal modulus $\mu(x_1, x_2, x_3, x_4)$ for any four points on the knot chosen in that cyclic order, since any separating zone of (x_1, x_2, x_3, x_4) is a non-trivial zone for K.

Fixing three points x_1, x_2, x_3 defines a function μ_{x_1,x_2,x_3} by $\mu_{x_1,x_2,x_3}(x) = \mu(x_1, x_2, x_3, x)$. It is a continuous function, the zero level of which is the arc γ of the circle trough (x_1, x_2, x_3) which does not contain the point x_2. Moreover, given a small value ε of μ_{x_1,x_2,x_3}, if the sphere S^2 is endowed with a metric such that the length of the circle through x_1, x_2, x_3 is of the order of 1, then the distance from the level $\mu_{x_1,x_2,x_3} = \varepsilon$ to the circle γ satisfies

$$a \cdot \operatorname{length}(\gamma) < d(x, \gamma) < A \cdot \operatorname{length}(\gamma) \quad \forall x \in \{\mu_{x_1,x_2,x_3} = \varepsilon\}.$$

Let us now suppose that the curve K has a small modulus, say, less than $\frac{1}{10\,000}$, and chose a stereographic projection of S^3 on $\mathbb{R}^3$ such that the two boundary spheres S_1 and S_2 of a maximal zone Z for K are concentric with centre the origin (the north pole of the projection is one of the limit points of the pencil generated by S_1 and S_2, the tangency point of S^3 and $\mathbb{R}^3$,which we chose as origin of $\mathbb{R}^3$, is the other limit point). Finally, compose the stereographic projection with a homothety to transform the inner sphere into the unit sphere centred at the origin.

Lemma 7.19. *The knot K is contained in a thin tubular neighbourhood of a geodesic circle of the middle sphere S_m (defined by the intersection of the ray containing $\frac{1}{2}(\sigma_1+\sigma_2)$ and Λ, where σ_1 and σ_2 are the points in Λ corresponding to the spheres S_1 and S_2) of the zone Z.*

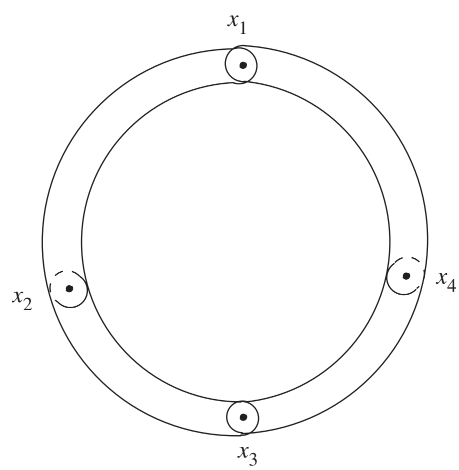

Figure 20. The knot is trapped in a neighbourhood of a circle.

Proof. We know that the knot K is tangent to S_1 in two antipodal points, they will be x_1 and x_3. We chose x_2 on the intersection of the knot with the 'equatorial' plane associated to the north and south poles x_1 and x_3. This defines a strand γ_1, with end points x_1 and x_3, containing x_2, of K. The strand of K joining x_3 to x_1 which does not contain x_2, that we will call γ_2, have to stay in a neighbourhood of the arc with end points x_1 and x_3, of the circle defined by the three points x_1, x_2, x_3 which does not contain x_2. Let x_4 be a point of the intersection of γ_2 with the equatorial plane previously defined. Using now the circle through x_1, x_2, x_4, we deduce that the strand γ_1 is contained in a neighbourhood of the arc with end points x_1 and x_2 of the circle determined by x_1, x_2, x_4 which does not contain x_4.

As the two circles containing x_1, x_2, x_3 and containing x_1, x_2, x_4 are close to each other, and close to a great circle Γ_1 of the sphere S_m, this completes the proof (Figure 20). □

Consider now the tube of radius δ_1 around Γ_1 containing K, and geodesic discs $D_1^1, \ldots, D_{n_1}^1$ of this tube, normal to Γ_1 through equidistant point of Γ_1, say, such that the length of those arcs is roughly 100 times the diameter δ_1 of the tube (Figure 21). Choose a point x_i^2 of K in each disc D_i^1. Joining consecutive (for the cyclic order) points x_i^2 and x_{i+1}^2 by a small arc of the circle defined by the two consecutive points x_i^2 and x_{i+1}^2 and one of the almost antipodal points to x_i^2, x_I^2, that we will call γ_i^2, we get an unknotted polygon Γ_2 with all the angles almost flat (the tangent of those angle is at most, say, $\varphi_2 < 1.5 \cdot \arctan(\frac{1}{100}) < \frac{3}{100}$).

Using the same idea as for the proof of the Lemma 7.19, we deduce that the 'small' arc of the knot joining x_i^2 to x_{i+1}^2 has to stay in a neighbourhood of the small arc of the circle γ_i^2 of 'diameter' of the order of $\delta_1 \cdot$ (length of γ_i^2).

The knot is now confined in a thin neighbourhood of Γ_2. Let us call δ_2 the diameter of this tube, which is also of the order of $\delta_1 \cdot$ (length of γ_i^2). Consider now in the tube a sequence of consecutive normal geodesic discs $D_1^2 \cdots D_{n_2}^2$ of radius $2 \cdot \delta_2$. We choose them to be a distance of roughly $100 \cdot \delta_2$. We can define them with no ambiguity, except

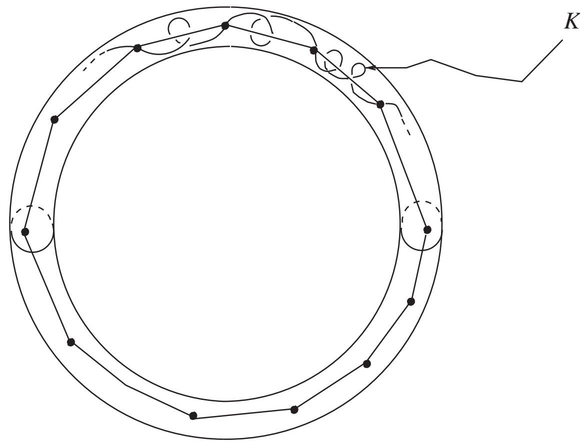

Figure 21. The first polygonal approximation.

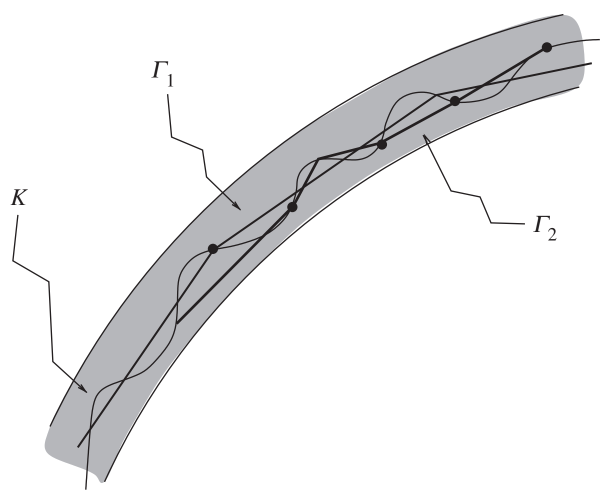

Figure 22. The second polygon Γ_2 inscribed in K.

in a neighbourhood of the vertices of Γ_2. The choice of the discs near the vertices of Γ_2 has to be made with more care: they should be roughly at a distance of $50\delta_2$ from the vertices of Γ_2. Again, we chose a point x_i^3 in each normal disc D_i^2. In this way, we get a new unknotted polygon Γ_3. The knot K is now contained in a thin tubular neighbourhood of Γ_3. The diameters δ_i of the successive tubes are related to the of one order of magnitude thinner.

The only obstruction left to proceed with inductive construction of unknotted polygons inscribed in K is the angles of the polygons. We need to guarantee they stay flat enough. The angles θ_i^2 of Γ_2 are bounded by φ_2 (see Figure 22).

That is also true for the angles at all the vertices of the successive polygons except for the ones which are adjacent to some vertex of the previous polygon. *A priori*, the angle cannot grow more than linearly with the index of the polygon. In fact, $8 \cdot \varphi_2$ bounds all the angles of all the Γ_k. If the angle θ at a vertex of Γ_{k-1} is larger than $5 \cdot \varphi_2$, then our construction will replace it by two angles of Γ_k smaller than $\frac{1}{2}\theta + 3\varphi_2$, therefore never reaching $8 \cdot \varphi_2$.

Getting to a polygon Γ_k such that the diameter δ_k of its tubular neighbourhood containing the knot K is smaller than $\frac{1}{3} \cdot \Delta(K)$, where $\Delta(K)$ is the global radius of curvature defined by Gonzalez and Maddocks [**13**] (see § 8.3), we prove that the knot K is trivial. This ends the proof of the Theorem 7.18.

Remark 7.20. Freedman and He [**10**] give a definition of the modulus of a solid torus using the degree of maps from the solid torus $\boldsymbol{T}$ to the circle $\mathbb{R}/\mathbb{Z}$. From our viewpoint (topology implies a jump of some geometrical invariant), it has the defect of being very small when the solid torus is very long and very thin.

But, in the same article, Freedman and He define a dual notion which is bounded below by a positive power of the average crossing number of knot type of $\boldsymbol{T}$. It would be very interesting to understand possible relations between this modulus (which they denote by $m^*(\boldsymbol{T})$) and our modulus of a knot, for example, via a 'thickest' tubular neighbourhood of a representative of a knot in its isotopy class.

7.4. Jump of the measure of acyclicity for non-trivial knots

Given the curve K, the spheres contained in a non-trivial zone Z intersect K in at least four points. The region R_Z in Λ corresponding to the spheres contained in the annulus A is bounded by two light cones (half-light cones to be precise) with vertices the boundary spheres S_1 and S_2 of Z. The volume of R_Z is a monotonous function of the modulus of Z. Therefore, the existence of a strictly larger than 0 lower bound for the moduli of maximal non-trivial zones of non-trivial knots implies the existence of a strictly positive constant $c > 0$ such that, for any non-trivial knot, the measure $mnts_1(C)$ of the set of non-trivial spheres is larger or equal to c.

The modulus and the measure of acyclicity probably do not behave the same way for connected sums of knots. Let $\rho([K])$ (or $mnts([K])$) denote the infimum of the modulus (or the measure of acyclicity respectively) of a knot that belongs to an isotopy class $[K]$.

Question 7.21. *Is it true that*

$$\rho([K_1 \sharp K_2]) = \max\{\rho([K_1]), \rho([K_2])\}?$$

Question 7.22. *Is it true that*

$$mnts([K_1 \sharp K_2]) = mnts([K_1]) + mnts([K_2])?$$

Question 7.23. *Do the modulus and the measure of acyclicity take their minimum values for non-trivial knots at a* $(2, 3)$*-torus knot on a torus of revolution?*

7.5. Explosion of the measure of acyclicity for singular knots

Theorem 7.24. *The measure of acyclicity is an energy functional for knots.*

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Proof. Fix δ $(0<\delta\leqslant\frac{1}{2})$. For $0<d\leqslant\delta$, put

$$\mathcal{K}(d)=\mathcal{K}_\delta(d)$$
$$=\left\{K: \text{a knot with length } l(K)\;\middle|\;\begin{array}{l}\exists x,y\in K \text{ such that (i) the shorter}\\ \text{arc-length between } x \text{ and } y \text{ is } \delta l(K),\\ \text{and (ii) } |x-y|\leqslant \mathrm{d}l(K)\end{array}\right\}.$$

and

$$\rho(d)=\inf_{K\in\mathcal{K}(d)}\{mnts(K)\}.$$

We remark that ρ is a monotone decreasing function of d because $d_1<d_2$ implies $\mathcal{K}(d_1)\subset\mathcal{K}(d_2)$, and that $\rho(d)=0$ for $d\geqslant(\sin\pi\delta)/\pi$ because $\mathcal{K}(d)$ contains the standard circle.

Assume that there is a positive constant M' such that

$$\sup_{d>0}\rho(d)=\lim_{d\to+0}\rho(d)=M'.$$

There is a positive constant $M=M(M')$ such that, if the measure of acyclicity of K is smaller than $1.1M'$, then the ratio of the radii of the two spheres of any concentric non-trivial zone for K is smaller than M.

Let K_d be a knot with length 1 in $\mathcal{K}(d)$ whose measure of acyclicity is smaller than $1.1M'$. Let x, y be a pair of points on K_d such that the shorter arc-length between them is δ and that $d_0=|x-y|\leqslant d$.* The knot K is divided into two arcs, A_1 and A_2, by x and y. Put

$$a=\min\Big\{\sup_{z\in A_1}|z-\tfrac{1}{2}(x+y)|,\ \sup_{w\in A_2}|w-\tfrac{1}{2}(x+y)|\Big\}.$$

Let Σ_r denote the 2-sphere with centre $\frac{1}{2}(x+y)$ and radius r. Since $(\Sigma_a,\Sigma_{d_0/2})$ forms a non-trivial zone, $a\leqslant\frac{1}{2}Md_0$, and hence $a\leqslant\frac{1}{2}Md$. Let $\bar{K}_d$ be the part of K_d which is contained in $\Sigma_{Md/2}$. The length $l(\bar{K}_d)$ of $\bar{K}_d$ is greater than or equal to δ since $\Sigma_{Md/2}$ contains at least one of the arcs A_1 and A_2. Then, by Poincaré's formula (see [**30**, p. 259; see also pp. 111, 277]), there holds

$$\int_G \#(g(\Sigma_r)\cap\bar{K}_d)\,\mathrm{d}g=\frac{O_3O_2O_1\cdot O_0}{O_2O_1}\cdot\operatorname{area}(\Sigma_r)\cdot l(\bar{K}_d),$$

where O_n denotes the volume of the n-dimensional unit sphere, G denotes the group of the orientation-preserving motions of $\mathbb{R}^3$, which is isomorphic to the semidirect product of $\mathbb{R}^3$ and $SO(3)$, and $\mathrm{d}g$ denotes the kinematic density (see [**30**, p. 256]). We have $\mathrm{d}g=\mathrm{d}P\wedge\mathrm{d}K_{[P]}$, where $P\in\mathbb{R}^3$, $\mathrm{d}P$ is the volume element of $\mathbb{R}^3$ and $\mathrm{d}K_{[P]}$ is the kinematic density of the group of special rotations around P, which is isomorphic to $SO(3)$. Since

$$\int \mathrm{d}K_{[P]}=O_2O_1,$$

* We use the axiom of choice here.

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Poincaré's formula implies

$$\int_{\Sigma_r(X,Y,Z)\cap K_d\neq\phi} \#(\Sigma_r(X,Y,Z)\cap K_d)\,\mathrm{d}X\,\mathrm{d}Y\,\mathrm{d}Z = 2\pi r^2 l(\bar{K}_d),$$

where $\Sigma_r(X,Y,Z)$ denotes the sphere with radius r and centre (X,Y,Z). Suppose $\frac{1}{2}d \leqslant r \leqslant \frac{1}{2}Md$. Put $n = \frac{1}{2}\#(\Sigma_r(X,Y,Z)\cap K_d)$. Then the measure of acyclicity of K_d satisfies

$$\begin{aligned} mnts(K_d) &= \int_{NT(K_d)} \binom{n}{2} \cdot \frac{1}{r^4}\,\mathrm{d}X\,\mathrm{d}Y\,\mathrm{d}Z\,\mathrm{d}r \\ &\geqslant \int_{d/2}^{Md/2} \frac{1}{r^4}\left\{\int_{D_R^3(c)} (\tfrac{1}{2}\#(\Sigma_r(X,Y,Z)\cap \bar{K}_d) - 1)\,\mathrm{d}X\,\mathrm{d}Y\,\mathrm{d}Z\right\}\mathrm{d}r, \end{aligned}$$

where $D_R^3(c)$ denotes the 3-ball with centre $c = \frac{1}{2}(x+y)$ and radius $R = \frac{1}{2}(Md) + r$. Thus

$$\begin{aligned} mnts(K_d) &\geqslant \frac{1}{2}\int_{d/2}^{Md/2} \frac{1}{r^4}\{2\pi r^2 l(\bar{K}_d) - \tfrac{4}{3}\pi(\tfrac{1}{2}Md + r)^3\}\,\mathrm{d}r \\ &\geqslant \frac{1}{2}\left\{2\pi\delta\left[-\frac{1}{r}\right]_{d/2}^{Md/2} - \tfrac{4}{3}\pi(Md)^3\left[-\frac{1}{3r^3}\right]_{d/2}^{Md/2}\right\}, \end{aligned}$$

which blows up as d goes down to 0, which contradicts the assumption that

$$\lim_{d\to+0}\rho(d) \leqslant M < \infty.$$

□

8. Appendix

8.1. The maximal modulus and cross-ratio of four points

In this subsection we give a formula to express the maximal Lorentzian modulus $\mu_{\mathrm{L}}(x^1, x^2, x^3, x^4)$ of the four points in terms of the cross-ratio $(x^2, x^3; x^1, x^4)$. It implies that the integrand of $E^{(2)}$ is equal to the *infinitesimal maximal modulus*

$$\mu_{\mathrm{L}}(x, x+\mathrm{d}x, y, y+\mathrm{d}y).$$

But we start with an alternative proof of Lemma 7.13 by showing it in lower dimension by one. The terms in the following lemma can be defined in a parallel way.

Lemma 8.1. *Let x_1, x_2, x_3 and x_4 be ordered four points on S^2. Suppose the cross-ratio $(x_2, x_3; x_1, x_4)$ is not a real number between 0 and 1.*

Then the following hold.

(1) *The maximal modulus of a separating annulus is attained by a separating annulus, which will be called a maximal separating annulus. Then the pair x_1, x_3 (or x_2, x_4) is on a circle of the pencil whose base points are the limit points of the pencil defined by the boundary circles of the maximal separating annulus.*

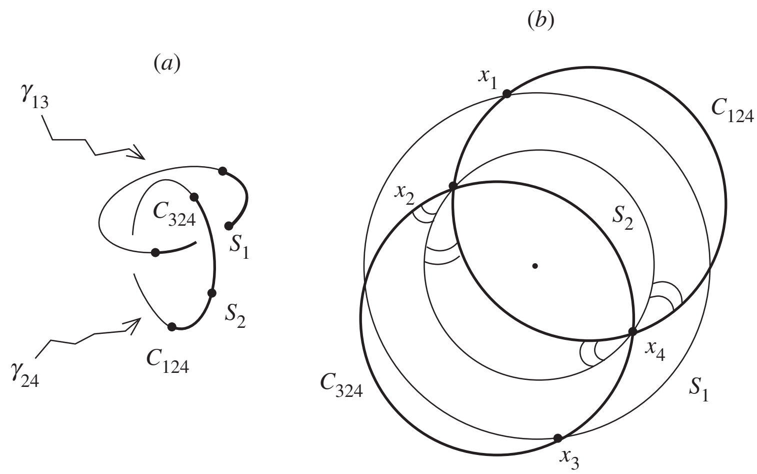

Figure 23. Characterization of the boundary circles of a maximal separating annulus ((*a*) in $\mathbb{P}\Lambda$).

(2) *There is exactly one maximal separating annulus. The position of the boundary circles of the annulus is explicitly determined in function of the four points.*

Proof. (1) First observe that the two boundary circles C_1 and C_2 of a separating annulus with the maximal modulus should contain, one x_1 and x_3, the other x_2 and x_4. The idea of the proof is the same as that of the proof of Lemma 7.13. Suppose these points were not on a circle Γ through the limit points generated by the two boundary circles. Then, for $x_1 \in C_1$ and $x_3 \in C_1$, rotation from C_1 in the pencil of base points x_1 and x_3 will define a curve in the quadric Λ of circles in S^2 which is transverse at C_1 to the level surface $\{C \in \Lambda \mid L(C_2, C) = L(C_2, C_1)\}$ of L. Therefore, this curve is transverse to the level surface defined by $m(C_2, C) = m(C_2, C_1)$, where $m(C, C')$ denotes the modulus of an annulus bounded by C and C'. It contradicts the fact that a maximum is a critical point.

(2) Let $\mathbb{P}\Lambda$ be the set of non-oriented spheres $\mathbb{P}\Lambda = \Lambda / \pm 1$. The pencils of circles through x_1, x_3 and through x_2, x_4 can be seen as two circles γ_{13} and γ_{24} in $\mathbb{P}\Lambda$. Consider the four circles determined by three of the four points x_1, x_2, x_3, x_4. Two of them bound on γ_{13} an open segment which is the set of circles contained in the pencil γ_{13} separating (in S^2) x_1, x_3 from x_2, x_4. We have a similar situation on the pencil γ_{24}.

Let us prove that the boundary circles of a maximal annulus are the middle points (for the arc-length in $\mathbb{P}\Lambda$) of the segments we just defined. This proves the uniqueness of the maximal separating annulus.

The arc-length on a pencil in $\mathbb{P}\Lambda$ is just the angle through a base point of the pencil.

In Figure 23 we have represented the pencil γ_{24}, the circles C_{124} through x_1, x_2, x_4 and C_{324} through x_3, x_2, x_4, and the circles S_1 and S_2, boundary of a maximal separating annulus.

The angles between C_{124} and S_2 and the angle between C_{324} and S_2 are equal, since the figure is symmetric with respect to the origin and since angles on two sides of a point of intersection of two circles are equal. That completes the proof. □

Lemma 8.2. *Let C_1 and C_2 be a pair of concentric circles on $\mathbb{R}^2 \subset \mathbb{R}^3$. Then, among the zones Z with $\partial Z = S_1 \cup S_2$ satisfying $(S_1 \cup S_2) \cap \mathbb{R}^2 = C_1 \cup C_2$, the maximal modulus is attained by the unique zone which has concentric boundary spheres whose centre is in the plane $\mathbb{R}^2$; these spheres are therefore orthogonal to the plane $\mathbb{R}^2$.*

Proof. Just notice that, when we presented (in Lemma 7.13) a maximal non-trivial zone using two concentric spheres, the four pairwise antipodal points x_1, x_3 and x_2, x_4 belong to the same plane, which is orthogonal to the two concentric spheres. □

Corollary 8.3. *Let x_1, x_2, x_3 and x_4 be ordered four points in $\mathbb{R}^3$ or S^3, and let Σ be a 2-sphere passing through them. Then the maximal modulus $\mu(x_1, x_2, x_3, x_4)$ of the four points is equal to the maximal modulus of a separating annulus in Σ.*

Claim 8.4. *The maximal Lorentzian modulus $\mu_{\mathrm{L}}(x^1, x^2, x^3, x^4)$ is expressed in terms of the cross-ratio $\mathrm{cr} = (x^2, x^3; x^1, x^4)$ as*

$$\mu_{\mathrm{L}}(x^1, x^2, x^3, x^4) = \sqrt{1 + 2|1 - \mathrm{cr}\,|^2 \left\{ \left| \frac{\mathrm{cr}}{1 - \mathrm{cr}} \right| - \mathrm{Re}\left(\frac{\mathrm{cr}}{1 - \mathrm{cr}} \right) \right\}}.$$

Remark 8.5. Lemma 7.13 implies the above claim as follows. The boundary spheres of the maximal separating zone can be mapped into a concentric position by a conformal transformation. Then Lemma 7.13 asserts that x_1 and x_3 are antipodal in one of the boundary spheres, and x_2 and x_4 are antipodal in another. We can assume, without loss of generality, that $x_1, x_3 = \pm 1$ and $x_2, x_4 = \pm z$ in $\mathbb{C} \subset \mathbb{R}^3$, and the boundary spheres of the maximal separating zone are concentric spheres with centre the origin and radii 1 and $|z|$. Then the maximal Lorentzian modulus $\mu_{\mathrm{L}}(x^1, x^2, x^3, x^4)$ is given by $\frac{1}{2}(|z| + 1/|z|)$ and the cross-ratio $\mathrm{cr} = (x^2, x^3; x^1, x^4)$ is given by $-(z-1)^2/(4z)$, and therefore $\mathrm{cr}/(1 - \mathrm{cr}) = (z-1)^2/(z+1)^2$. One can verify the equality by the direct calculation.

Lemma 8.6. *Let Π be a plane and Σ be a 2-sphere in $\mathbb{R}^3$ such that the minimum and maximum distance between Π and Σ are a and b $(0 < a < b)$, respectively. Then the modulus $\rho(\Sigma, \Pi)$ of the zone bounded by Σ and Π is given by*

$$\rho(\Sigma, \Pi) = \log\left(\frac{\sqrt{b} + \sqrt{a}}{\sqrt{b} - \sqrt{a}} \right).$$

Proof. We may assume that Π is the y-z plane and Σ has $(\frac{1}{2}(a+b), 0, 0)$ as its centre. Then any inversion with respect to a 2-sphere with centre $(\pm\sqrt{ab}, 0, 0)$ maps Σ and Π to a concentric position. □

This lemma immediately implies the following lemma.

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Lemma 8.7. *Let Σ be a 2-sphere in $\mathbb{R}^3$ with centre O, and $A \in \mathbb{R}^3$ be a point outside Σ. Then, among planes P passing through A, the plane P_0 perpendicular to the line OA gives the maximal modulus $\rho(\Sigma, P)$.*

Let T_0 be an inversion with respect to a 2-sphere whose centre lies on the line OA that maps Σ and P_0 to a concentric position as is given in the proof of the previous lemma. Then $T_0(A)$ and $T_0(\infty)$ are antipodal in $T_0(P_0)$. Therefore, this lemma gives an alternative computational proof of Lemma 7.13.

Lemma 8.8. *Let C be a circle with centre O in a plane Π, and $A \in \Pi$ be a point outside C. Then, among pairs of a sphere Σ passing through C and a plane P passing through A, the pair of the sphere Σ_0 whose centre belongs to Π and the plane P_0 perpendicular to the line OA gives the maximal modulus.*

Proof. Let r be the radius of C and $a = |O - A|$. Let $\Sigma(h)$ denote the 2-sphere whose centre is apart from Π by h ($h \geqslant 0$). Then the preceding two lemmas imply that the maximum of the modulus $\rho(\Sigma(h), P)$ with $P \ni A$ is given by

$$\log\left(\sqrt{1 + \frac{a^2 - r^2}{r^2 + h^2}} + \sqrt{\frac{a^2 - r^2}{r^2 + h^2}}\right),$$

which is a decreasing function of h. $\square$

Proof of Claim 8.4. Without loss of generality, we can assume that $x^1 = \infty$, $x^2 = 0$, $x^3 = 1$ and $x^4 = z = u + \mathrm{i}v$ in $\mathbb{C} \cup \{\infty\} \cong \mathbb{R}^2 \cup \{\infty\} \subset \mathbb{R}^3 \cup \{\infty\}$. Then the cross-ratio $\mathrm{cr} = (0, 1; \infty, z) = 1 - 1/z$, hence $\mathrm{cr}/(1 - \mathrm{cr}) = z - 1$. We assume that $z \notin \{z \in \mathbb{R} \mid z > 1\}$, otherwise both sides of the formula coincide with 1. The previous lemma implies that the maximal modulus $\mu_{\mathrm{L}}(\infty, 0, 1, z)$ is attained by a zone $Z(\xi)$ bounded by $S_1(\xi)$ and $S_2(\xi)$ for some $\xi \in \mathbb{R}$, where $S_2(\xi)$ has centre

$$O(\xi) = \left(\tfrac{1}{2}u - \frac{v}{\sqrt{u^2 + v^2}}\xi, \tfrac{1}{2}v + \frac{u}{\sqrt{u^2 + v^2}}\xi\right) \in \mathbb{R}^2$$

and $S_1(\xi)$ is a plane perpendicular to the line joining $O(\xi)$ and 1. Then $\rho(S_1(\xi), S_2(\xi))$ is given by

$$\rho(Z(\xi)) = \log\left(\frac{\sqrt{1 - u + \frac{1}{4}(u^2 + v^2) + (2v/\sqrt{u^2 + v^2})\xi + \xi^2} + \sqrt{1 - u + (2v/\sqrt{u^2 + v^2})\xi}}{\sqrt{\frac{1}{4}(u^2 + v^2) + \xi^2}}\right),$$

which takes the maximum value

$$\tfrac{1}{2}\log\left(1 + \frac{2\{\sqrt{(u-1)^2 + v^2} - (u - 1)\}}{u^2 + v^2}\right).$$

$\square$

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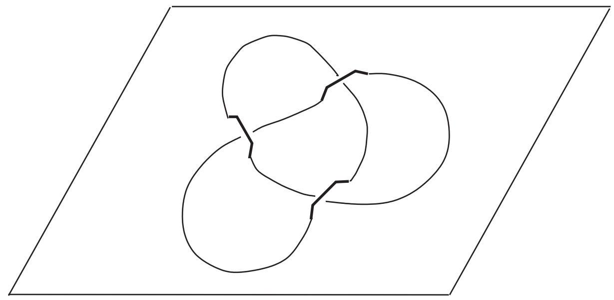

Figure 24. A knot in 'thin position'.

As a corollary of Claim 8.4, we have the following result.

Corollary 8.9. *The integrand* $|\Omega_{\mathrm{CR}}| - \mathrm{Re}\,\Omega_{\mathrm{CR}}$ *of* $E^{(2)}(K)$ *can be interpreted as the maximal Lorentzian modulus* $\mu_{\mathrm{L}}(x, x{+}\mathrm{d}x, y, y{+}\mathrm{d}y){-}1$ *of a pair of infinitesimal segments.*

8.2. The circular Gauss map and the inverted open knots

Let $C(y, y, x)$ be as in Definition 3.3 and $v_y(x)$ be as in § 5.1. We remark, that when y approaches x, then $C(y, y, x)$ approaches the *osculating circle* at x, which will be denoted by $C(x, x, x)$, and $v_y(x)$ approaches the tangent vector at x, which will be denoted by $v_x(x)$.

Definition 8.10. The *circular Gauss map* $\mathring{\Phi}_K$ of a knot K is defined by

$$\mathring{\Phi}_K : S^1 \times S^1 \ni (s, t) \mapsto v_{f(s)}(f(t)) \in S^2.$$

We remark that $\mathring{\Phi}_K$ is well defined at the diagonal set, but it is not a symmetric function.

Remark 8.11. The circular Gauss map $\mathring{\Phi}_K$ is not conformally invariant, namely, for a conformal transformation T, there is generally no element g in $O(3)$ that satisfies $\mathring{\Phi}_{T(K)}(s, t) = g(\mathring{\Phi}_K(s, t))$ for any $(s, t) \in S^1 \times S^1$. To see this, one can put $T = I_x$ as an extreme case, when '$v_{T(x)}(T(y))$' $= I_{x*}(v_x(y))$ is constantly equal to $-v_x(x)$.

Claim 8.12. *The degree of* $\mathring{\Phi}_K$ *vanishes for any knot* K*.*

Proof. Any knot K can be deformed continuously by an ambient isotopy to a very 'thin position', so that K is contained in xy-plane except for some 'bridges' which are contained in $\{0 \leqslant z \leqslant \varepsilon\}$, as illustrated in Figure 24. Then the pre-image of the vector $(0, 0, 1) \in S^2$ by $\mathring{\Phi}_K$ consists of pairs of points near the crossing points.

Suppose a knot satisfies

$$f(t) = \begin{cases} (t, 0, \varepsilon), & -\frac{1}{8} \leqslant t \leqslant \frac{1}{8}, \\ (0, t - \frac{1}{2}, 0), & \frac{1}{2} - \frac{1}{8} \leqslant t \leqslant \frac{1}{2} + \frac{1}{8}, \end{cases}$$

for a small ε $(0 < \varepsilon < \frac{1}{8})$. Put

$$U = [-\tfrac{1}{8}, \tfrac{1}{8}] \cup [\tfrac{1}{2} - \tfrac{1}{8}, \tfrac{1}{2} + \tfrac{1}{8}].$$

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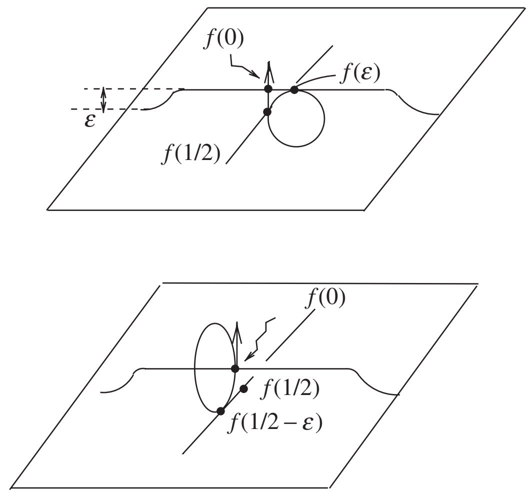

Figure 25. $(\mathring{\Phi}_K)^{-1}((0,0,1))$.

The pre-image $(\mathring{\Phi}_K|_{U\times U})^{-1}((0,0,1)) \in U \times U$ is a pair of points $(\varepsilon, \frac{1}{2})$ and $(\frac{1}{2} - \varepsilon, 0)$, where the signatures of $(\mathring{\Phi}_K|_{U\times U})_*$ are opposite, and hence the contribution of $U \times U$ to the degree of $\mathring{\Phi}_K$ is 0. □

Let us introduce two non-trivial functionals derived from $\mathring{\Phi}_K$.

Definition 8.13.

(1) Let ω_{S^2} be the unit volume 2-form of S^2,

$$\omega_{S^2} = \frac{1}{4\pi}\frac{x_1\,\mathrm{d}x_2 \wedge \mathrm{d}x_3 + x_2\,\mathrm{d}x_3 \wedge \mathrm{d}x_1 + x_3\,\mathrm{d}x_1 \wedge \mathrm{d}x_2}{\{(x_1)^2 + (x_2)^2 + (x_3)^2\}^{3/2}}.$$

The *absolute circular self-linking number à la Gauss*, |csl|, is defined by

$$|\mathrm{csl}|(K) = \int_{T^2} |\mathring{\Phi}_K^*(\omega_{S^2})|.$$

(2) Let $l_K(x)$ be the length of the curve $\bigcup_{y\in K} v_y(x) = \mathring{\Phi}_K(S^1, s)$ on S^2. The *total variation of the conformally translated tangent vectors*, I_{tv}, is defined by

$$I_{\mathrm{tv}}(K) = \int_{S^1} l_K(x)\,\mathrm{d}x.$$

By definition, $I_{\mathrm{tv}}(K) \geqslant |\mathrm{csl}|(K)$ for any knot K.

Let us give a geometric interpretation of I_{tv} using the inverted open knot. Let I_x, $\tilde{K}_x$ and $\tilde{y}$ be as in § 3.2. Then $I_x(C(y,y,x))$ is the (oriented) tangent line to $\tilde{K}_x$ at $\tilde{y}$. Let $\tilde{v}_{\tilde{y}}(\tilde{y})$ be the unit tangent vector to $I_x(C(y,y,x))$ at $\tilde{y}$. Then $-v_y(x) = I_{x*}(v_y(x)) = \tilde{v}_{\tilde{y}}(\tilde{y})$. Therefore, $l_K(x)$ is equal to the length of the curve $\bigcup_{\tilde{y}\in\tilde{K}_x} \tilde{v}_{\tilde{y}}(\tilde{y}) \subset S^2$. Thus $I_{\mathrm{tv}}(K)$ can be considered as the *total variation of the tangent vectors to the inverted open knots.*

If $T : \mathbb{R}^3 \cup \{\infty\} \to \mathbb{R}^3 \cup \{\infty\}$ is a conformal transformation that fixes $\{\infty\}$, then $T|_{\mathbb{R}^3}$ is a homothety. Therefore, we have the following.

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Claim 8.14. *The homothety class of the inverted open knot $\tilde{K}_x$ is a conformal invariant of K. Namely, $I_{T(x)}(T(K))$ is homothetic to $\tilde{K}_x$ for any conformal transformation T.*

Therefore, the functional I_{tv} is a conformally invariant functional.

Although I_{tv} is conformally invariant, it cannot be expressed in terms of the infinitesimal cross-ratio like $E^{(2)}$ and $E_{\sin\theta}$, because I_{tv} is determined by up to the second-order derivatives of the knot.

Claim 8.15. *Neither $|\mathrm{csl}|$ nor I_{tv} is an energy functional for knots.*

Proof. It suffices to show that I_{tv} is not an energy functional because $I_{\mathrm{tv}} \geqslant |\mathrm{csl}|$ for any knot.

We show that the contribution to I_{tv} of a pair of straight line segments of a fixed length with the closest distance ε does not blow up even if ε goes down to 0. Let

$$A_1 = \{x(s) \mid a \leqslant s \leqslant b\} \quad \text{and} \quad A_2 = \{y(t) \mid a' \leqslant t \leqslant b'\}$$

be straight line segments with $\min_{x\in A_1, y\in A_2} |x-y| = \varepsilon$. Let us consider $I_{\mathrm{tv}}|_{A_1\cup A_2}$. Put

$$u = f'(s), \quad v = f'(t) \quad \text{and} \quad w = \frac{f(t)-f(s)}{|f(t)-f(s)|},$$

as before. Then u and v are constant. Fix t and put $\gamma(s) = v_x(y)$. Then, since $\gamma(s) = 2(u,w)w - u$, we have

$$\frac{\mathrm{d}\gamma}{\mathrm{d}s} = 2\left(u, \frac{\mathrm{d}w}{\mathrm{d}s}\right)w + 2(u,w)\frac{\mathrm{d}w}{\mathrm{d}s},$$

and hence

$$\left|\frac{\mathrm{d}\gamma}{\mathrm{d}s}\right| \leqslant 2\sqrt{2}\left|\frac{\mathrm{d}w}{\mathrm{d}s}\right|.$$

Therefore,

$$l_{A_1}(y) = \int_a^b \left|\frac{\mathrm{d}\gamma}{\mathrm{d}s}\right| \mathrm{d}s \leqslant 2\sqrt{2}\int_a^b \left|\frac{\mathrm{d}w}{\mathrm{d}s}\right| \mathrm{d}s \leqslant 2\sqrt{2}\pi,$$

and hence

$$I_{\mathrm{tv}}|_{A_1\cup A_2} = \int_{a'}^{b'} l_{A_1}(y)\,\mathrm{d}t + \int_a^b l_{A_2}(x)\,\mathrm{d}s \leqslant 2\sqrt{2}\pi(b'-a'+b-a),$$

which is independent of ε. □

We show that I_{tv} can detect the unknot.

Example 8.16. Let $K_\circ$ be the standard planar circle. Then $v_y(x) = f'(s)$ for any y and therefore $I_{\mathrm{tv}}(K_\circ) = |\mathrm{csl}|(K_\circ) = 0$.

Theorem 8.17. *If K is a non-trivial knot, then $I_{\mathrm{tv}}(K) \geqslant \pi$.*

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Proof. The unit tangent vector $\tilde{v}_{\tilde{y}}(\tilde{y})$ of the inverted open knot $\tilde{K}_x$ is asymptotic to $-v_x(x)$ as $\tilde{y}$ goes to ∞. If the angle between $\tilde{v}_{\tilde{y}}(\tilde{y})$ and $-v_x(x)$ is smaller than $\frac{1}{2}\pi$ for any $\tilde{y}$, then $\tilde{K}_x$ is unknotted, which contradicts the assumption. Therefore, $l_K(x) \geqslant \pi$ for any $x \in K$. □

Conjecture 8.18. *There is a positive constant C such that, if K is a non-trivial knot, then $|\mathrm{csl}|(K) \geqslant C$.*

8.3. The global radius of curvature

Let us make a remark on the relation between the infimum of the radii of non-trivial spheres and the global radius of curvature by Gonzalez and Maddocks [**13**]. Let us consider a knot K in $\mathbb{R}^3$.

Let $r(C(x, y, z))$ be the radius of the circle $C(x, y, z)$ that passes through x, y and z in K. When two (or three) of them coincide, $C(x, y, z)$ means the tangent (or, respectively, osculating) circle. The *global radius of curvature* $\rho_K^{(3)}(x)$ of a knot K at x is defined by

$$\rho_K^{(3)}(x) = \min_{y,z\in K} r(C(x, y, z)).$$

This $\rho_K^{(3)}(x)$ is attained by a triple (x, y, y) and, especially, when it is attained by a triple (x, x, x), $\rho_K^{(3)}(x)$ is the radius of curvature in the ordinary sense.

Let $\sigma(x, y, z, w)$ denote the smallest sphere that passes through x, y, z and w in K, where the points in $\sigma \cap K$ are counted with multiplicity according to the order of the tangency. Generically, $\sigma(x, y, z, w)$ is uniquely determined. Let $r(\sigma(x, y, z, w))$ be the radius of $\sigma(x, y, z, w)$. Put

$$\rho_K^{(4)}(x) = \inf_{(y,z,w)\in K} r(\sigma(x, y, z, w)).$$

Since $r(\sigma(x, y, z, w)) \geqslant r(C(x, y, z))$, there holds $\rho_K^{(4)}(x) \geqslant \rho_K^{(3)}(x)$. Put

$$\Delta(K) = \min_{x\in K} \rho_K^{(3)}(x) = \min_{x,y,z\in K} r(C(x, y, z)),$$
$$\Box(K) = \inf_{x\in K} \rho_K^{(4)}(x) = \inf_{(x,y,z,w)\in K} r(\sigma(x, y, z, w)).$$

Then $\Delta(K)$ is equal to the *thickness* [**16**, **24**]. As is shown in [**13**], $\Delta(K)$ is either the minimum local radius of curvature or the strictly smaller radius of a sphere $\sigma = \partial D^3$, with $\mathrm{Int}\, D^3 \cap K = \phi$ which is twice tangent to K at antipodal points.

Claim 8.19 (cf. J. H. Maddocks and J. Smutny (personal communication) and [**14**]**).** *We have that $\rho_K^{(3)}(x) = \rho_K^{(4)}(x)$ for any x. Therefore, $\Delta(K) = \Box(K)$.*

8.4. Links

One can ask similar questions for links $\mathcal{L} = C_1 \cup C_2$.

We say that the link is *splittable* if there exist two disjoint closed balls B_1 and B_2 such that $C_1 \subset B_1$ and $C_2 \subset B_2$.

The 'cross' energy of a link $\mathcal{L}$ is given by

$$E^{(2)}(C_1, C_2) = \int_{x \in C_1} \int_{y \in C_2} \frac{\mathrm{d}x\,\mathrm{d}y}{|x-y|^2}.$$

The minimizers of $E^{(2)}$ were studied in [**15**]. The interpretation in terms of the infinitesimal cross-ratio was given in [**21**].

(1) What can be said about the measure of spheres (*non-trivial spheres*) intersecting the two components if the link is not splittable?

(2) Define a non-trivial zone for a link as a zone crossed by the two components (then at least two strands of one and two strands of the other component cross the zone), and the modulus of a link as the maximum of the modulus of a non-trivial zone for the link. Give a lower bound for the modulus of a non-splittable link.

A recent result of Langevin and Moniot [**19**] is as follows.

Claim 8.20. *The modulus of a non-splittable link is bounded below by the modulus of the Hopf Link,*

$$\mathcal{H} = C_1 \cup C_2, \quad C_1 = \{x = 0\} \cap S^3, \quad C_2 = \{y = 0\} \cap S^3, \quad S^3 \subset \mathbb{C}.$$

As in the case of knots, the claim provides a lower bound for the measure of non-trivial spheres for a non-splittable link.

Note added in proof. As a corollary of Proposition 4.14, ω in Lemma 4.12 is invariant under the diagonal action of the conformal group on $S^n \times S^n \setminus \Delta$. But this fact can be shown more easily.

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