

MÖBIUS ENERGY OF GRAPHS.

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INTRODUCTION.

The study of knot energies was initiated by the work of Moffatt (1969) [13], and was developed by him in [14] following Arnold's work [2]. The first discrete energy of knots were produced by W. Fukuhara in 1988, for the details see his work [5]. Möbius energy was discovered by J. O'Hara [6] in 1991. Further investigations of Möbius energy properties were made by M. H. Freedman, Z. -H. He, and Z. Wang in [4]. Particularly, the authors introduced variational principles for Möbius energy and found some upper estimates for the minimal possible energy of knots with the given crossing number in their work. Conformal properties of Möbius energy allow us to calculate explicitly some critical values for toric knots, see the work [12]. The following articles were dedicated to general theory of knot energies: [1], [7], [8], [10], [11], [15] etc. Recently A. Bobenko in [3] introduced Möbius energy for simplicial surfaces. A good overview of properties for knot energies, the techniques of the approximation constructions of extremal knots, and some generalizations of energies can be found in the book of J. O'Hara [9].

In the present paper we introduce *Möbius energy for the embedded graphs*. This energy is invariant under Möbius transformations. This paper is organized as follows. In Section 1 we give the definition of Möbius energy. Further in Section 2 we formulate the main properties of this energy and outline the main ideas of their proofs. In the last section we study critical configurations for the angles at vertices of degree less than five. We

Date: 14 September 2005.

Key words and phrases. Energies of graphs, variational principles, Möbius transformation.

Partially supported by RFBR grant SS-1972.2003.1 and by RFBR grant 05-01-01012a.

conclude the paper with a few words about the techniques of construction of symmetric toric embedded graphs with critical values of Möbius energy.

The author is grateful to A. Sossinski for constant attention to this work and useful remarks and discussions.

1. DEFINITION OF MÖBIUS ENERGY FOR THE GRAPHS.

We will start with the definition of Möbius energy for knots in a conformal form proposed by P. Doyle and O. Schramm (see, for example, [9], page 39). In the present paper by oriented *knot* we mean the C^2 -smooth embedding of the circle $S^1 = \mathbb{R}/(2\pi\mathbb{Z})$ in \mathbb{R}^3 . Let $\tau : S^1 \rightarrow \mathbb{R}^3$ be an oriented knot. Denote by $C(\tau(t_1), \tau(t_1), \tau(t_2))$ the circle (or the line) tangent to the knot at the point $\tau(t_1)$ and containing the point $\tau(t_2)$. We orient this circle such that the obtained orientation coincides with the knot orientation at the tangency point $\tau(t_1)$. Denote the angle between the oriented circles $C(\tau(t_1), \tau(t_1), \tau(t_2))$ and $C(\tau(t_2), \tau(t_2), \tau(t_1))$ by $\theta_\gamma(t_1, t_2)$. By definition the angle θ_γ is from the segment $[0, \pi]$. By $|\ast|$ we denote the absolute value of the vector in \mathbb{R}^3 .

By *Möbius energy* of the knot τ we mean the following value:

$$M(\tau) = \iint_{S^1 \times S^1} \left(\frac{\dot{\tau}(t_1)\dot{\tau}(t_2)}{|\tau(t_1) - \tau(t_2)|^2} - \cos \theta_\tau(t_1, t_2) \frac{\dot{\tau}(t_1)\dot{\tau}(t_2)}{|\tau(t_1) - \tau(t_2)|^2} \right) dt_1 dt_2.$$

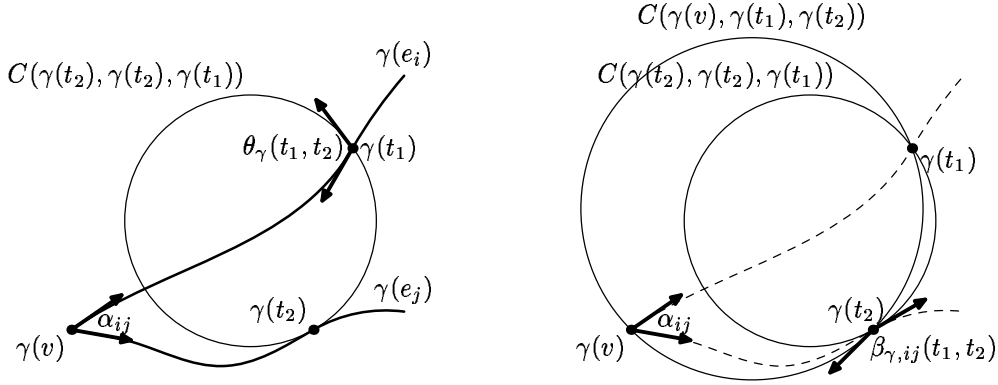
Möbius energy is well-defined, positive, does not depend on orientation and parametrization of the knot. If we C^2 -smoothly perturb the knot then Möbius energy changes in the continuous way. The energy is invariant under the group of Möbius transformations (i.e. the group of transformations in \mathbb{R}^3 generated by all inversions), see [4]. The minuend of the integrand is called the *principal term*, the subtrahend is called the *normalization term*.

Suppose now we have some graph G with edges e_i , $i=1, \dots, n$, and vertices v_k , $k=1, \dots, m$. For the simplicity we suppose that the graph G does not contain loops and multiple edges (note that the construction below can be easily generalized to the arbitrary graph). So let $\gamma : G \rightarrow \mathbb{R}^3$ be an embedding or an immersion that is C^2 -smooth on open edges and such that at any vertex the one-sided first and second derivatives are well-defined and continuous. Suppose also that for any couple of edges e_i and e_j adjacent to the same vertex the angle α_{ij} between the vectors of the corresponding one-sided first derivatives at this vertex is non-zero. Denote the set of all angles α_{ij} for all vertices of the graph G by α . Such embedding or immersion is called an α -*embedding* or an α -*immersion*. Note that for any fixed set α of angles, C^2 -topology on the space of all α -embeddings (or all α -immersions) is defined in the natural way.

First, we define Möbius energy for edges and for couples of edges.

1). Möbius energy for some edge e_i is calculated similar to the case of Möbius energy for knots:

$$M(\gamma; e_i, e_i) = \iint_{e_i \times e_i} \left(\frac{\dot{\gamma}(t_1)\dot{\gamma}(t_2)}{|\gamma(t_1) - \gamma(t_2)|^2} - \cos \theta_\gamma(t_1, t_2) \frac{\dot{\gamma}(t_1)\dot{\gamma}(t_2)}{|\gamma(t_1) - \gamma(t_2)|^2} \right) dt_1 dt_2.$$

FIGURE 1. The angles $\theta_\gamma(t_1, t_2)$ and $\beta_{\gamma,ij}(t_1, t_2)$.

2). Let edges e_i and e_j do not have any common vertex. Orient them in an arbitrary way and define

$$M(\gamma; e_i, e_j) = \iint_{e_i \times e_j} \left(\frac{\dot{\gamma}(t_1)\dot{\gamma}(t_2)}{|\gamma(t_1) - \gamma(t_2)|^2} - (\cos \theta_\gamma(t_1, t_2) + \cos(\pi - \theta_\gamma(t_1, t_2))) \frac{\dot{\gamma}(t_1)\dot{\gamma}(t_2)}{2|\gamma(t_1) - \gamma(t_2)|^2} \right) dt_1 dt_2 = \iint_{e_i \times e_j} \frac{\dot{\gamma}(t_1)\dot{\gamma}(t_2)}{|\gamma(t_1) - \gamma(t_2)|^2} dt_1 dt_2.$$

3). Consider now the case of an ordered couple of edges e_i and e_j adjacent to their common vertex v with the corresponding angle α_{ij} . Let t_1 and t_2 be some points of edges e_i and e_j respectively. Orient the edge e_i in the direction to the common vertex v , and the edge e_j in the direction from the common vertex v . Denote by $C(\gamma(v), \gamma(t_1), \gamma(t_2))$ the circle passing through the points $\gamma(v)$, $\gamma(t_1)$, and $\gamma(t_2)$ with the orientation corresponding to the following order of points: $\gamma(v)$, $\gamma(t_1)$, $\gamma(t_2)$. Denote the angle between the oriented circles $C(\gamma(v), \gamma(t_1), \gamma(t_2))$ and $C(\gamma(t_2), \gamma(t_2), \gamma(t_1))$ by $\beta_{\gamma,ij}(t_1, t_2)$. Möbius energy for the ordered couple of edges e_i and e_j is defined as follows:

$$M(\gamma; e_i, e_j) = \iint_{e_i \times e_j} \left(\frac{\dot{\gamma}(t_1)\dot{\gamma}(t_2)}{|\gamma(t_1) - \gamma(t_2)|^2} - \cos(\theta_\gamma(t_1, t_2) + 2\beta_{\gamma,ij}(t_1, t_2) - \alpha_{ij} - \pi) \frac{\dot{\gamma}(t_1)\dot{\gamma}(t_2)}{|\gamma(t_1) - \gamma(t_2)|^2} \right) dt_1 dt_2.$$

Again the minuend of the integrand is called the *principal term*, and the subtrahend is called the *normalization term*.

Definition 1.1. Let $\gamma : G \rightarrow \mathbb{R}^3$ be a C^2 -smooth embedding of some graph G . By *Möbius energy* of the embedding γ we mean the following value:

$$M(\gamma, G) = \sum_{i=1}^n \sum_{j=1}^n M(\gamma; e_i, e_j).$$

2. MAIN PROPERTIES OF MÖBIUS ENERGY FOR GRAPHS.

Let G be some graph with edges e_i where $i = 1, \dots, n$ and vertices v_k for $k = 1, \dots, m$. We suppose also that the graph G does not have simple loops and multiple edges. Let $\gamma : G \rightarrow \mathbb{R}^3$ be an α -embedding.

Theorem 2.1. *The following statements hold.*

- i). Möbius energy $M(\gamma, G)$ is well-defined.
- ii). The value $M(\gamma, G)$ does not depend on the parametrization and orientation choice for the edges of the graph G .
- iii). Möbius energy is nonnegative.
- iv). Let $T : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ be some Möbius transformation such that the its preimage of infinity does not contain points of the embedded graph $\gamma(G)$. Then $M(\gamma, G) = M(T \circ \gamma, G)$.

Proof. Since for any couple of open edges the integrand is bounded from above and continuous, all integrals converge (for adjacent edges the boundedness follows from the explicit angle calculations for the corresponding embedded angle obtained with two straight rays). Therefore, Möbius energy of the graph $M(\gamma, G)$ is well-defined. This proves the first property. The second Property is obviously satisfied. Since all integrands are nonnegative, Möbius energy is also nonnegative. Hence the third property holds.

To prove the last property we remind that the set of all straight lines and circles maps to itself under (conformal) Möbius transformations, and also the angles between them are invariant. Hence the angles α_{ij} , $\beta_{\gamma,ij}(t_1, t_2)$ and $\theta_\gamma(t_1, t_2)$ are invariant. Besides that the cross-ratio is also invariant under Möbius transformations. Thus the following value is Möbius invariant:

$$\frac{\dot{\gamma}(t_1)\dot{\gamma}(t_2)}{|\gamma(t_1) - \gamma(t_2)|^2}$$

Therefore, Möbius energy of graphs is invariant under Möbius transformations. \square

Remark 2.2. If we multiply the integrand by some smooth arbitrary function of θ_γ then we will obtain a new functional on the space of graphs invariant under Möbius group action.

Further we fix all angles at the vertices in families of α -embeddings (i.e. all α are equal to each other).

Theorem 2.3. *Consider an arbitrary graph G and an arbitrary set of angles α , corresponding to the graph G .*

- i). Let γ_δ where $0 \leq \delta \leq 1$ be a continuous family of α -embeddings, then the function $M(\gamma_\delta, G)$ is continues in the variable δ .
- ii). Let γ_δ for $0 \leq \delta \leq 1$ be a continuous family of α -immersions where γ_0 is an immersion with the unique point of transversal double self-intersection and γ_δ for any $\delta \neq 0$ is an embedding, then

$$\lim_{\delta \rightarrow 0} M(\gamma_\delta, G) = +\infty.$$

Sketch of the proof. i). Consider an arbitrary couple of open edges e_i and e_j . Since the integrand (considered as a function in t_1 , t_2 , and δ variables) is continuous, non-negative, and bounded from above on the set $e_i \times e_j \times [0, 1]$, the first statement of theorem holds.

ii). Let the edges e_i and e_j (where $i \neq j$) of the immersion γ_0 transversely intersect with the angle φ . Suppose that the edges e_i and e_j are adjacent to some common edge. Consider an embedding γ_δ and denote the parts of the edges e_i and e_j which images under γ_δ are contained in complement of the ball of radius $(\sqrt{\delta}d)$ to the ball of radius d both centered at the self-intersection point of the immersion γ_0 by $e_i(d, \delta)$ and $e_j(d, \delta)$ respectively.

For any positive ε there exists some positive d such that for any positive $\delta < d$ for all points of the set $e_i(d, \delta) \times e_j(d, \delta)$ holds

$$\left| \beta_{\gamma_\delta, ji}(t_1, t_2) - (\pi - \varphi - \beta_{\gamma_\delta, ij}(t_1, t_2)) \right| < \varepsilon.$$

Let us estimate the integral for the corresponding sets $e_i(d, \delta) \times e_j(d, \delta)$. Let us sum up the integrands for the ordered couples $(e_i(d, \delta), e_j(d, \delta))$ and $(e_j(d, \delta), e_i(d, \delta))$. The normalization term will be as follows:

$$\frac{(\cos(\theta_{\gamma_\delta}(t_1, t_2) + 2\beta_{\gamma_\delta, ij}(t_1, t_2) - \alpha_{ij} - \pi) + \cos(\theta_{\gamma_\delta}(t_1, t_2) + 2\beta_{\gamma_\delta, ji}(t_1, t_2) - \alpha_{ij} - \pi)) \times \gamma_\delta(t_1)\dot{\gamma}_\delta(t_2)}{|\gamma_\delta(t_1) - \gamma_\delta(t_2)|^2}.$$

Since for the set under consideration the following holds:

$$\left| \beta_{\gamma_\delta, ji}(t_1, t_2) - (\pi - \varphi - \beta_{\gamma_\delta, ij}(t_1, t_2)) \right| < \varepsilon,$$

the sum of cosines of the normalization term differ from

$$2 \cos(\theta_{\gamma_\delta}(t_1, t_2) - \alpha_{ij} - \varphi) \cos(2\beta_{\gamma_\delta, ij} + \varphi - \pi)$$

less than by ε .

The absolute value of the second factor is less than or equal to the unity. The absolute value of the first factors essentially varies and there exist a subset of $e_i(d, \delta) \times e_j(d, \delta)$ of positive measure such that its absolute value is bounded from above by some constant less than unity. Hence for any positive C there exist sufficiently small d such that for δ tending to zero the value of the functional of Möbius energy on the set $e_i(d, \delta) \times e_j(d, \delta)$ tends to some real number greater than C . Therefore,

$$\lim_{\delta \rightarrow 0} M(\gamma_\delta, G) = +\infty.$$

The case of self-intersection of one edge is similar to the classical case of knot Möbius energy. The case of self-intersection of two edges that do not have the common vertex is trivial. □

3. ON SOME CRITICAL OBJECTS FOR MÖBIUS ENERGY FUNCTIONAL.

In this section we formulate some statements and question related to the critical configurations of angles at vertices, and discuss the techniques of construction of special embedded graphs with critical values of Möbius energy.

3.1. Critical configurations of angles at vertices. By the *intensity* of an angle $\alpha \in (0, \pi]$ we mean the following value:

$$\psi(\alpha) = \begin{cases} 1 - \frac{\pi - \alpha}{\sin(\alpha)} & \text{for } 0 < \alpha < \pi \\ 0 & \text{for } \alpha = \pi \end{cases}.$$

Consider an arbitrary graph G and an embedding γ . Take a couple of edges e_i and e_j adjacent to some common vertex v with the corresponding angle α_{ij} . Let $V_\varepsilon \subset e_i \times e_j$ be the set of couples (t_1, t_2) such that the images $\gamma(t_1)$ and $\gamma(t_2)$ are not contained in the ball of radius ε centered at the point $\gamma(v)$.

Statement 3.1. *The integral of the principal term estimates as follows*

$$\iint_{V_\varepsilon} \frac{\dot{\gamma}(t_1)\dot{\gamma}(t_2)}{|\gamma(t_1) - \gamma(t_2)|^2} dt_1 dt_2 = \psi(\alpha_{ij}) \ln\left(\frac{1}{\varepsilon}\right) + C(\gamma) + o(1),$$

while ε tends to zero. The constant $C(\gamma)$ here does not depend on ε . □

Now consider the configuration space Ω_k of k -tuples non-coinciding enumerated unit segments in \mathbb{R}^3 with the common vertex at the origin. Consider an arbitrary k -tuple ω of Ω_k . Denote the angle between the i -th and the j -th segments by α_{ij} where $0 < \alpha_{ij} \leq \pi$.

Definition 3.2. Let ω be some k -tuple of Ω_k . The following value

$$\Psi(\omega) = \sum_{i=1}^k \sum_{j>i}^k \psi(\alpha_{ij})$$

is called the *intensity* of the k -tuple ω .

Let v be some vertex of G of order k , and γ — some α -embedding of G that maps v to the origin. Denote by $\omega(\gamma; v)$ the k -tuple of Ω_k whose segments are tangent to the corresponding edges of $\gamma(G)$ at the origin.

Definition 3.3. A vertex v of the order k is said to be *critical* (*extremal*, *minimal*), if the k -tuple $\omega(\gamma; v)$ is critical (extremal, minimal) for the function Ψ .

Since all angles between vectors of the first derivatives are fixed, the value $\Psi(\omega(\gamma; v))$ does not depend on an embedding γ . Therefore, the property of the vertex to be critical (extremal, minimal) also does not depend on the embedding γ .

The question of finding vertices with the least intensity is natural here. Here we show some examples of extremal vertices.

Statement 3.4. *i). The angle at any critical vertex of order two is straight. This critical vertex is also the minimal vertex.*

ii). All angles at any critical vertex of order three are equal to $\frac{2\pi}{3}$. The critical vertex is also the minimal vertex at that.

iii). There exist at least two critical configurations of angles for the vertices of order four:

a) the first one corresponds to the diagonals of the square;

b) the second one corresponds to the segments that join the mass center of the homogeneous regular tetrahedron with the vertices of this tetrahedron. \square

The further classification of critical vertices is unknown for the author.

Problem 1. Find all angle configurations at vertices of degree four, five (of degree n) that corresponds to critical, extremal, and minimal vertices. To which convex polyhedra do these angle configurations correspond?

It is supposed that the vertex of degree four that corresponds to the square is not extremal; the vertex of degree four that corresponds to the regular tetrahedron is minimal; all other vertices of order four are not critical.

3.2. Some examples of critical graphs. In conclusion of this paper we study some examples of critical graphs that were constructed by the techniques of D. Kim and R. Kusner [12]. Namely, consider a three-dimensional space as a subspace a four-dimensional space. By some Möbius transformation in the four-dimensional space this subspace is taken to the unit sphere defined by the following equation: $x^2+y^2+z^2+t^2=1$. This sphere contains a family of "symmetric tori" that are obtained as intersections of the sphere and surfaces of type $x^2+y^2=\lambda^2$, where $\lambda \in (0, 1)$ is a parameter of the family. The torus $T_{1/2}$ divides the sphere into two symmetric with respect to this torus parts. Now by symmetry reasons any symmetric graph of $T_{1/2}$ that corresponds to some regular quadratic lattice of $T_{1/2}$ is critical.

The rectangular symmetric graphs of the torus $T_{1/2}$ are parametrized (up to the length preserving transformations of \mathbb{R}^4) by 4-tuples of integers $(p, q; m, n)$. Here p and q are either relatively prime and $p \geq q \geq 1$ or $p=1$ and $q=0$; and also m and n satisfy the following conditions: $m \geq n \geq 1$. Let us call one of the lattice directions of the rectangular symmetric graph *horizontal* and the perpendicular to it — *vertical*. The couple (p, q) is defined by the torus winding corresponding to the horizontal direction. The integers m and n equal to the numbers of horizontal and respectively vertical "circles" in the graph. Some lattice is square iff $m = n$. So critical graphs are the graphs of the type $(p, q; n, n)$. This critical graphs are taken to some critical graph embeddings in \mathbb{R}^3 by some stereographic projection.

See the examples of symmetric toric square graphs $(1, 0; 3, 3)$, $(1, 1; 2, 2)$, $(2, 1; 1, 1)$ and $(3, 1; 1, 1)$ on Fig. 2 (from the left to the right). The approximate calculations show that

$$M((2, 1; 1, 1)) \approx 25.137,$$

$$M((1, 1; 2, 2)) \approx 68.789,$$

$$M((1, 0; 3, 3)) \approx 95.979,$$

$$M((3, 1; 1, 1)) \approx 109.91.$$

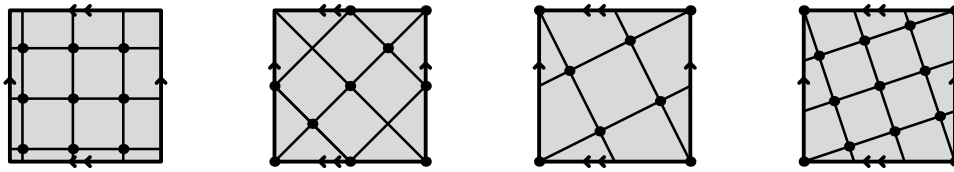


FIGURE 2. Symmetric toric graphs $(1, 0; 3, 3)$, $(1, 1; 2, 2)$, $(2, 1; 1, 1)$ and $(3, 1; 1, 1)$.

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