

# THE SUM OF LAGRANGE NUMBERS

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ABSTRACT. Combining McShane’s identity on a hyperbolic punctured torus with Schmutz’s work on the Markov Uniqueness Conjecture (MUC), we find that MUC is equivalent to the identity

$$\sum_{n=1}^{\infty} (3 - L_n) = 4 - \varphi - \sqrt{2}$$

where  $L_n$  is the  $n$ th Lagrange number and  $\varphi = \frac{1+\sqrt{5}}{2}$  is the golden ratio.

## 1. PRELIMINARIES

**1.1. Lagrange and Markov numbers.** The *Lagrange numbers*  $\mathcal{L} = \{L_n\}_{n=1}^{\infty} = \{\sqrt{5}, \sqrt{8}, \dots\}$  are a sequence of real numbers that naturally arise in Diophantine approximation. Hurwitz’s theorem states that for any irrational number  $x$ , there exists a sequence of rationals  $p_n/q_n$  converging to  $x$  with  $\left|x - \frac{p_n}{q_n}\right| < \frac{1}{\sqrt{5}q_n^2}$ . In this expression,  $\sqrt{5}$  is optimal, as can be shown by taking  $x = \varphi$  (golden ratio). It turns out that when  $x = \varphi$  is excluded,  $\sqrt{8}$  is the new best constant. By definition,  $L_1 = \sqrt{5}$  is the first Lagrange number,  $L_2 = \sqrt{8}$  is the second Lagrange number, etc.

The *Markov numbers*  $\mathcal{M} = \{m_n\}_{n=1}^{\infty} = \{1, 2, 5, 13, \dots\}$  are the positive integers that appear in a Markov triple, i.e. a solution  $(x, y, z) \in \mathbb{Z}^3$  to the cubic

$$(1) \quad x^2 + y^2 + z^2 = 3xyz.$$

In 1880, Markov [Mar79, Mar80] discovered a remarkable connection between this cubic and the theory of binary quadratic forms, and proved the unexpected relation between Markov and Lagrange numbers:

$$(2) \quad L_n = \sqrt{9 - \frac{4}{m_n^2}}.$$

Using the Vieta involution  $(x, y, z) \mapsto (x, y, 3xy - z)$ , it is easy to see that for any Markov number  $m$ , one can always find a Markov triple  $(x, y, m)$  with  $0 < x \leq y \leq m$ . The *Markov Uniqueness Conjecture* (MUC) asserts that such a triple is always unique. MUC was initially offered by Frobenius in 1913 [Fro13] and is notoriously difficult [Guy83]. For more context, we refer to [Aig15, CF89].

**1.2. The sum of Lagrange numbers.** It is clear from (2) that  $L_n$  is an increasing sequence of positive numbers that converges to 3 when  $n \rightarrow +\infty$ . Moreover, we have  $3 - L_n \sim \frac{2}{3m_n^2}$ , and since  $m_n \geq n$  (actually  $m_n$  is much greater, see § 3), the series  $\sum_{n=1}^{\infty} (3 - L_n)$  is convergent. In this paper, we prove:

**Theorem 1.1.** *The Markov Uniqueness Conjecture holds if and only if*

$$(3) \quad \sum_{n=1}^{\infty} (3 - L_n) = 4 - \varphi - \sqrt{2}.$$

The proof is easily derived from the McShane identity on a hyperbolic punctured torus and a result of Schmutz regarding the well-known relationship between hyperbolic geometry and Markov numbers. It is nonetheless a striking identity, and could optimistically open a new path towards probing MUC.

*Remark 1.2.* Several authors have developed similar ideas, for instance [Bow96], [LT07, §4.3].

*Remark 1.3.* Numerical computation confirms the identity (3) convincingly, as we shall see in § 3. This is not surprising since MUC has also directly been checked by computers for high values of  $n$ .

**1.3. Markov numbers and the modular torus.** The beautiful relationship between Markov numbers and hyperbolic geometry was discovered by Gorshkov [Gor81] and Cohn [Coh55]. Let  $T^*$  denote the once-punctured torus, i.e. the topological surface obtained by removing a point from the torus  $T^2$ . For a certain hyperbolic metric on  $T^*$ , the lengths of simple closed geodesics on  $T^*$  are given by the Markov numbers. We briefly explain this connection and refer to e.g. [Ser85] for more discussion.

The *character variety* of the once-punctured torus is the cubic surface  $\mathcal{X}$  defined by the equation

$$(4) \quad x^2 + y^2 + z^2 = xyz.$$

Hyperbolic metrics on  $T^*$  with finite volume correspond to real points of  $\mathcal{X}$ . Indeed, let  $\pi_1(T^*) = \langle a, b \rangle$  where  $a$  and  $b$  are the standard generators of  $\pi_1(T^2) \approx \mathbb{Z}^2$ . Hyperbolic structures on  $T^*$  are parametrized by  $x = \text{tr}(A)$ ,  $y = \text{tr}(B)$ ,  $z = \text{tr}(AB)$  where  $A, B \in \text{SL}_2(\mathbb{R})$  are (lifts of) the holonomies of  $a, b \in \pi_1(T^*)$ . The condition that the metric has finite volume amounts to the peripheral curve  $aba^{-1}b^{-1}$  having parabolic holonomy, i.e.  $\text{tr}(ABA^{-1}B^{-1}) = -2$ . Using the classical trace relations in  $\text{SL}_2(\mathbb{R})$ , this equation is rewritten  $x^2 + y^2 + z^2 = xyz$ . We refer to e.g. [Gol03] for more details on this correspondence.

The integer solutions  $(x, y, z) \in \mathbb{Z}^3$  of (4) are clearly in bijection with Markov triples:  $x, y, z$  must all be divisible by 3, and the reduced triple  $(x/3, y/3, z/3)$  verifies (1). Thus Markov triples are the integral points of  $\mathcal{X}$  (up to  $1/3$ ). On the other hand, the mapping class group  $\text{Mod}(T^*)$  acts transitively on such triples, i.e. all corresponding hyperbolic tori are isometric. This hyperbolic torus is called the *modular torus*  $X$ , a 6-fold cover of the modular orbifold. Since  $\text{Mod}(T^*)$  acts transitively on simple closed curves, Markov numbers can alternatively be described as one third of traces of simple closed geodesics on  $X$ :

$$3\mathcal{M} = \{3m_n, n \in \mathbb{N}\} = \{\tau(\gamma), \gamma \in \mathcal{S}\}$$

where we denote  $\mathcal{S}$  the set of simple closed geodesics on  $X$  and  $\tau(\gamma)$  the trace of the holonomy of  $\gamma \in \mathcal{S}$ .

It is natural to ask whether for any  $m \in \mathcal{M}$ , the geodesic  $\gamma$  such that  $\tau(\gamma) = 3m$  is unique up to an isometry of  $X$ . It was proved by Schmutz [Sch96] that this statement is equivalent to MUC.

## 1.4. Acknowledgments.

## 2. PROOF OF THE THEOREM

Greg McShane showed that, for any finite-volume hyperbolic metric on the punctured torus  $T^*$ ,

$$\sum_{\gamma \in \mathcal{S}} \frac{1}{1 + e^{\ell(\gamma)}} = \frac{1}{2}$$

where  $\mathcal{S}$  is the set of simple closed geodesics and  $\ell(\gamma)$  indicates the length of  $\gamma$  [McS98]. Recalling that the trace and length of  $\gamma$  are related by  $\tau(\gamma) = 2 \cosh(\ell(\gamma)/2)$ , McShane's identity can be rewritten

$$(5) \quad \begin{aligned} 1 &= \sum_{\gamma} \frac{2}{1 + e^{\ell(\gamma)}} = \sum_{\gamma} e^{-\ell(\gamma)/2} \text{sech}(\ell(\gamma)/2) \\ &= \sum_{\gamma} \frac{2}{\tau(\gamma) + \sqrt{\tau(\gamma)^2 - 4}} \cdot \frac{2}{\tau(\gamma)} = \sum_{\gamma} 1 - \sqrt{1 - \frac{4}{\tau(\gamma)^2}}. \end{aligned}$$

When  $T^*$  with its hyperbolic metric is chosen to be the modular torus  $X$ , let us denote  $m(\gamma) := \tau(\gamma)/3$  the associated Markov number (see § 1.3) and  $L(\gamma) := \sqrt{9 - \frac{4}{m(\gamma)^2}}$  the associated Lagrange number. Rewriting (5), McShane's identity on the modular torus is simply rewritten:

$$(6) \quad \sum_{\gamma \in \mathcal{S}} (3 - L(\gamma)) = 3.$$

It remains to investigate the fibers of the map  $\gamma \mapsto L(\gamma)$  from simple closed geodesics on  $X$  to Lagrange numbers. It is not hard to show that all fibers are nonempty: this is because Vieta involutions act transitively on the Markov tree, and act as mapping classes on  $\mathcal{S}$ . By Schmutz's theorem [Sch96], MUC is equivalent to each fiber of  $\gamma \mapsto L(\gamma)$  being the  $\text{Aut}(X)$ -orbit of a single simple closed geodesic on  $X$ . To finish the proof of Theorem 1.1, we just need to count the number of elements of each orbit.

**Lemma 2.1.** *Let  $\mathcal{S}_0 \subset \mathcal{S}$  indicate the six shortest geodesics on  $X$ , and let  $\mathcal{S}_1 = \mathcal{S} - \mathcal{S}_0$ . Each orbit  $\text{Aut}(X) \curvearrowright \mathcal{S}_0$  has three elements, and each orbit of  $\text{Aut}(X) \curvearrowright \mathcal{S}_1$  has six elements.*

*Proof.* There is an  $\text{Aut}(X)$ -equivariant correspondence of  $\mathcal{S}$  with lines in  $H := H_1(X, \mathbb{Z})$ . The standard generators  $a, b$  of  $\pi_1(X) \approx \pi_1(T^*)$  (as in § 1.3) provide a basis of  $H \approx \mathbb{Z}^2$ . The image of the homomorphism  $\text{Aut}(X) \rightarrow \text{GL}(2, \mathbb{Z})$  is the dihedral group with six elements, generated by

$$r = \begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix} \text{ and } \sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The actions of  $r$  and  $\sigma$  on  $\mathbb{P}^1 H$  have fixed points  $\text{Fix}(r) = \emptyset$  and  $\text{Fix}(\sigma) = \{[1 : 1], [1 : -1]\}$ . This implies that all simple closed geodesics on  $X$  have six images under the action of  $\text{Aut}(X)$ , except for the two geodesics corresponding to  $ab$  and  $ab^{-1}$ , which have three such images apiece. These six geodesics are precisely the six shortest geodesics on  $X$ .  $\square$

Let us now prove Theorem 1.1, in fact the slightly more precise version:

**Theorem 2.2.** *We have  $\sum_{n=1}^{\infty} (3 - L_n) \leq 4 - \varphi - \sqrt{2}$ , with equality if and only if MUC holds.*

*Proof.* Recall that  $X$  denotes the modular torus and  $\mathcal{S}$  the set of simple closed geodesics on  $X$ . Let  $\mathcal{S}/\text{Aut}(X)$  indicate the set of  $\text{Aut}(X)$ -orbits in  $\mathcal{S}$ . By (6), the McShane identity on  $X$  is rewritten:

$$\sum_{\gamma \in \mathcal{S}} (3 - L(\gamma)) = \sum_{A \in \mathcal{S}/\text{Aut}(X)} \sum_{\gamma \in A} 3 - L(\gamma) = 3.$$

By Lemma 2.1, the map  $\gamma \mapsto \tau(\gamma)$  is 6-to-1 for  $\gamma \in \mathcal{S}_1$  and 3-to-1 for  $\gamma \in \mathcal{S}_0$ . Therefore, we get

$$\left( 6 \sum_{[\gamma] \in \mathcal{S}_1/\text{Aut}(X)} + 3 \sum_{[\gamma] \in \mathcal{S}_0/\text{Aut}(X)} \right) (3 - L(\gamma)) = 3.$$

The six curves in  $\mathcal{S}_0$  are the shortest geodesics in  $\mathcal{S}$ , so the two Lagrange numbers they determine are the two smallest Lagrange numbers  $L_1 = \sqrt{5}$  and  $L_2 = \sqrt{8}$ . The previous equality can be rearranged:

$$\left( 6 \sum_{[\gamma] \in \mathcal{S}/\text{Aut}(X)} (3 - L(\gamma)) \right) - 3 \left( (3 - L_1) + (3 - L_2) \right) = 3$$

which we rewrite:

$$\sum_{[\gamma] \in \mathcal{S}/\text{Aut}(X)} (3 - L(\gamma)) = 4 - \varphi - \sqrt{2}.$$

The map  $[\gamma] \mapsto L(\gamma)$  from  $\mathcal{S}/\text{Aut}(X)$  to the set of Lagrange numbers  $\mathcal{L} = \{L_n, n \in \mathbb{N}\}$  is onto, and one-to-one if and only if MUC holds (see discussion above Lemma 2.1). The conclusion follows.  $\square$

## 3. NUMERICAL EVIDENCE

Numerical computation suggests that the series  $\sum_{n=1}^{\infty} (3 - L_n)$  indeed converges to  $L = 4 - \varphi - \sqrt{2}$ . Denoting  $R_n := L - \sum_{k=1}^n (3 - L_k)$  the presumed remainder, we find for instance  $R_n \approx 7.34169 \times 10^{-455}$  for  $n = 50\,000$ . Of course, MUC has also been checked directly by computers, at least for Markov numbers  $m_n$  up to  $10^{140}$  (see [Met15]) i.e.  $n \leq 18\,906$ , but it is interesting to see a different confirmation.

Pushing the analysis further, we obtain new numerical evidence of Zagier's estimate  $m_n \sim \frac{1}{3}e^{C\sqrt{n}}$  where  $C = 2.35234\dots$ . Let us recall that this estimate is still open but was proved in weaker forms in [Zag82] and [MR95]. Elementary calculus involving the comparison of the remainder  $R_n$  with the integral  $6 \int_n^{+\infty} e^{-2C\sqrt{t}} dt$  translates Zagier's estimate to  $R_n \sim \frac{6\sqrt{n}}{C} e^{-2C\sqrt{n}}$ . On Figure 1 it appears that the graph of  $R_n$  in Log scale is indeed asymptotic to the expected curve.

*Remark 3.1.* We wrote a simple recursive algorithm in Python to generate the list of Markov numbers. It takes a few seconds on a PC to write out all  $m_n \leq 10^{400}$ , i.e. up to  $n = 153\,665$ . We then used Mathematica to compute  $R_n$  up to  $n = 50\,000$  and plot. Our code is freely available on GitHub [js20].

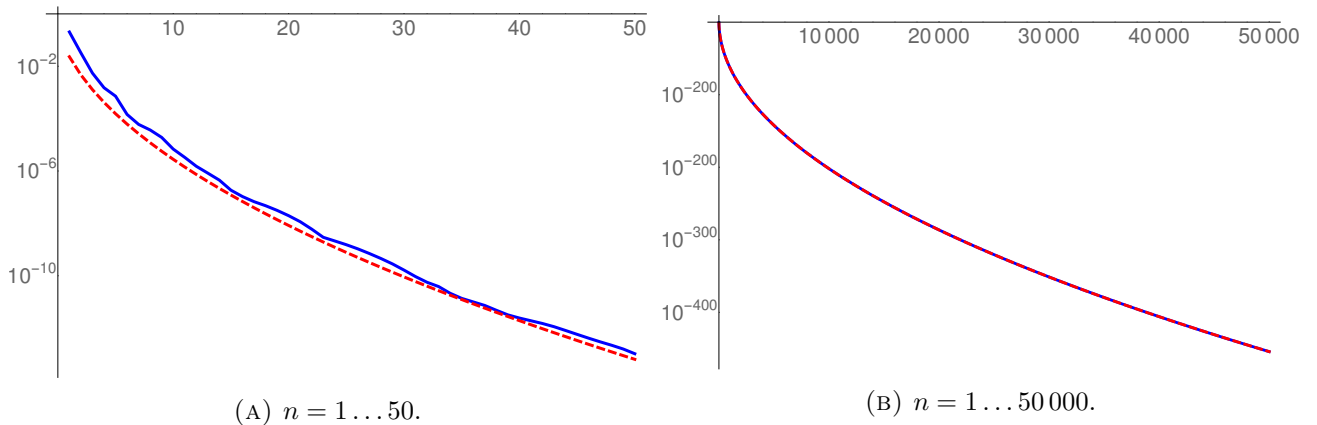


FIGURE 1. Numerical computation of the remainder  $R_n = (4 - \varphi - \sqrt{2}) - \sum_{k=1}^n (3 - L_k)$ . The dashed curve shows the expected asymptotic profile  $\frac{6\sqrt{n}}{C} e^{-2C\sqrt{n}}$ .

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