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Markoff–Lagrange spectrum and extremal numbers

by

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1. Introduction

The purpose of this paper is to present a link between two relatively distant topics of Diophantine approximation. The first one concerns the *Lagrange constant* $\nu(\xi)$ of a real number ξ defined as the infimum of all real numbers $c>0$ for which the inequality

$$\left|\xi-\frac{p}{q}\right|\leqslant\frac{c}{q^2}$$

admits infinitely many solutions $(p,q)\in\mathbb{Z}^2$ with $q\geqslant 1$. This constant, which vanishes when $\xi\in\mathbb{Q}$, provides a measure of approximation to ξ by rational numbers. It is also given by

$$\nu(\xi)=\liminf_{q\to\infty} q\|q\xi\|,$$

where $\|x\|$ stands for the distance from a real number x to a closest integer. The *Lagrange spectrum* is the set $\nu(\mathbb{R})$ of values of ν. It is a subset of the interval $[0,1/\sqrt{5}\,]$. Due to work of Markoff, the portion of the spectrum in the subinterval $\left(\frac{1}{3},1/\sqrt{5}\,\right]$ is well understood (see [3, Chapter II, §6]). It forms a countable discrete subset of this subinterval with $\frac{1}{3}$ as its only accumulation point. Moreover the real numbers ξ for which $\nu(\xi)>\frac{1}{3}$ are all quadratic. As a consequence, any transcendental real number ξ has $\nu(\xi)\leqslant\frac{1}{3}$. In the range $\left[0,\frac{1}{3}\right]$, the situation becomes more complicated. Although, with respect to Lebesgue measure, almost all real numbers ξ have $\nu(\xi)=0$, we know in particular that there are uncountably many $\xi\in\mathbb{R}$ with $\nu(\xi)=\frac{1}{3}$.

The second topic is the problem of simultaneous rational approximations to a real number and its square, from a uniform perspective. Let $\gamma=\frac{1}{2}(1+\sqrt{5}\,)$ denote the golden

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ratio. In 1969, Davenport and Schmidt showed [6, Theorem 1a] that, for each non-quadratic irrational real number ξ, there exists a constant $c>0$ with the property that, for arbitrarily large values of X, the inequalities

$$|x_0|\leqslant X, \quad |x_0\xi-x_1|\leqslant cX^{-1/\gamma} \quad \text{and} \quad |x_0\xi^2-x_2|\leqslant cX^{-1/\gamma}$$

admit no non-zero solution $(x_0,x_1,x_2)\in\mathbb{Z}^3$. Recently, it was established [14, Theorem 1.1] that their result is best possible in the sense that, conversely, there are countably many non-quadratic irrational real numbers ξ which we henceforth call *extremal* such that, for a larger value of c, the same inequalities admit a non-zero integer solution for each $X\geqslant 1$. Our objective here is to show the existence of extremal numbers ξ with $\nu(\xi)=\frac{1}{3}$ and to show how this set is intimately linked with Markoff's theory.

In the next section, we present the main results of Markoff's theory from a point of view pertaining to the study of extremal numbers. Then, in §3, we construct a family of extremal numbers $\xi_{\mathbf{m}}$ parameterized by all solutions in positive integers $\mathbf{m}=(m,m_1,m_2)$ of the Markoff equation

$$m^2+m_1^2+m_2^2=3mm_1m_2, \tag{1}$$

up to permutation, except $\mathbf{m}=(1,1,1)$. Our main result is that these numbers $\xi_{\mathbf{m}}$ constitute a system of representatives of the equivalence classes of extremal numbers ξ with $\nu(\xi)=\frac{1}{3}$, under the action of $\mathrm{GL}_2(\mathbb{Z})$ on $\mathbb{R}\setminus\mathbb{Q}$ by linear fractional transformations. To prove this, we develop further the properties of approximation to extremal numbers by quadratic real numbers obtained in [14, §8]. Each extremal number ξ comes with a sequence of best quadratic approximations $\{\alpha_i\}_{i\geqslant 1}$ which is uniquely determined by ξ up to its first terms. In §4, we show that the sequence of their conjugates $\{\bar\alpha_i\}_{i\geqslant 1}$ admits exactly two accumulation points ξ' and ξ'' which are also extremal numbers and which we call the *conjugates* of ξ. Then, in §5, we show that $\nu(\xi)=\nu(\xi')=\nu(\xi'')$ and that these Lagrange constants can be computed as the infima of the absolute values of the binary real quadratic forms

$$|\xi-\xi'|^{-1}(T-\xi U)(T-\xi' U) \quad \text{and} \quad |\xi-\xi''|^{-1}(T-\xi U)(T-\xi'' U)$$

on $\mathbb{Z}^2\setminus\{(0,0)\}$. The latter quantities admit handy representations in terms of doubly infinite words attached to the continued fraction expansions of ξ and ξ' on one hand, and of ξ and ξ'' on the other hand. This is at the basis of Markoff's original approach. However, it requires that $0<\xi<1$ and $\max\{\xi',\xi''\}<-1$. In §6, we show that each extremal number is $\mathrm{GL}_2(\mathbb{Z})$-equivalent to exactly one extremal number ξ satisfying $0<\xi<1$ and having conjugates ξ' and ξ'' of unequal negative integral parts. We say that such an extremal number is *balanced.* We also provide a characterization of the numbers $\xi_{\mathbf{m}}$ in terms of their continued fraction expansions. Finally, we conclude in §7 with the proof of our main result by showing that any balanced extremal number ξ with $\nu(\xi)=\frac{1}{3}$ is equivalent to some $\xi_{\mathbf{m}}$ on the basis of the strong combinatorial properties shared by the two doubly infinite words attached to ξ. As a corollary, we obtain that an extremal number ξ has $\nu(\xi)=\frac{1}{3}$ if and only if its sequence of best quadratic approximations $\{\alpha_i\}_{i\geqslant 1}$ satisfies $\nu(\alpha_i)>\frac{1}{3}$ for infinitely many indices i.

2. Markoff's theory

A general reference for this section is the exposition given by Cassels in [3, Chapter II]. In the presentation below, we reinterpret his constructions in [3, §II.3], from a point of view closer to the approach of Cohn in [4], to align them with similar constructions arising from the study of extremal numbers.

We first recall that the group $\mathrm{GL}_2(\mathbb{Q})$ acts on the set $\mathbb{R}\setminus\mathbb{Q}$ of irrational numbers by

$$g\cdot\xi=\frac{a\xi+b}{c\xi+d},\quad \text{if } g=\begin{pmatrix} a & b\\ c & d\end{pmatrix}\in\mathrm{GL}_2(\mathbb{Q}), \tag{2}$$

and that we have $\nu(g\cdot\xi)=\nu(\xi)$ for any $g\in\mathrm{GL}_2(\mathbb{Z})$ and any $\xi\in\mathbb{R}\setminus\mathbb{Q}$ [3, §I.3, Corollary]. Consequently, the Lagrange spectrum can be described as the set of values taken by ν on a set of representatives of the equivalence classes of $\mathbb{R}\setminus\mathbb{Q}$ under $\mathrm{GL}_2(\mathbb{Z})$.

A real binary quadratic form $F(U,T)=rU^2+qUT+sT^2\in\mathbb{R}[U,T]$ is said to be *indefinite* if its *discriminant* $\mathrm{disc}(F)=q^2-4rs$ is positive. For such a form, one is interested in the quantity

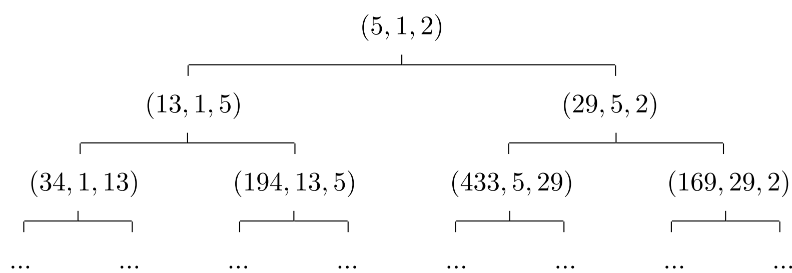
$$\mu(F):=\inf\{|F(x,y)|:(x,y)\in\mathbb{Z}^2\setminus\{(0,0)\}\}.$$

Keeping the same notation as in (2), the group $\mathbb{R}^*\times\mathrm{GL}_2(\mathbb{Z})$ acts on the set of real indefinite binary quadratic forms by

$$(\lambda,g)\cdot F(U,T)=\lambda F((U,T)g)=\lambda F(aU+cT,\, bU+dT),$$

and this action fixes the ratio $\mu(F)/\sqrt{\mathrm{disc}(F)}$. The *Markoff spectrum* is the set of values of these quotients $\mu(F)/\sqrt{\mathrm{disc}(F)}$, where F runs through the set of all real indefinite binary quadratic forms or equivalently through a system of representatives of the equivalence classes of these forms under the above action of $\mathbb{R}^*\times\mathrm{GL}_2(\mathbb{Z})$. Although this spectrum contains strictly the Lagrange spectrum [5, Chapter 3, Theorem 1], a remarkable feature of Markoff's theory is that the intersections of the two spectra with the interval $\left(\frac{1}{3},1/\gamma\right]$ are equal (recall that $\gamma=\frac{1}{2}(1+\sqrt{5}\,)$).

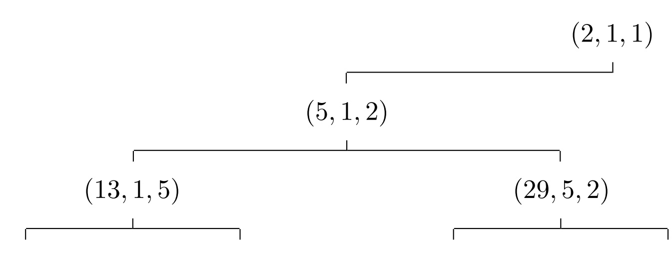
The theory provides explicit sets of representatives both for the equivalence classes of real numbers ξ with $\nu(\xi)>\frac{1}{3}$ and for the equivalence classes of real indefinite binary quadratic forms F with $\mu(F)/\sqrt{\mathrm{disc}(F)}>\frac{1}{3}$. They are parameterized by the solutions in positive integers $\mathbf{m}=(m, m_1, m_2)$ of Markoff's equation (1) upon identifying two solutions when one is a permutation of the other. Setting aside the "degenerate solutions" $(1,1,1)$ and $(2,1,1)$ which have at least two equal entries, all other solutions in positive integers appear once and only once in the rooted binary tree



(3)

where each node (m, m_1, m_2) has successors given by $(3mm_1-m_2, m_1, m)$ on the left and by $(3mm_2-m_1, m, m_2)$ on the right. Moreover [3, §II.2] all nodes (m, m_1, m_2) satisfy $m>\max\{m_1, m_2\}$.

The same construction starting with $(2,1,1)$ as a root provides a tree which contains exactly once each triple (m, m_1, m_2) satisfying (1) and $m>\max\{m_1, m_2\}>0$. In this new tree, each non-degenerate solution occurs twice, with the tree (3) appearing as its left half. This suggests to extend the latter by adding $(2,1,1)$ as a right ancestor of $(5,1,2)$:



(4)

In this extended tree, a node $\mathbf{m}=(m, m_1, m_2)$ has $m_1>m_2$ if and only if $\mathbf{m}$ has a left ancestor. In the sequel, we denote by Σ^* the set of all nodes of the tree (4), and by $\Sigma=\Sigma^*\cup\{(1,1,1)\}$ the set of all positive solutions of the Markoff equation (1).

The next proposition lifts (3) to a tree whose nodes are triples of symmetric matrices in $\mathrm{SL}_2(\mathbb{Z})$ (compare with [3, §II.3] and [4, §5]).

Proposition 2.1. *Put*

$$M=\begin{pmatrix}3 & 1\\ -1 & 0\end{pmatrix}$$

and consider the binary rooted tree

$$\left(\begin{pmatrix}5 & 3\\ 3 & 2\end{pmatrix},\begin{pmatrix}1 & 1\\ 1 & 2\end{pmatrix},\begin{pmatrix}2 & 1\\ 1 & 1\end{pmatrix}\right)$$

$$\left(\begin{pmatrix}13 & 8\\ 8 & 5\end{pmatrix},\begin{pmatrix}1 & 1\\ 1 & 2\end{pmatrix},\begin{pmatrix}5 & 3\\ 3 & 2\end{pmatrix}\right)\qquad\left(\begin{pmatrix}29 & 17\\ 17 & 10\end{pmatrix},\begin{pmatrix}5 & 3\\ 3 & 2\end{pmatrix},\begin{pmatrix}2 & 1\\ 1 & 1\end{pmatrix}\right)$$

$$\ldots\qquad\ldots\qquad\ldots\qquad\ldots\tag{5}$$

where each node $(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$ *has successors* $(\mathbf{x}_1M\mathbf{x},\mathbf{x}_1,\mathbf{x})$ *on the left and* $(\mathbf{x}M\mathbf{x}_2,\mathbf{x},\mathbf{x}_2)$ *on the right. Then each node* $(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$ *of this tree is a triple of symmetric matrices in* $\mathrm{SL}_2(\mathbb{Z})$ *with positive entries of the form*

$$\mathbf{x}=\begin{pmatrix}m & k\\ k & l\end{pmatrix},\quad \mathbf{x}_1=\begin{pmatrix}m_1 & k_1\\ k_1 & l_1\end{pmatrix}\quad\text{and}\quad \mathbf{x}_2=\begin{pmatrix}m_2 & k_2\\ k_2 & l_2\end{pmatrix}\tag{6}$$

satisfying both $\mathbf{x}=\mathbf{x}_1M\mathbf{x}_2$ *and* $\max\{k,l\}\leqslant m\leqslant 2k$. *Moreover, the tree formed by replacing each of these triples of matrices* $(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$ *by the triple of their upper left entries* (m,m_1,m_2) *is exactly the tree* (3) *of non-degenerate solutions of the Markoff equation.*

Proof. We first note that the triple of upper left entries of the root of this tree is the root $(5,1,2)$ of the Markoff tree (3). Now, suppose that a node $(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$ of the tree consists of symmetric matrices in $\mathrm{SL}_2(\mathbb{Z})$ satisfying $\mathbf{x}=\mathbf{x}_1M\mathbf{x}_2$, and that the corresponding triple (m,m_1,m_2) is a node of the Markoff tree. Using Cayley–Hamilton's theorem, we find that

$$\begin{aligned}\mathbf{x}_1M\mathbf{x}&=(\mathbf{x}_1M)^2\mathbf{x}_2=(\mathrm{tr}(\mathbf{x}_1M)\mathbf{x}_1M-\det(\mathbf{x}_1M)I)\mathbf{x}_2=3m_1\mathbf{x}-\mathbf{x}_2,\\ \mathbf{x}M\mathbf{x}_2&=\mathbf{x}_1(M\mathbf{x}_2)^2=\mathbf{x}_1(\mathrm{tr}(M\mathbf{x}_2)M\mathbf{x}_2-\det(M\mathbf{x}_2)I)=3m_2\mathbf{x}-\mathbf{x}_1.\end{aligned}\tag{7}$$

Since $\mathbf{x}$, $\mathbf{x}_1$ and $\mathbf{x}_2$ are symmetric matrices in $\mathrm{SL}_2(\mathbb{Z})$ and since $M\in\mathrm{SL}_2(\mathbb{Z})$, we conclude that these products are also symmetric matrices in $\mathrm{SL}_2(\mathbb{Z})$. Moreover, if we write

$$\mathbf{x}_1M\mathbf{x}=\begin{pmatrix}m_2' & k_2'\\ k_2' & l_2'\end{pmatrix}\quad\text{and}\quad \mathbf{x}M\mathbf{x}_2=\begin{pmatrix}m_1' & k_1'\\ k_1' & l_1'\end{pmatrix},$$

then we get $m_2'=3mm_1-m_2$ and $m_1'=3mm_2-m_1$, showing that the triples (m_2',m_1,m) and (m_1',m,m_2) associated with the left and right successors of $(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$ are respectively the left and right successors of (m, m_1, m_2) in the Markoff tree. By recurrence, this proves all the assertions of the proposition besides the constraints on the coefficients of the matrices. To prove the latter, suppose that the node $(\mathbf{x}, \mathbf{x}_1, \mathbf{x}_2)$ satisfies conditions of the form

$$\varphi(\mathbf{x}) \geqslant \varphi(\mathbf{x}_i) \geqslant c \quad \text{for } i = 1, 2, \tag{8}$$

for some constant $c \geqslant 0$ and some linear form φ on the space of 2×2 matrices. Then, using the fact that m_1 and m_2 are positive (because $(m, m_1, m_2) \in \Sigma^*$), the relations (7) lead to

$$\begin{aligned}\varphi(\mathbf{x}_1 M \mathbf{x}) &= 3m_1\varphi(\mathbf{x}) - \varphi(\mathbf{x}_2) \geqslant \varphi(\mathbf{x}) \geqslant \varphi(\mathbf{x}_1) \geqslant c,\\ \varphi(\mathbf{x} M \mathbf{x}_2) &= 3m_2\varphi(\mathbf{x}) - \varphi(\mathbf{x}_1) \geqslant \varphi(\mathbf{x}) \geqslant \varphi(\mathbf{x}_2) \geqslant c,\end{aligned}$$

showing by induction on the level that (8) holds for each node of the tree (5) as soon as it holds for its root. Since the latter satisfies $m \geqslant m_i \geqslant 1$, $k \geqslant k_i \geqslant 1$ and $l \geqslant l_i \geqslant 1$ for $i = 1, 2$, we conclude that each node of the tree meets these conditions and so consists of matrices with positive entries. Moreover, since the root also satisfies $m - k \geqslant m_i - k_i \geqslant 0$ and $2k - m \geqslant 2k_i - m_i \geqslant 0$ for $i = 1, 2$, each node meets these additional conditions and in particular satisfies $k \leqslant m \leqslant 2k$. Finally, since $(m, m_1, m_2) \in \Sigma^*$, we have $m > \max\{m_1, m_2\} \geqslant 1$. Thus $m \geqslant 2$ and, from $1 = \det(\mathbf{x}) = ml - k^2$, we deduce that $l = (k^2+1)/m \leqslant m + 1/m < m + 1$, and therefore $l \leqslant m$. □

For each node $\mathbf{m} = (m, m_1, m_2)$ of (3), we denote by

$$\mathbf{x}_{\mathbf{m}} = \begin{pmatrix} m & k \\ k & l \end{pmatrix} \tag{9}$$

the first component of the corresponding node (6) of the tree (5), and we extend this definition to all of Σ by putting

$$\mathbf{x}_{(1,1,1)} = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix} \quad \text{and} \quad \mathbf{x}_{(2,1,1)} = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}. \tag{10}$$

Then, for each $\mathbf{m} \in \Sigma$, we define

$$F_{\mathbf{m}}(U, T) = (T \quad -U)\mathbf{x}_{\mathbf{m}} M \begin{pmatrix} U \\ T \end{pmatrix} = mT^2 + (3m - 2k)TU + (l - 3k)U^2, \tag{11}$$

using the notation (9). Since $\det(\mathbf{x}_{\mathbf{m}}) = ml - k^2 = 1$, we find that $\operatorname{disc}(F_{\mathbf{m}}) = 9m^2 - 4$. As $\operatorname{disc}(F_{\mathbf{m}}) \equiv 2 \bmod 3$, the form $F_{\mathbf{m}}$ is irreducible over $\mathbb{Q}$. Therefore it factors as a product

$$F_{\mathbf{m}}(U, T) = m(T - \alpha_{\mathbf{m}} U)(T - \bar{\alpha}_{\mathbf{m}} U),$$

where

$$\alpha_{\mathbf{m}} = \frac{2k-3m+\sqrt{9m^2-4}}{2m} \quad \text{and} \quad \bar{\alpha}_{\mathbf{m}} = \frac{2k-3m-\sqrt{9m^2-4}}{2m} \tag{12}$$

are conjugate quadratic real numbers.

In his presentation of Markoff's theory, Cassels also defines quadratic forms indexed by solutions $\mathbf{m}$ of Markoff's equation, except that, assuming the uniqueness conjecture, he denotes them simply F_m, where m is the largest entry of $\mathbf{m}$, the conjecture being that this entry determines uniquely the solution (see [3, p. 33] or [1, Appendix B]). In view of the discussion in [3, §II.4], the corollary below shows that the above forms $F_{\mathbf{m}}$ are equivalent to the corresponding forms defined by Cassels.

COROLLARY 2.2. *For each* $\mathbf{m}=(m,m_1,m_2)\in\Sigma$ *the off-diagonal entry* k *of* $\mathbf{x_m}$ *satisfies*

$$k \equiv \frac{m_1}{m_2} \equiv -\frac{m_2}{m_1} \mod m \quad \textit{and} \quad 0<k\leqslant m. \tag{13}$$

Note that condition (13) makes sense since each triple of Σ has pairwise relatively prime components [3, §II.3, Lemma 5]. It also determines k uniquely.

Proof. This is readily checked when $\mathbf{m}$ is $(1,1,1)$ or $(2,1,1)$. Now, assume that $\mathbf{m}$ is non-degenerate and write the corresponding triple of symmetric matrices $(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$ in the form (6). Since $\mathbf{x}=\mathbf{x_m}$, this notation is consistent with (9). Then, by Proposition 2.1, we have $0<k\leqslant m$. As $\mathbf{x}$, $\mathbf{x}_1$ and $\mathbf{x}_2$ are symmetric, taking the transpose of both sides of the equality $\mathbf{x}=\mathbf{x}_1 M\mathbf{x}_2$ gives $\mathbf{x}=\mathbf{x}_2\,{}^tM\mathbf{x}_1$, and so we obtain $\mathbf{x}\mathbf{x}_2^{-1}=\mathbf{x}_1M$ and $\mathbf{x}\mathbf{x}_1^{-1}=\mathbf{x}_2\,{}^tM$. Comparing the upper right entries in the latter matrix equalities, we find that $km_2-mk_2=m_1$ and $km_1-mk_1=-m_2$, from which the requested congruences follow. □

Combining Theorems II and III in [3, Chapter II], we then recover the following main results of Markoff [11], [12].

THEOREM 2.3. (Markoff, 1879/80) *The real numbers* $\alpha_{\mathbf{m}}$ *with* $\mathbf{m}\in\Sigma$ *form a system of representatives of the equivalence classes of real numbers* ξ *with* $\nu(\xi)>\frac{1}{3}$, *while the forms* $F_{\mathbf{m}}$ *with* $\mathbf{m}\in\Sigma$ *constitute a system of representatives of the equivalence classes of real indefinite binary quadratic forms* F *with* $\mu(F)/\sqrt{\mathrm{disc}(F)}>\frac{1}{3}$. *Moreover, for each* $\mathbf{m}=(m,m_1,m_2)\in\Sigma$, *the numbers* $\alpha_{\mathbf{m}}$ *and* $\bar{\alpha}_{\mathbf{m}}$ *are equivalent and we have*

$$\nu(\alpha_{\mathbf{m}})=\nu(\bar{\alpha}_{\mathbf{m}})=\frac{\mu(F_{\mathbf{m}})}{\sqrt{\mathrm{disc}(F_{\mathbf{m}})}}=\frac{1}{\sqrt{9-4m^{-2}}}.$$

3. Extremal numbers

Let $\mathcal{P}$ denote the set of 2×2 matrices with relatively prime integer coefficients and non-zero determinant. It is a group for the product $*$ given by $\mathbf{y}_1 * \mathbf{y}_2 = c^{-1}\mathbf{y}_1\mathbf{y}_2$, where c is the greatest positive common divisor of the coefficients of $\mathbf{y}_1\mathbf{y}_2$. This group contains $\mathrm{GL}_2(\mathbb{Z})$ as a subgroup, and its quotient $\mathcal{P}/\{\pm I\}$ is isomorphic to $\mathrm{PGL}_2(\mathbb{Q})$. With this notation, we state the following characterization of extremal numbers reproduced from [17, Lemma 3.1], which collects results from [14] and [15].

Proposition 3.1. *Let ξ be an extremal real number. Then, there exists an unbounded sequence of symmetric matrices $\{\mathbf{x}_i\}_{i\geqslant 1}$ in $\mathcal{P}$ such that, for each $i\geqslant 1$, we have*

$$\|\mathbf{x}_{i+1}\| \asymp \|\mathbf{x}_i\|^{\gamma}, \quad \|(\xi,-1)\mathbf{x}_i\| \asymp \|\mathbf{x}_i\|^{-1} \quad \textit{and} \quad |\det \mathbf{x}_i| \asymp 1, \tag{14}$$

with implied constants that are independent of i. Such a sequence $\{\mathbf{x}_i\}_{i\geqslant 1}$ is uniquely determined by ξ up to its first terms and up to multiplication of each of its terms by ± 1. Moreover, for any such sequence, there exists a non-symmetric and non-skew-symmetric matrix $M\in\mathcal{P}$ such that

$$\mathbf{x}_{i+2} = \pm\begin{cases} \mathbf{x}_{i+1} * M * \mathbf{x}_i, & \textit{if } i \textit{ is odd},\\ \mathbf{x}_{i+1} * {}^tM * \mathbf{x}_i, & \textit{if } i \textit{ is even}, \end{cases} \tag{15}$$

for any sufficiently large index i. Conversely, if $\{\mathbf{x}_i\}_{i\geqslant 1}$ is an unbounded sequence of symmetric matrices in $\mathcal{P}$ which satisfies a recurrence relation of the type (15) *for some non-symmetric matrix $M\in\mathcal{P}$, and if for each $i\geqslant 1$ we have*

$$\|\mathbf{x}_{i+2}\| \gg \|\mathbf{x}_{i+1}\|\,\|\mathbf{x}_i\| \quad \textit{and} \quad |\det \mathbf{x}_i| \ll 1, \tag{16}$$

then $\{\mathbf{x}_i\}_{i\geqslant 1}$ also satisfies the estimates (14) *for some extremal real number ξ.*

In the above statement, the choice of a norm for matrices is secondary, since it only affects the implied constants in all estimates. However, for definiteness, we choose the norm $\|\mathbf{x}\|$ of a matrix $\mathbf{x}$ with real coefficients to be the largest absolute value of its coefficients. Then, for an extremal number ξ with a corresponding unbounded sequence of symmetric matrices $\{\mathbf{x}_i\}_{i\geqslant 1}$ in $\mathcal{P}$ satisfying (14), we find that

$$\|(\xi,-1)\mathbf{x}_i\| = \max\{|x_{i,0}\xi - x_{i,1}|, |x_{i,1}\xi - x_{i,2}|\} \quad \text{upon writing } \mathbf{x}_i = \begin{pmatrix} x_{i,0} & x_{i,1}\\ x_{i,1} & x_{i,2}\end{pmatrix},$$

and therefore $\xi = \lim_{i\to\infty} x_{i,1}/x_{i,0} = \lim_{i\to\infty} x_{i,2}/x_{i,1}$.

It can be shown directly from the definition that the set of extremal numbers is stable under the action of $\mathrm{GL}_2(\mathbb{Q})$ by linear fractional transformations on $\mathbb{R}\setminus\mathbb{Q}$ [17, §2]. In particular, it is stable under the action of the subgroup $\mathrm{GL}_2(\mathbb{Z})$. The next corollary shows how the latter action affects the corresponding sequences of symmetric matrices $\{\mathbf{x}_i\}_{i\geqslant 1}$ and the corresponding matrices M.

Corollary 3.2. *Let ξ be an extremal number, let $\{\mathbf{x}_i\}_{i\geqslant 1}$ be an unbounded sequence of symmetric matrices in $\mathcal{P}$ satisfying* (14) *and let $M\in\mathcal{P}$ be such that* (15) *holds. For any*

$$g=\begin{pmatrix} a & b \\ c & d \end{pmatrix}\in \mathrm{SL}_2(\mathbb{Z}),$$

the number $\xi':=g\cdot\xi$ is also extremal with corresponding sequence $\{\mathbf{x}'_i\}_{i\geqslant 1}$ and matrix M' given by

$$\mathbf{x}'_i={}^t(g')^{-1}\mathbf{x}_i(g')^{-1} \quad \textit{and} \quad M'=g'M\,{}^tg', \quad \textit{where} \ \ g'=\begin{pmatrix} a & -b \\ -c & d \end{pmatrix}. \tag{17}$$

Proof. It is clear that the above matrices $\mathbf{x}'_i$ and M' belong to $\mathcal{P}$ and satisfy the recurrence relation (15) instead of $\mathbf{x}_i$ and M. Moreover, the matrices $\mathbf{x}'_i$ are symmetric while M' is both non-symmetric and non-skew-symmetric. We also find that $\|\mathbf{x}'_i\|\asymp\|\mathbf{x}_i\|$,

$$\|(\xi',-1)\mathbf{x}'_i\|=|c\xi+d|^{-1}\|(\xi,-1)\mathbf{x}_i(g')^{-1}\|\asymp\|(\xi,-1)\mathbf{x}_i\|,$$

and $\det(\mathbf{x}'_i)=\det(\mathbf{x}_i)$. Therefore $\{\mathbf{x}'_i\}_{i\geqslant 1}$ and ξ' also satisfy (14) instead of $\{\mathbf{x}_i\}_{i\geqslant 1}$ and ξ. In particular, $\{\mathbf{x}'_i\}_{i\geqslant 1}$ satisfies (16) and so, by the last part of Proposition 3.1, it obeys (14) for some extremal number ξ'' instead of ξ. This forces $\xi'=\xi''$, and therefore ξ' is extremal. □

It follows from Proposition 3.1 that the matrix $M\in\mathcal{P}$ attached to an extremal number ξ is uniquely determined by ξ within the set $\{M,-M,{}^tM,-{}^tM\}$. When the sequence of symmetric matrices attached to ξ is contained in $\mathrm{SL}_2(\mathbb{Z})$, the matrix M also belongs to $\mathrm{SL}_2(\mathbb{Z})$ and the recurrence relation (15) can be put in a simpler form. Then, applying an identity of Fricke like Cohn in [4], we obtain the following result.

Lemma 3.3. *Let ξ be an extremal number with a corresponding sequence of symmetric matrices $\{\mathbf{x}_i\}_{i\geqslant 1}$ in $\mathrm{SL}_2(\mathbb{Z})$. Choose $M\in\mathrm{SL}_2(\mathbb{Z})$ and the above sequence so that, for each $i\geqslant 1$, we have*

$$\mathbf{x}_{i+2}=\mathbf{x}_{i+1}M_{i+1}\mathbf{x}_i, \quad \textit{where} \ \ M_i=\begin{cases} M, & \textit{if } i \textit{ is even}, \\ {}^tM, & \textit{if } i \textit{ is odd}. \end{cases}$$

Then, for each $i\geqslant 1$, the traces $q_i:=\mathrm{tr}(\mathbf{x}_iM_i)\in\mathbb{Z}$ satisfy

$$q_{i+2}^2+q_{i+1}^2+q_i^2=q_{i+2}q_{i+1}q_i+\mathrm{tr}({}^tMM^{-1})+2. \tag{18}$$

Proof. In [9] Fricke shows that for any $A, B \in \mathrm{SL}_2(\mathbb{R})$ we have

$$\mathrm{tr}(A)^2+\mathrm{tr}(B)^2+\mathrm{tr}(AB)^2=\mathrm{tr}(A)\,\mathrm{tr}(B)\,\mathrm{tr}(AB)+\mathrm{tr}(ABA^{-1}B^{-1})+2.$$

Putting $A=\mathbf{x}_{i+1}M_{i+1}$ and $B=\mathbf{x}_iM_i$, the recurrence relation gives

$$AB=\mathbf{x}_{i+2}M_i=\mathbf{x}_{i+2}M_{i+2},$$

and so $\mathrm{tr}(AB)=q_{i+2}$. Since $\mathbf{x}_{i+2}$ is symmetric, we also find that

$$AB={}^t\mathbf{x}_{i+2}M_i=\mathbf{x}_iM_i\mathbf{x}_{i+1}M_i=BAM_{i+1}^{-1}M_i,$$

and so $\mathrm{tr}(ABA^{-1}B^{-1})=\mathrm{tr}(M_{i+1}^{-1}M_i)$. The conclusion follows since

$$\mathrm{tr}(M_{i+1}^{-1}M_i)=\mathrm{tr}({}^tM_{i+2}^{-1}\,{}^tM_{i+1})=\mathrm{tr}(M_{i+2}^{-1}M_{i+1})$$

is independent of i. □

We observed in [13] that the arithmetic of extremal numbers is particularly simple when the corresponding sequence of symmetric matrices $\{\mathbf{x}_i\}_{i\geqslant 1}$ is contained in $\mathrm{GL}_2(\mathbb{Z})$ and the lower right entry of the corresponding matrix M is 0. When all these matrices belong to $\mathrm{SL}_2(\mathbb{Z})$, the preceding result applies and we find the following result.

Lemma 3.4. *Let u be a non-zero integer and let $\mathcal{E}_u^+$ denote the set of all extremal numbers with a corresponding sequence of symmetric matrices*

$$\mathbf{x}_i=\begin{pmatrix} x_{i,0} & x_{i,1}\\ x_{i,1} & x_{i,2}\end{pmatrix}\in\mathrm{SL}_2(\mathbb{Z})$$

satisfying, for each $i\geqslant 1$,

$$\mathbf{x}_{i+2}=\mathbf{x}_{i+1}M_{i+1}\mathbf{x}_i,\quad \textit{where } M_i=\begin{pmatrix} u & (-1)^i\\ (-1)^{i+1} & 0\end{pmatrix}. \tag{19}$$

Then, the set $\mathcal{E}_u^+=\mathcal{E}_{-u}^+$ is empty if $u\neq\pm 3$. Moreover, if $\xi\in\mathcal{E}_3^+$, then, upon choosing the matrices $\mathbf{x}_i$ as above, each triple $(x_{i+2,0},x_{i+1,0},x_{i,0})$ is a solution of Markoff's equation (1).

Proof. Let $\xi\in\mathcal{E}_u^+$. Using the notation of the lemma, a simple computation shows that the matrix $M{:=}M_2$ satisfies $\mathrm{tr}({}^tM\,M^{-1})=-2$ and that, for each $i\geqslant 1$, we have $\mathrm{tr}(\mathbf{x}_iM_i)=ux_{i,0}$. Therefore, Lemma 3.3 gives

$$x_{i+2,0}^2+x_{i+1,0}^2+x_{i,0}^2=u\,x_{i+2,0}\,x_{i+1,0}\,x_{i,0} \tag{20}$$

for each $i\geqslant 1$. Since -1 is not a square modulo 3 and since $1=\det(\mathbf{x}_i)\equiv -x_{i,1}^2 \bmod x_{i,0}$, we also note that $x_{i,0}$ is prime to 3 for each $i\geqslant 1$. Then, looking at the equation (20) modulo 3, we deduce that u is divisible by 3 and so, each triple $\frac{1}{3}u(x_{i+2,0},x_{i+1,0},x_{i,0})$ provides a solution of Markoff's equation in integers not all zero. Since each such solution has relatively prime entries, this is possible only if $u=\pm 3$. □

Lemma 3.5. *Two elements ξ and ξ' of $\mathcal{E}_3^+$ are equivalent (under $\mathrm{GL}_2(\mathbb{Z})$) if and only if $\xi'=\pm\xi+b$ for some $b\in\mathbb{Z}$. Each element of $\mathcal{E}_3^+$ is equivalent to one and only one element of $\mathcal{E}_3^+$ in the open interval $\left(\frac{1}{2},1\right)$.*

Proof. The second assertion follows from the first one, since, for each $\xi\in\mathbb{R}\setminus\mathbb{Q}$, there is a unique integer b and a unique choice of sign such that $\pm\xi+b\in\left(\frac{1}{2},1\right)$. To prove the first assertion, suppose that $\xi\in\mathcal{E}_3^+$ and let

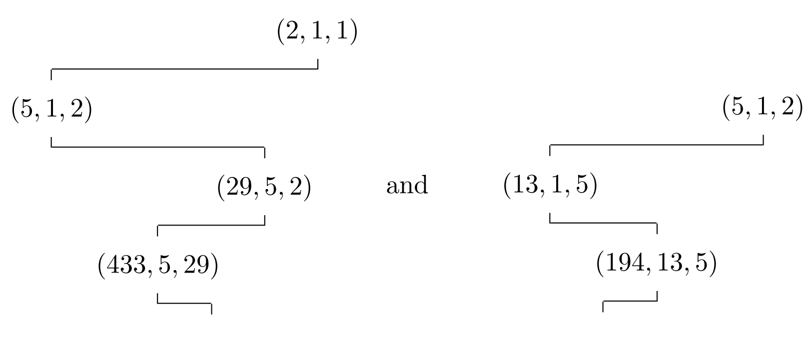
$$g=\begin{pmatrix} a & b \\ c & d \end{pmatrix}\in\mathrm{GL}_2(\mathbb{Z}).$$

By Corollary 3.2, we have $g\cdot\xi\in\mathcal{E}_3^+$ if and only if

$$\begin{pmatrix} a & -b \\ -c & d \end{pmatrix}\begin{pmatrix} 3 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} a & -c \\ -b & d \end{pmatrix}=\varepsilon_1\begin{pmatrix} 3 & \varepsilon_2 \\ -\varepsilon_2 & 0 \end{pmatrix}$$

for some choices of $\varepsilon_1,\varepsilon_2\in\{1,-1\}$. Equating coefficients, this translates into the conditions $3a^2=3\varepsilon_1$, $3c^2=0$ and $\det(g)\pm 3ac=\varepsilon_1\varepsilon_2$, which mean that $\varepsilon_1=1$, $a=\pm1$, $c=0$, $ad=\varepsilon_2$ and impose no restriction on b. For such a, c and d, we find $g\cdot\xi=\varepsilon_2(\xi\pm b)$. □

A *zigzag* in the tree (4) is a sequence of nodes $\mathbf{m}^{(1)},\mathbf{m}^{(2)},\mathbf{m}^{(3)},\dots$ of that tree such that, for each $i\geqslant1$, the node $\mathbf{m}^{(i+1)}$ is a successor of $\mathbf{m}^{(i)}$ on some side (left or right) and $\mathbf{m}^{(i+2)}$ is a successor of $\mathbf{m}^{(i+1)}$ on the other side. A *maximal zigzag* is a zigzag $\mathbf{m}^{(1)},\mathbf{m}^{(2)},\mathbf{m}^{(3)},\dots$ which cannot be extended by inserting an ancestor of $\mathbf{m}^{(1)}$ as the first element. With the convention that the root $(2,1,1)$ has no ancestor in (4), it follows that each $\mathbf{m}\in\Sigma^*$ is the first element of a unique maximal zigzag. Examples of maximal zigzags in (4) are



Recall that, in §2, we attached a symmetric matrix $\mathbf{x}_{\mathbf{m}}\in\mathrm{SL}_2(\mathbb{Z})$ to each $\mathbf{m}\in\Sigma$. Thus, each maximal zigzag in (4) leads to a sequence of symmetric matrices in $\mathrm{SL}_2(\mathbb{Z})$. We can now state and prove the main result of this section.

Theorem 3.6. *Given* $\mathbf{m}\in\Sigma^*$, *consider the maximal zigzag* $\mathbf{m}=\mathbf{m}^{(1)},\mathbf{m}^{(2)},\mathbf{m}^{(3)},\dots$ *in the tree* (4) *originating from* $\mathbf{m}$. *Then* $\{\mathbf{x}_{\mathbf{m}^{(i)}}\}_{i\geqslant 1}$ *is a sequence of symmetric matrices in* $\mathrm{SL}_2(\mathbb{Z})$ *corresponding to an extremal number* $\xi_{\mathbf{m}}$ *in* $\mathcal{E}_3^+\cap\left(\frac{1}{2},1\right)$, *and we have*

$$\xi_{\mathbf{m}}=\lim_{i\to\infty}\alpha_{\mathbf{m}^{(i)}}=\lim_{i\to\infty}(\bar\alpha_{\mathbf{m}^{(i)}}+3) \tag{21}$$

in terms of the quadratic numbers given by (12). *Each element of* $\mathcal{E}_3^+$ *is equivalent to* $\xi_{\mathbf{m}}$ *for one and only one* $\mathbf{m}\in\Sigma^*$.

Proof. Let

$$M=\begin{pmatrix}3&1\\-1&0\end{pmatrix}$$

be as in Proposition 2.1 and let $\{\mathbf{m}^{(i)}\}_{i\geqslant 1}$ be a maximal zigzag in (4) originating from a point $\mathbf{m}=\mathbf{m}^{(1)}$ in Σ^*. For simplicity, we write $\mathbf{x}_i$ to denote the matrix $\mathbf{x}_{\mathbf{m}^{(i)}}$. If, for some index i, the point $\mathbf{m}^{(i+1)}$ is the left successor of $\mathbf{m}^{(i)}$, then the node of the tree (5) corresponding to $\mathbf{m}^{(i+1)}$ takes the form $(\mathbf{x}_{i+1},*,\mathbf{x}_i)$ and, as $\mathbf{m}^{(i+2)}$ is the right successor of $\mathbf{m}^{(i+1)}$, we find that $\mathbf{x}_{i+2}=\mathbf{x}_{i+1}M\mathbf{x}_i$. Similarly, if $\mathbf{m}^{(i+1)}$ is the right successor of $\mathbf{m}^{(i)}$, then the node of (5) corresponding to $\mathbf{m}^{(i+1)}$ takes the form $(\mathbf{x}_{i+1},\mathbf{x}_i,*)$ and $\mathbf{m}^{(i+2)}$ is the left successor of $\mathbf{m}^{(i+1)}$. Thus $\mathbf{x}_{i+2}=\mathbf{x}_iM\mathbf{x}_{i+1}=\mathbf{x}_{i+1}\,{}^tM\mathbf{x}_i$. As the parity of i decides which alternative holds, we deduce that condition (15) of Proposition 3.1 is satisfied for each $i\geqslant 1$ with the present choice of M or with M replaced by its transpose ${}^tM$. The above considerations also show that, for each $i\geqslant 1$, the node of (5) corresponding to $\mathbf{m}^{(i+2)}$ is either $(\mathbf{x}_{i+2},\mathbf{x}_{i+1},\mathbf{x}_i)$ or $(\mathbf{x}_{i+2},\mathbf{x}_i,\mathbf{x}_{i+1})$ and so $\mathbf{m}^{(i+2)}$ can be described as the node of the Markoff tree (4) formed by the upper left entries of $\mathbf{x}_{i+2}$, $\mathbf{x}_{i+1}$ and $\mathbf{x}_i$.

To verify conditions (16) of Proposition 3.1, we write

$$\mathbf{x}_i=\begin{pmatrix}m_i&k_i\\k_i&l_i\end{pmatrix}.$$

With this notation, Proposition 2.1 gives $\|\mathbf{x}_i\|=m_i$ and $k_i\leqslant m_i\leqslant 2k_i$ for each $i\geqslant 1$. Thus, if $\mathbf{x}_{i+2}=\mathbf{x}_{i+1}M\mathbf{x}_i$, we find that

$$m_{i+2}=(3m_{i+1}-k_{i+1})m_i+m_{i+1}k_i\geqslant\tfrac{5}{2}m_{i+1}m_i.$$

Otherwise, we have $\mathbf{x}_{i+2}=\mathbf{x}_iM\mathbf{x}_{i+1}$ and the same computation applies with the indices i and $i+1$ permuted. This means that $\|\mathbf{x}_{i+2}\|\geqslant\frac{5}{2}\|\mathbf{x}_{i+1}\|\,\|\mathbf{x}_i\|$ for each $i\geqslant 1$. As $\det(\mathbf{x}_i)=1$ for each i, conditions (16) of Proposition 3.1 are fulfilled and therefore $\{\mathbf{x}_i\}_{i\geqslant 1}$ satisfies the conditions (14) of the same proposition for some extremal number $\xi=\xi_{\mathbf{m}}$. We have $\xi_{\mathbf{m}}\in\mathcal{E}_3^+$ by definition, and moreover $\xi_{\mathbf{m}}=\lim_{i\to\infty}k_i/m_i\in\left[\frac{1}{2},1\right]$. Then (21) follow from formulas (12) and, as $\xi_{\mathbf{m}}$ is irrational, we conclude that $\xi_{\mathbf{m}} \in \mathcal{E}_3^+ \cap \left(\frac{1}{2}, 1\right)$. The first assertion of the theorem is proved.

Now assume that $\xi_{\mathbf{m}} = \xi_{\mathbf{n}}$ for some $\mathbf{n} \in \Sigma^*$, and let $\{\mathbf{n}^{(i)}\}_{i \geqslant 1}$ denote the maximal zigzag starting with $\mathbf{n}^{(1)} = \mathbf{n}$. Then, $\{\mathbf{x}_{\mathbf{m}^{(i)}}\}_{i \geqslant 1}$ and $\{\mathbf{x}_{\mathbf{n}^{(i)}}\}_{i \geqslant 1}$ are two sequences of symmetric matrices with positive entries corresponding to the same extremal number. By Proposition 3.1, this is possible if and only if there exists an integer s such that $\mathbf{x}_{\mathbf{m}^{(i)}} = \mathbf{x}_{\mathbf{n}^{(i+s)}}$ for each sufficiently large i. However, we observed that, for each $i \geqslant 1$, the triple $\mathbf{m}^{(i+2)}$ is the node of (4) formed by the upper left entries of $\mathbf{x}_{\mathbf{m}^{(i+2)}}$, $\mathbf{x}_{\mathbf{m}^{(i+1)}}$ and $\mathbf{x}_{\mathbf{m}^{(i)}}$. Similarly, $\mathbf{n}^{(i+2)}$ is formed by the upper left entries of $\mathbf{x}_{\mathbf{n}^{(i+2)}}$, $\mathbf{x}_{\mathbf{n}^{(i+1)}}$ and $\mathbf{x}_{\mathbf{n}^{(i)}}$. This forces $\mathbf{m}^{(i)} = \mathbf{n}^{(i+s)}$ for each sufficiently large i, and therefore $\mathbf{m} = \mathbf{n}$ because each zigzag in (4) is contained in a unique maximal zigzag.

Lemma 3.5 together with the preceding observation reduce the last assertion of the theorem to proving that each element of $\mathcal{E}_3^+ \cap \left(\frac{1}{2}, 1\right)$ is equal to $\xi_{\mathbf{m}}$ for some $\mathbf{m} \in \Sigma^*$. To this end, we fix a point $\xi \in \mathcal{E}_3^+ \cap \left(\frac{1}{2}, 1\right)$ and a corresponding sequence $\{\mathbf{x}_i\}_{i \geqslant 1}$ of symmetric matrices in $\mathrm{SL}_2(\mathbb{Z})$ obeying the recurrence relation (19) of Lemma 3.4 with $u = 3$. Using the notation of that lemma for the entries of $\mathbf{x}_i$, we have $\xi = \lim_{i \to \infty} x_{i,1}/x_{i,0}$. Since ξ belongs to $\left(\frac{1}{2}, 1\right)$, the ratio $x_{i,1}/x_{i,0}$ must also belong to that interval for each sufficiently large integer i. Without loss of generality, we may assume that this already holds for each $i \geqslant 1$. Upon multiplying $\mathbf{x}_1$ and $\mathbf{x}_2$ by ± 1 and adjusting the following $\mathbf{x}_i$ so that (19) continues to hold, we may also assume that $x_{1,0}$ and $x_{2,0}$ are positive. Then a simple recurrence argument based on (19) shows that $x_{i,0} > \max\{x_{i-1,0}, x_{i-2,0}\} > 0$ for each $i \geqslant 3$. By Lemma 3.4, this means that, for each $i \geqslant 3$, exactly one of the points $(x_{i,0}, x_{i-1,0}, x_{i-2,0})$ and $(x_{i,0}, x_{i-2,0}, x_{i-1,0})$ is a node $\mathbf{m}^{(i)}$ of the tree (4). In particular, the integers $x_{i,0}$, $x_{i-1,0}$ and $x_{i-2,0}$ are pairwise relatively prime.

We claim that $\mathbf{x}_i = \mathbf{x}_{\mathbf{m}^{(i)}}$ for each $i \geqslant 3$. Since the symmetric matrices $\mathbf{x}_i$ and $\mathbf{x}_{\mathbf{m}^{(i)}}$ have the same upper left entries and the same determinant, this reduces to showing that the off-diagonal entry k of $\mathbf{x}_{\mathbf{m}^{(i)}}$ is $x_{i,1}$. In the notation of Lemma 3.4 (with $u = 3$), we have $\mathbf{x}_i \mathbf{x}_{i-2}^{-1} = \mathbf{x}_{i-1} M_{i-1}$ which, by comparing the upper right entries of the matrices on both sides (as in the proof of Corollary 2.2), gives $x_{i,1} x_{i-2,0} - x_{i,0} x_{i-2,1} = (-1)^{i-1} x_{i-1,0}$, and therefore

$$x_{i,1} \equiv (-1)^{i-1} \frac{x_{i-1,0}}{x_{i-2,0}} \mod x_{i,0}. \tag{22}$$

By comparison with the conditions that Corollary 2.2 imposes on k, this leads to $k \equiv \pm x_{i,1}$ mod $x_{i,0}$. As Proposition 2.1 gives $\frac{1}{2} x_{i,0} \leqslant k \leqslant x_{i,0}$ and as we know that $\frac{1}{2} x_{i,0} < x_{i,1} < x_{i,0}$, we conclude that $k = x_{i,1}$, and the claim is proved.

Comparing the congruence (22) with those of (13) shows moreover that, for $i \geqslant 3$,

$$\mathbf{m}^{(i)} = \begin{cases} (x_{i,0}, x_{i-1,0}, x_{i-2,0}), & \text{if } i \text{ is odd,} \\ (x_{i,0}, x_{i-2,0}, x_{i-1,0}), & \text{if } i \text{ is even.} \end{cases}$$

Since $\mathbf{m}^{(i+1)}$ has two coordinates in common with $\mathbf{m}^{(i)}$ and a larger first coordinate, this implies that, in the Markoff tree (4), $\mathbf{m}^{(i+1)}$ is the left successor of $\mathbf{m}^{(i)}$ if i is odd, and its right successor if i is even (see [3, §II.3]). Thus, the sequence $\{\mathbf{m}^{(i)}\}_{i\geqslant 3}$ is a zigzag in (4) and $\{\mathbf{x}_{\mathbf{m}^{(i)}}\}_{i\geqslant 3}$ is a sequence of symmetric matrices associated with the extremal number ξ. We conclude that $\xi = \xi_{\mathbf{m}}$, where $\mathbf{m}$ is the first element of the maximal zigzag containing $\{\mathbf{m}^{(i)}\}_{i\geqslant 3}$. □

The main goal of this paper is to show that the set $\{\xi_{\mathbf{m}} : \mathbf{m} \in \Sigma^*\}$ constitutes a system of representatives of the equivalence classes of extremal numbers ξ with $\nu(\xi) = \frac{1}{3}$. By Lemma 3.5, we know that they belong to distinct equivalence classes. The next step is to show that $\nu(\xi_{\mathbf{m}}) = \frac{1}{3}$ for each $\mathbf{m} \in \Sigma^*$. This will be achieved in §5.

4. Conjugates of an extremal number

This section deals with approximation to extremal numbers by quadratic real numbers, and introduces the notion of conjugates of an extremal number, a concept which will play an important role in the sequel. With respect to notation, we define the *norm* $\|F\|$ of a polynomial F over $\mathbb{R}$ to be the largest absolute value of its coefficients, and we define the *height* $H(\alpha)$ of an algebraic number α to be the norm of its minimal polynomial in $\mathbb{Z}[T]$.

Throughout the section, we fix an arbitrary extremal number ξ, a corresponding unbounded sequence of symmetric matrices $\{\mathbf{x}_i\}_{i\geqslant 1}$ in $\mathcal{P}$ satisfying the condition (14) of Proposition 3.1, and a matrix $M \in \mathcal{P}$ which is assumed to satisfy (15) for each $i \geqslant 1$ (this condition on the range of i carries no loss of generality). For each $i \geqslant 1$, we write

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad \mathbf{x}_i = \begin{pmatrix} x_{i,0} & x_{i,1} \\ x_{i,1} & x_{i,2} \end{pmatrix} \quad \text{and} \quad X_i = \|\mathbf{x}_i\|.$$

We also define new matrices

$$W_i = \mathbf{x}_i * M_i, \quad \text{where } M_i = \begin{cases} M, & \text{if } i \text{ is even,} \\ {}^tM, & \text{if } i \text{ is odd,} \end{cases}$$

and real quadratic forms

$$F_i(U,T) = -(U \quad T) J W_i \begin{pmatrix} U \\ T \end{pmatrix} \quad \text{and} \quad G_i(U,T) = -(U \quad T) J \begin{pmatrix} 1 & \xi \\ \xi & \xi^2 \end{pmatrix} M_i \begin{pmatrix} U \\ T \end{pmatrix}.$$

It is clear from the above definition that G_i depends only on the parity of i. A short computation gives the following formulas.

LEMMA 4.1. *For each integer $i \geqslant 1$, we have*

$$G_i(U,T) = \begin{cases} G'(U,T) := (c+d\xi)(T-\xi U)(T-\xi' U), & \text{if } i \text{ is odd}, \\ G''(U,T) := (b+d\xi)(T-\xi U)(T-\xi'' U), & \text{if } i \text{ is even}, \end{cases} \tag{23}$$

where

$$\xi' = -\frac{a+b\xi}{c+d\xi} \quad \text{and} \quad \xi'' = -\frac{a+c\xi}{b+d\xi}. \tag{24}$$

The sets $\{\xi', \xi''\}$ and $\{\pm G', \pm G''\}$ depend only on ξ. Moreover, ξ, ξ' and ξ'' are three distinct extremal numbers.

Proof. The second assertion of the lemma follows from the facts that M is uniquely determined by ξ within the set $\{\pm M, \pm {}^tM\}$ (see §3), and that replacing M by $\pm M$ or by $\pm {}^tM$ just permutes the elements of $\{\xi', \xi''\}$ and $\{\pm G', \pm G''\}$. The real numbers ξ' and ξ'' are extremal because they belong to the $\mathrm{GL}_2(\mathbb{Q})$-orbit of ξ (see [17, §2]). Finally, the numbers ξ, ξ' and ξ'' are distinct because ξ is not quadratic over $\mathbb{Q}$ and, by Proposition 3.1, M is neither symmetric nor skew-symmetric. □

Definition 4.2. The extremal numbers ξ' and ξ'' given by (24) are called the *conjugates* of ξ, while the polynomials G' and G'' given by (23) are called the *real quadratic forms associated* with ξ.

For example, the extremal numbers $\xi_{\mathbf{m}}$ constructed by Theorem 3.6 have associated matrix

$$M = \begin{pmatrix} 3 & 1 \\ -1 & 0 \end{pmatrix},$$

and so a short computation gives the following result.

LEMMA 4.3. *For each $\mathbf{m} \in \Sigma^*$, the conjugates of $\xi_{\mathbf{m}}$ are $\xi_{\mathbf{m}}-3$ and $\xi_{\mathbf{m}}+3$ and its associated quadratic forms are, up to sign,*

$$G_{\mathbf{m}}(U,T) := (T-\xi_{\mathbf{m}}U)(T-(\xi_{\mathbf{m}}-3)U) \quad \text{and} \quad G_{\mathbf{m}}(U, T-3U).$$

In the computations below, we use the fact that, for any $A, B \in \mathcal{P}$, the integer c determined by $A*B = c^{-1}AB$ is a common divisor of $\det(A)$ and $\det(B)$. We also use the estimate $X_{i+1} \asymp X_i^{\gamma}$ coming from (14). The next lemma relates the forms F_i and G_i.

LEMMA 4.4. *For each $i \geqslant 1$, there exists a non-zero rational number r_i with $|r_i| \asymp X_i$ such that $F_i = r_i G_i + \mathcal{O}(X_i^{-1})$.*

Proof. As $W_i = \mathbf{x}_i * M_i$, we have $W_i = c_i^{-1}\mathbf{x}_i M_i$ for some divisor c_i of $\det(M)$. Thus, for i large enough, the rational number $r_i = x_{i,0}/c_i$ is non-zero and satisfies

$$|r_i| \asymp |x_{i,0}| \asymp X_i$$

as well as

$$\|F_i - r_i G_i\| \ll \left\| \mathbf{x}_i - x_{i,0}\begin{pmatrix} 1 & \xi \\ \xi & \xi^2 \end{pmatrix} \right\| \asymp \|(\xi,-1)\mathbf{x}_i\| \asymp X_i^{-1}. \qquad \square$$

The next result provides an alternative formula for the forms F_i, showing that they are essentially homogenous versions of the quadratic polynomials of [14, §8].

LEMMA 4.5. *For each $i \geqslant 1$, we have*

$$F_i(U,T) = \frac{1}{d_i} \begin{vmatrix} U^2 & UT & T^2 \\ x_{i+1,0} & x_{i+1,1} & x_{i+1,2} \\ x_{i+2,0} & x_{i+2,1} & x_{i+2,2} \end{vmatrix}, \tag{25}$$

where d_i is a divisor of $\det(\mathbf{x}_{i+1})$. Moreover, the content of F_i as a polynomial in $\mathbb{Z}[U,T]$ is bounded above independently of i.

Proof. Due to the formulas of [14, §2], the determinant in the right-hand side of (25) can be rewritten as

$$\operatorname{tr}\left(\begin{pmatrix} U^2 & UT \\ UT & T^2 \end{pmatrix} J\mathbf{x}_{i+2} J\mathbf{x}_{i+1} J \right).$$

As $\mathbf{x}_{i+2} = W_i * \mathbf{x}_{i+1} = \varkappa_i^{-1} W_i \mathbf{x}_{i+1}$ for some divisor $\varkappa_i$ of $\det(\mathbf{x}_{i+1})$ and since $\mathbf{x}_{i+1} J \mathbf{x}_{i+1} J = -\det(\mathbf{x}_{i+1}) I$, this expression becomes

$$-\frac{\det(\mathbf{x}_{i+1})}{\varkappa_i} \operatorname{tr}\left(\begin{pmatrix} U^2 & UT \\ UT & T^2 \end{pmatrix} J W_i \right) = \frac{\det(\mathbf{x}_{i+1})}{\varkappa_i} F_i(U,T).$$

This proves the first assertion. Identifying any symmetric matrix

$$\begin{pmatrix} m & k \\ k & l \end{pmatrix}$$

with the triple (m,k,l), formula (25) implies that the content of F_i divides

$$\det(\mathbf{x}_i, \mathbf{x}_{i+1}, \mathbf{x}_{i+2}).$$

The second assertion follows as, by [14, Theorem 5.1], the absolute value of this determinant is bounded above independently of i. $\square$

Combining the above lemma with the results of [14, §8], we obtain the following result.

Proposition 4.6. *There exists an integer* $i_0 \geqslant 1$ *such that, for each* $i \geqslant i_0$, *the polynomial* $F_i(U,T)$ *is irreducible over* $\mathbb{Q}$ *and the root* α_i *of* $F_i(1,T)$ *which is closest to* ξ *is algebraic over* $\mathbb{Q}$ *of degree* 2 *with*

$$H(\alpha_i) \asymp \|F_i\| \asymp X_i \quad \textit{and} \quad |\xi-\alpha_i| \asymp H(\alpha_i)^{-2\gamma-2}.$$

Moreover, for every algebraic number $\alpha \in \mathbb{C}$ *of degree* $\leqslant 2$ *over* $\mathbb{Q}$ *with* $\alpha \neq \alpha_i$ *for each* $i \geqslant i_0$, *we have* $|\xi-\alpha| \gg H(\alpha)^{-4}$.

Proof. According to [14, Theorem 8.2], the polynomial $Q_{i+1}(T) := d_i F_i(1,T)$ is irreducible over $\mathbb{Q}$ for each sufficiently large i. So, for those i, the quadratic form $F_i(U,T)$ is irreducible over $\mathbb{Q}$ and α_i is algebraic over $\mathbb{Q}$ of degree 2. Since by Lemma 4.5 the integer d_i and the content of F_i are bounded, we deduce that $H(\alpha_i) \asymp \|F_i\| \asymp \|Q_{i+1}\|$. According to [14, Proposition 8.1], we also have $\|Q_{i+1}\| \asymp X_i$. The remaining estimates follow from [14, Theorem 8.2]. □

Definition 4.7. In view of the above proposition, the sequence $\{\alpha_i\}_{i \geqslant i_0}$ is uniquely determined by the extremal number ξ up to its first terms. We refer to it as a sequence of *best quadratic approximations* to ξ.

The next lemma provides such sequences for the extremal numbers $\xi_{\mathbf{m}}$ defined in Theorem 3.6, in terms of the quadratic numbers $\alpha_{\mathbf{m}}$ given by (12).

Lemma 4.8. *Let* $\mathbf{m} \in \Sigma^*$ *and let* $\{\mathbf{m}^{(i)}\}_{i \geqslant 1}$ *denote the maximal zigzag in the tree* (4) *starting with* $\mathbf{m}^{(1)} = \mathbf{m}$. *Put* $r=1$ *if* $\mathbf{m}^{(2)}$ *is the right successor of* $\mathbf{m}^{(1)}$ *and* $r=0$ *otherwise. Then a sequence* $\{\alpha_i\}_{i \geqslant 1}$ *of best quadratic approximations to* $\xi_{\mathbf{m}}$ *is given by*

$$\alpha_i = \begin{cases} \alpha_{\mathbf{m}^{(i)}}, & \textit{if } i \equiv r \bmod 2, \\ \bar{\alpha}_{\mathbf{m}^{(i)}} + 3, & \textit{if } i \not\equiv r \bmod 2. \end{cases} \tag{26}$$

Proof. Define $\mathbf{x}_i = \mathbf{x}_{\mathbf{m}^{(i)}}$ for each $i \geqslant 1$ so that $\{\mathbf{x}_i\}_{i \geqslant 1}$ is a sequence of symmetric matrices in $\mathrm{SL}_2(\mathbb{Z})$ corresponding to $\xi_{\mathbf{m}}$ (see Theorem 3.6). By virtue of the choice of r, the triple $\mathbf{m}^{(i+1)}$ is a right successor of $\mathbf{m}^{(i)}$ in (4) if and only if $i \equiv r \bmod 2$. From this we deduce that

$$\mathbf{x}_{i+2} = \mathbf{x}_{i+1} \begin{pmatrix} 3 & (-1)^{i-r+1} \\ (-1)^{i-r} & 0 \end{pmatrix} \mathbf{x}_i$$

for each $i \geqslant 1$ (same argument as in the first paragraph of the proof of Theorem 3.6). Thus, in view of Proposition 4.6, it remains simply to show that, for each sufficiently large i, the real number defined by (26) is the root of the polynomial

$$-(1 \quad T)J\mathbf{x}_i\begin{pmatrix} 3 & (-1)^{i-r} \\ (-1)^{i-r-1} & 0 \end{pmatrix}\begin{pmatrix} 1 \\ T \end{pmatrix},$$

which is closest to $\xi_{\mathbf{m}}$. If $i \equiv r \bmod 2$, this polynomial is simply $F_{\mathbf{m}^{(i)}}(1,T)$ (with the notation of (11)). If $i \not\equiv r \bmod 2$, a short computation shows that it is equal to $-F_{\mathbf{m}^{(i)}}(1,T-3)$. The conclusion follows since the roots of $F_{\mathbf{m}^{(i)}}(1,T)$ are $\alpha_{\mathbf{m}^{(i)}}$ and $\bar{\alpha}_{\mathbf{m}^{(i)}}$ which, according to (21), converge respectively to $\xi_{\mathbf{m}}$ and $\xi_{\mathbf{m}}-3$, as $i \to \infty$. □

The next result justifies the terminology of Definition 4.2.

Proposition 4.9. *Let $\{\alpha_i\}_{i \geqslant i_0}$ be as in Proposition 4.6. Then, as $i \to \infty$, we have*

$$|\xi' - \bar{\alpha}_{2i-1}| \asymp H(\alpha_{2i-1})^{-2} \quad \textit{and} \quad |\xi'' - \bar{\alpha}_{2i}| \asymp H(\alpha_{2i})^{-2}. \tag{27}$$

Therefore, the sequence of conjugates of a sequence of best quadratic approximations to ξ admits exactly two accumulation points, namely the conjugates ξ' and ξ'' of ξ.

Proof. We simply prove (27), since the second assertion follows from it. For each $i \geqslant i_0$, let $p_i := F_i(0,1)$ denote the coefficient of T^2 in $F_i(U,T)$. If $i \geqslant i_0$ is odd, Lemma 4.4 gives

$$(T-\alpha_i U)(T-\bar{\alpha}_i U) = p_i^{-1} F_i(U,T) = (T-\xi U)(T-\xi' U) + \mathcal{O}(X_i^{-2}),$$

and therefore $\alpha_i + \bar{\alpha}_i = \xi + \xi' + \mathcal{O}(X_i^{-2})$, by comparing the coefficients of UT. Since Proposition 4.6 gives $\|F_i\| \asymp X_i$ and $|\alpha_i - \xi| \asymp X_i^{-2\gamma-2}$, we deduce that

$$|p_i| \asymp X_i \quad \text{and} \quad |\bar{\alpha}_i - \xi'| \ll X_i^{-2}.$$

To bound $|\bar{\alpha}_i - \xi'|$ from below, we first note that, since $\xi' \neq \xi$, the above estimates imply

$$|\alpha_i - \alpha_{i+2}| \asymp X_i^{-2\gamma-2}, \quad |\bar{\alpha}_i - \alpha_{i+2}| \asymp 1 \quad \text{and} \quad |\alpha_i - \bar{\alpha}_{i+2}| \asymp 1,$$

and so the resultant of F_i and F_{i+2} satisfies

$$\begin{aligned} |\mathrm{Res}(F_i, F_{i+2})| &= p_i^2 p_{i+2}^2 \, |\alpha_i - \alpha_{i+2}| \, |\bar{\alpha}_i - \alpha_{i+2}| \, |\alpha_i - \bar{\alpha}_{i+2}| \, |\bar{\alpha}_i - \bar{\alpha}_{i+2}| \\ &\ll X_i^2 X_{i+2}^2 X_i^{-2\gamma-2} (|\bar{\alpha}_i - \xi'| + \mathcal{O}(X_{i+2}^{-2})) \\ &\ll X_i^2 |\bar{\alpha}_i - \xi'| + \mathcal{O}(X_{i+1}^{-2}). \end{aligned}$$

If i is large enough this resultant is a non-zero integer. Its absolute value is then bounded below by 1, and the above estimate leads to $|\bar{\alpha}_i - \xi'| \gg X_i^{-2}$. Thus

$$|\bar{\alpha}_i - \xi'| \asymp X_i^{-2} \asymp H(\alpha_i)^{-2}.$$

The proof for i even is similar: it suffices to replace everywhere ξ' by ξ''. □

COROLLARY 4.10. *For each $A \in \mathrm{GL}_2(\mathbb{Q})$, the conjugates of $A\cdot\xi$ are $A\cdot\xi'$ and $A\cdot\xi''$.*

Proof. Fix $A \in \mathrm{GL}_2(\mathbb{Q})$ and a sequence $\{\alpha_i\}_{i\geqslant 1}$ of best quadratic approximations to ξ. Since

$$|A\cdot\xi - A\cdot\alpha_i| \asymp |\xi-\alpha_i| \asymp H(\alpha_i)^{-2\gamma-2} \asymp H(A\cdot\alpha_i)^{-2\gamma-2},$$

we deduce that $\{A\cdot\alpha_i\}_{i\geqslant 1}$ is a sequence of best quadratic approximations to the extremal number $A\cdot\xi$. Thus the conjugates of $A\cdot\xi$ are the accumulation points of the sequence $\{A\cdot\bar{\alpha}_i\}_{i\geqslant 1}$, namely $A\cdot\xi'$ and $A\cdot\xi''$. □

Based on this proposition, a simple computation gives the following result.

COROLLARY 4.11. *Let*

$$N = \begin{pmatrix} b & a \\ -d & -c \end{pmatrix}.$$

Then we have $\xi' = N\cdot\xi$ and $\xi'' = N^{-1}\cdot\xi$. Moreover, for each $i\in\mathbb{Z}$, the conjugates of $N^i\cdot\xi$ are $N^{i-1}\cdot\xi$ and $N^{i+1}\cdot\xi$.

In particular, this shows that ξ is one of the two conjugates of ξ' and also one of the two conjugates of ξ''. Although we will not need the next result in the sequel, we decided to include it, as it provides an attractive complement to Proposition 4.6.

THEOREM 4.12. *Let $\{\alpha_i\}_{i\geqslant i_0}$ be as in Proposition 4.6. For each $i\geqslant i_0$, define*

$$\alpha_i' = \begin{cases} \alpha_i, & \text{if } i \text{ is odd,} \\ N\cdot\bar{\alpha}_i, & \text{if } i \text{ is even,} \end{cases}$$

where N is the integral matrix of Corollary 4.11, then

$$|\xi-\alpha_i'|\,|\xi'-\bar{\alpha}_i'| \asymp H(\alpha_i')^{-2\gamma-4}. \tag{28}$$

For each quadratic or rational number $\alpha\in\mathbb{C}$ not belonging to the sequence $\{\alpha_i'\}_{i\geqslant i_0}$, we have instead

$$|\xi-\alpha|\,|\xi'-\bar{\alpha}| \gg H(\alpha)^{-6}, \tag{29}$$

where $\bar{\alpha}$ denotes the conjugate of α over $\mathbb{Q}$.

Proof. If i is odd, the estimate (28) follows from Propositions 4.6 and 4.9, since $\alpha_i'=\alpha_i$ and $\bar{\alpha}_i'=\bar{\alpha}_i$. If i is even, we find that

$$|\xi-\alpha_i'|\,|\xi'-\bar{\alpha}_i'| = |\xi-N\cdot\bar{\alpha}_i|\,|\xi'-N\cdot\alpha_i| \asymp |N^{-1}\cdot\xi-\bar{\alpha}_i|\,|N^{-1}\cdot\xi'-\alpha_i| = |\xi''-\bar{\alpha}_i|\,|\xi-\alpha_i|,$$

and (28) again follows from Propositions 4.6 and 4.9, because $H(\alpha_i)\asymp H(\alpha_i')$.

To prove the second part of the theorem, we first note that, if $\alpha=\alpha_i$ for some even integer i, then Proposition 4.6 provides $|\xi-\alpha|\asymp H(\alpha)^{-2\gamma-2}$, while the estimates of Proposition 4.9 lead to $|\xi'-\bar{\alpha}|\asymp 1$ since $\xi'\neq\xi''$. Similarly, if $\alpha=N\cdot\bar{\alpha}_i$ for some odd integer i, we find that

$$|\xi'-\bar{\alpha}|=|N\cdot\xi-N\cdot\alpha_i|\asymp|\xi-\alpha_i|\asymp H(\alpha)^{-2\gamma-2} \text{ and } |\xi-\alpha|\asymp|N^{-1}\cdot\xi-\bar{\alpha}_i|=|\xi''-\bar{\alpha}_i|\asymp 1.$$

In both cases, this leads to

$$|\xi-\alpha|\,|\xi'-\bar{\alpha}|\asymp H(\alpha)^{-2\gamma-2}\gg H(\alpha)^{-6}.$$

If $\alpha=\bar{\alpha}_i$ for an integer $i\geqslant i_0$, then we find instead $|\xi-\alpha|\asymp|\xi'-\bar{\alpha}|\asymp 1$ and so (29) holds again. This estimate also holds if $\alpha\in\mathbb{Q}$, because in that case we have $|\xi-\alpha|\gg H(\alpha)^{-3}$ and $|\xi'-\alpha|\gg H(\alpha)^{-3}$ by [14, Theorem 1.3]. We may therefore assume that α is irrational and different from α_i, $\bar{\alpha}_i$ and $N\cdot\bar{\alpha}_i$ for each $i\geqslant i_0$. In this case, Proposition 4.6 gives

$$|\xi-\alpha|\gg H(\alpha)^{-4} \quad\text{and}\quad |\xi'-\bar{\alpha}|\asymp|\xi-N^{-1}\cdot\bar{\alpha}|\gg H(\alpha)^{-4}. \tag{30}$$

Let p denote the positive integer for which the polynomial

$$F(U,T):=p(T-\alpha U)(T-\bar{\alpha}U)$$

has relatively prime integer coefficients. Then, F is an irreducible polynomial of $\mathbb{Z}[T]$ and, for each $i\geqslant i_0$, we have

$$1\leqslant|\mathrm{Res}(F,F_i)|=p^2p_i^2|\alpha-\alpha_i|\,|\alpha-\bar{\alpha}_i|\,|\bar{\alpha}-\alpha_i|\,|\bar{\alpha}-\bar{\alpha}_i|,$$

where $p_i=F_i(0,1)$. Since

$$\begin{aligned} p|p_i|\,|\alpha-\bar{\alpha}_i|\,|\bar{\alpha}-\alpha_i| &\leqslant p|p_i|(2\max\{1,|\alpha|\}\max\{1,|\bar{\alpha}_i|\})(2\max\{1,|\bar{\alpha}|\}\max\{1,|\alpha_i|\})\\ &=4(p\max\{1,|\alpha|\}\max\{1,|\bar{\alpha}|\})(|p_i|\max\{1,|\alpha_i|\}\max\{1,|\bar{\alpha}_i|\})\\ &\ll H(\alpha)H(\alpha_i), \end{aligned}$$

we deduce that

$$1\ll H(\alpha)^2H(\alpha_i)^2|\alpha-\alpha_i|\,|\bar{\alpha}-\bar{\alpha}_i|.$$

If i is odd, Propositions 4.6 and 4.9 also give

$$H(\alpha_i)\asymp X_i, \quad |\alpha-\alpha_i|\leqslant|\xi-\alpha|+\mathcal{O}(X_i^{-2\gamma-2}) \quad\text{and}\quad |\bar{\alpha}-\bar{\alpha}_i|\leqslant|\xi'-\bar{\alpha}|+\mathcal{O}(X_i^{-2}).$$

Combining these estimates, we deduce the existence of a constant $c>0$ such that

$$c\leqslant H(\alpha)^2X_i^2(|\xi-\alpha|+X_i^{-2\gamma-2})(|\xi'-\bar{\alpha}|+X_i^{-2})$$

for each odd integer i. If $|\xi-\alpha|\geqslant\frac{1}{4}cH(\alpha)^{-2}$ or $|\xi'-\bar{\alpha}|\geqslant\frac{1}{4}cH(\alpha)^{-2}$, then the required estimate (29) follows from (30) and we are done. Otherwise, we obtain

$$\tfrac{1}{2}c\leqslant H(\alpha)^2X_i^{-2\gamma-2}+H(\alpha)^2X_i^2|\xi-\alpha|\,|\xi'-\bar{\alpha}|.$$

Choose i to be the smallest positive odd integer such that $H(\alpha)^2X_i^{-2\gamma-2}\leqslant\frac{1}{4}c$. Then we have $X_i\ll H(\alpha)^{1/\gamma}$ and we obtain

$$\tfrac{1}{4}c\leqslant H(\alpha)^2X_i^2|\xi-\alpha|\,|\xi'-\bar{\alpha}|\ll H(\alpha)^{2\gamma}|\xi-\alpha|\,|\xi'-\bar{\alpha}|,$$

which is stronger than (29). □

Remark. A similar argument shows that Theorem 4.12 holds with ξ' replaced by ξ'' and α_i' replaced by α_i'', where

$$\alpha_i''=\begin{cases}\alpha_i, & \text{if } i \text{ is even},\\ N^{-1}\cdot\bar{\alpha}_i, & \text{if } i \text{ is odd}.\end{cases}$$

5. Minima of the associated real quadratic forms

We keep the notation of the preceding section. In particular we deal with a fixed arbitrary extremal number ξ with conjugates ξ' and ξ'' and associated quadratic forms G' and G''. The main result of this section is that

$$\nu(\xi)=\frac{\mu(G')}{\sqrt{\operatorname{disc}(G')}}=\frac{\mu(G'')}{\sqrt{\operatorname{disc}(G'')}}.$$

We will deduce from this that the extremal numbers $\xi_{\mathbf{m}}$, $\mathbf{m}\in\Sigma^*$, constructed by Theorem 3.6 have Lagrange constant $\nu(\xi_{\mathbf{m}})=\frac{1}{3}$. The proof goes through a series of lemmas.

LEMMA 5.1. *Let d denote the least common multiple of all integers* $\det(W_i)$ *with* $i\geqslant1$. *Suppose that* $W_i\equiv W_j \bmod 4d$ *for some indices* $i,j\geqslant1$. *Then,* $W_jW_i^{-1}\in\mathrm{SL}_2(\mathbb{Z})$.

Proof. This follows from the formula

$$W_jW_i^{-1}=\det(W_i)^{-1}W_j\operatorname{Adj}(W_i),$$

where $\operatorname{Adj}(W_i)$ denotes the adjoint of W_i. Since

$$W_j\operatorname{Adj}(W_i)\equiv W_i\operatorname{Adj}(W_i)\equiv\det(W_i)I \mod 4d,$$

and since $\det(W_i)$ divides d, the matrix $W_jW_i^{-1}$ has integer coefficients. Moreover, as $\det(W_i)$ and $\det(W_j)$ divide d and are congruent modulo $4d$, they must be equal, and so $\det(W_jW_i^{-1})=1$. □

Lemma 5.2. *Let $i_0\in\{0,1\}$. There exists an integer $k\geqslant 1$ such that $W_{i+2k}W_i^{-1}\in \mathrm{SL}_2(\mathbb{Z})$ for an infinite set of indices $i\geqslant 1$ with $i\equiv i_0 \bmod 2$.*

Proof. Let d be as in Lemma 5.1, and let $N=(4d)^4$ denote the number of congruence classes of 2×2 integral matrices modulo $4d$. For each integer $j\geqslant 1$ with $j\equiv i_0 \bmod 2$, at least two matrices among $W_j, W_{j+2}, ..., W_{j+2N}$ are congruent modulo $4d$. So there exist integers i and k, with $i\geqslant j$, $i\equiv i_0 \bmod 2$ and $1\leqslant k\leqslant N$, such that $W_i\equiv W_{i+2k} \bmod 4d$. By varying j, we get infinitely many such pairs (i,k). As k stays within a finite set, at least one value of k arises infinitely many times. The conclusion follows by Lemma 5.1. □

Lemma 5.3. *For each $i\geqslant 2$, we have $\|W_iW_{i-1}W_i-W_{i-1}W_i^2\|\asymp X_{i-1}$.*

Proof. As $W_i=\mathbf{x}_i*M_i$ and $W_{i-1}=\mathbf{x}_{i-1}*M_{i-1}$ are respectively quotients of $\mathbf{x}_iM_i$ and $\mathbf{x}_{i-1}M_{i-1}$ by divisors of $\det(M)$, this amounts to showing that

$$\|(\mathbf{x}_iM_i\mathbf{x}_{i-1}M_{i-1}-\mathbf{x}_{i-1}M_{i-1}\mathbf{x}_iM_i)\mathbf{x}_iM_i\|\asymp X_{i-1}.$$

Since $\mathbf{x}_iM_i\mathbf{x}_{i-1}=\mathbf{x}_{i-1}M_{i-1}\mathbf{x}_i$ is the product of $\mathbf{x}_{i+1}$ by a divisor $\varkappa$ of $\det(\mathbf{x}_i)\det(M)$, and since the latter is a bounded integer, this in turn amounts to showing that

$$\|\mathbf{x}_{i+1}(M_{i-1}-M_i)\mathbf{x}_iM_i\|\asymp X_{i-1}.$$

Finally, as $M_{i-1}-M_i=\pm(M-{}^tM)=\pm(b-c)J$, this last estimate follows from the fact that $\mathbf{x}_{i+1}J\mathbf{x}_i=\varkappa^{-1}\mathbf{x}_{i-1}M_{i-1}\mathbf{x}_iJ\mathbf{x}_i=\varkappa^{-1}\det(\mathbf{x}_i)\mathbf{x}_{i-1}M_{i-1}J$ has norm of the same order as $\|\mathbf{x}_{i-1}\|=X_{i-1}$. □

Lemma 5.4. *For each $i\geqslant 2$, we have*

$$\|F_{i+2}((U,T)\,{}^tW_i)-\det(W_i)F_{i+2}(U,T)\|\ll X_{i-1}. \tag{31}$$

Proof. The left-hand side of (31) is the norm of the polynomial

$$-(U\quad T)A\begin{pmatrix}U\\T\end{pmatrix},\quad \text{where } A={}^tW_iJW_{i+2}W_i-\det(W_i)JW_{i+2}.$$

Since $W_{i+2}=W_{i+1}*W_i=W_i*W_{i-1}*W_i$, we find that

$$\begin{aligned}\|A\|&\asymp\|{}^tW_iJW_iW_{i-1}W_i^2-\det(W_i)JW_iW_{i-1}W_i\|\\&=|\det W_i|\,\|JW_{i-1}W_i^2-JW_iW_{i-1}W_i\|\\&\ll X_{i-1},\end{aligned}$$

where the last estimate comes from Lemma 5.3. The conclusion follows. □

LEMMA 5.5. *For each $i \geqslant 2$, we have*

$$\|G_i((U,T)\,{}^tW_i) - \det(W_i)G_i(U,T)\| \ll X_i^{-2}.$$

Proof. Since $G_i = G_{i+2}$, Lemma 4.4 shows that $G_i = r_{i+2}^{-1}F_{i+2} + \mathcal{O}(X_{i+2}^{-2})$ for some non-zero rational number r_{i+2} with $|r_{i+2}| \asymp X_{i+2}$. As $\|W_i\| \asymp X_i$, this gives

$$\begin{aligned} G_i((U,T)\,{}^tW_i) &= r_{i+2}^{-1}F_{i+2}((U,T)\,{}^tW_i) + \mathcal{O}(X_i^2X_{i+2}^{-2}) \\ &= r_{i+2}^{-1}\det(W_i)F_{i+2}(U,T) + \mathcal{O}(X_{i+2}^{-1}X_{i-1}) \quad \text{by Lemma 5.4,} \\ &= \det(W_i)G_i(U,T) + \mathcal{O}(X_{i+2}^{-1}X_{i-1}). \end{aligned}$$

□

LEMMA 5.6. *For any integers $i \geqslant 1$ and $k \geqslant 0$, the matrix $S_{i,k} := W_{i+2k}W_i^{-1}$ satisfies*

$$\|G_{i+1}((U,T)\,{}^tS_{i,k}) - \det(S_{i,k})G_{i+1}(U,T)\| \leqslant cX_{i+1}^{-2},$$

with a constant $c>0$ which is independent of both i and k.

Proof. Define $H_{i,k}(U,T) = G_{i+1}((U,T)\,{}^tS_{i,k}) - \det(S_{i,k})G_{i+1}(U,T)$ for each $i \geqslant 1$ and $k \geqslant 0$. When $k \geqslant 1$, we have that

$$S_{i,k} = S_{i+2,k-1}W_{i+2}W_i^{-1} = a_i^{-1}S_{i+2,k-1}W_{i+1}$$

for some bounded positive integer a_i, and so

$$\begin{aligned} H_{i,k}(U,T) = {} & a_i^{-2}H_{i+2,k-1}((U,T)\,{}^tW_{i+1}) \\ & + a_i^{-2}\det(S_{i+2,k-1})(G_{i+1}((U,T)\,{}^tW_{i+1}) - \det(W_{i+1})G_{i+1}(U,T)). \end{aligned}$$

Since $|\det(S_{i+2,k-1})| \leqslant |\det(W_{i+2k})| \ll 1$, we deduce from Lemma 5.5 that

$$\|H_{i,k}\| \leqslant c_1\|H_{i+2,k-1}\|X_{i+1}^2 + c_1X_{i+1}^{-2}, \tag{32}$$

with a constant $c_1>0$ which is independent of i and k. Put $h_{i,k} = \|H_{i,k}\|X_{i+1}^2$ and choose $c_2>0$ such that $X_iX_{i+1} \leqslant c_2X_{i+2}$ for each $i \geqslant 1$. Then, we find that $X_{i+3}^{-2} \leqslant c_2^4X_i^{-2}X_{i+1}^{-4}$, and so (32) leads to

$$h_{i,k} \leqslant c_1 + c_1c_2^4X_i^{-2}h_{i+2,k-1} \tag{33}$$

for any $i, k \geqslant 1$. Our goal is to show that $h_{i,k}$ is bounded above independently of i and k. To this end, we choose an integer $i_0 \geqslant 1$ such that $X_i^2 \geqslant 2c_1c_2^4$ for each $i \geqslant 2i_0$. Then (33) gives $h_{i,k} \leqslant c_1 + \frac{1}{2}h_{i+2,k-1}$ for each $i \geqslant 2i_0$ and $k \geqslant 1$. Since $h_{i+2k,0} = 0$, this implies that $h_{i,k} \leqslant 2c_1$ whenever $i \geqslant 2i_0$. If $1 \leqslant i < 2i_0 \leqslant 2k$, estimate (33) leads to

$$h_{i,k} \ll 1 + h_{i+2i_0,k-i_0} \leqslant 1 + 2c_1.$$

We conclude that $h_{i,k} \ll 1$ for any $i \geqslant 1$ and $k \geqslant 0$. □

Lemma 5.7. *Let G stand for one of the polynomials G' or G''. For each $\delta>0$, there exists a matrix $S\in\mathrm{SL}_2(\mathbb{Z})$ which satisfies both*

$$\|(\xi,-1)S\|\leqslant\delta \quad \textit{and} \quad \|G((U,T)\,{}^tS)-G(U,T)\|\leqslant\delta. \tag{34}$$

Proof. Put

$$i_0=\begin{cases}0, & \text{if } G=G',\\ 1, & \text{if } G=G'',\end{cases}$$

so that $G=G_{i+1}$ for each integer $i\geqslant 1$ with $i\equiv i_0 \bmod 2$. By Lemma 5.2, there exists an integer $k\geqslant 1$ such that $S_{i,k}=W_{i+2k}W_i^{-1}\in\mathrm{SL}_2(\mathbb{Z})$ for an infinite set I of positive integers i with $i\equiv i_0 \bmod 2$. Since $W_i^{-1}=\det(W_i)^{-1}\,\mathrm{Adj}(W_i)$ and $W_{i+2k}=\mathbf{x}_{i+2k}*M_i$, we find that

$$\|(\xi,-1)S_{i,k}\|\ll\|(\xi,-1)\mathbf{x}_{i+2k}\|\,\|W_i\|\ll X_{i+2k}^{-1}X_i\ll X_{i+1}^{-1}.$$

This, combined with Lemma 5.6 shows that, given $\delta>0$, the matrix $S=S_{i,k}$ satisfies (34) for each sufficiently large $i\in I$. □

Theorem 5.8. *We have*

$$\nu(\xi)=\frac{\mu(G')}{\sqrt{\mathrm{disc}(G')}}=\frac{\mu(G'')}{\sqrt{\mathrm{disc}(G'')}}.$$

Proof. We have $\mathrm{disc}(G')=\theta^2$, where $\theta:=(c+d\xi)(\xi-\xi')$, and

$$G'(U,T)=(c+d\xi)(T-\xi U)(T-\xi' U)=(c+d\xi)(T-\xi U)^2+\theta(T-\xi U)U. \tag{35}$$

Fix a real ε with $0<\varepsilon<1$. By definition, there exists a non-zero point $(u,t)\in\mathbb{Z}^2$ for which $|G'(u,t)|\leqslant\mu(G')+\varepsilon$. Then, by Lemma 5.7, there exists $S\in\mathrm{SL}_2(\mathbb{Z})$ such that the point $(q,p)=(u,t)\,{}^tS\in\mathbb{Z}^2$ satisfies both

$$|q\xi-p|=\left|(\xi,-1)S\begin{pmatrix}u\\ t\end{pmatrix}\right|\leqslant\varepsilon \quad\text{and}\quad |G'(q,p)-G'(u,t)|\leqslant\varepsilon.$$

Combining this with (35), we deduce that

$$\mu(G')+2\varepsilon\geqslant|G'(q,p)|\geqslant|\theta|\,|q(q\xi-p)|-|c+d\xi|\varepsilon^2.$$

By letting ε tend to 0, the integer $|q|$ tends to infinity and we conclude that $\mu(G')\geqslant|\theta|\nu(\xi)$.

The reverse inequality follows directly from (35) by observing that, for each $\varepsilon>0$, there exists a point $(q,p)\in\mathbb{Z}^2$ with $q\geqslant 1$, $|q\xi-p|\leqslant\varepsilon$ and $q|q\xi-p|\leqslant\nu(\xi)+\varepsilon$, and so, by (35), we obtain $\mu(G')\leqslant|G'(q,p)|\leqslant|\theta|(\nu(\xi)+\varepsilon)+|c+d\xi|\varepsilon^2$, which upon letting $\varepsilon\to 0$ gives $\mu(G')\leqslant|\theta|\nu(\xi)$. This shows that $\mu(G')=\nu(\xi)\sqrt{\mathrm{disc}(G')}$. The proof for G'' is similar. □

COROLLARY 5.9. *We have* $\nu(\xi)=\nu(\xi')=\nu(\xi'')$.

Proof. By Corollary 4.11, ξ is one of the two conjugates of ξ'. Thus, G' is a constant multiple of one of the two real quadratic polynomials associated with ξ', and so Theorem 5.8 gives $\nu(\xi')=\mu(G')/\sqrt{\operatorname{disc}(G')}=\nu(\xi)$. Similarly, we find that $\nu(\xi'')=\nu(\xi)$. □

COROLLARY 5.10. *For any* $\mathbf{m}\in\Sigma^*$, *we have* $\nu(\xi_{\mathbf{m}})=\frac{1}{3}\mu(G_{\mathbf{m}})=\frac{1}{3}$, *where* $G_{\mathbf{m}}$ *is as in Lemma* 4.3.

Proof. Fix $\mathbf{m}\in\Sigma^*$. By Theorem 5.8, we have $\nu(\xi_{\mathbf{m}})=\frac{1}{3}\mu(G_{\mathbf{m}})$, since $\operatorname{disc}(G_{\mathbf{m}})=9$. According to Theorem 3.6, we also have $\xi_{\mathbf{m}}=\lim_{i\to\infty}\alpha_{\mathbf{m}^{(i)}}=\lim_{i\to\infty}(\bar{\alpha}_{\mathbf{m}^{(i)}}+3)$, where $\{\mathbf{m}^{(i)}\}_{i\geqslant 1}$ denotes the maximal zigzag in the tree (4) originating from $\mathbf{m}$. In terms of the quadratic forms (11), this means that

$$\frac{G_{\mathbf{m}}}{3}=\lim_{i\to\infty}\frac{F_{\mathbf{m}^{(i)}}}{\sqrt{\operatorname{disc}(F_{\mathbf{m}^{(i)}})}}$$

and thus $\frac{1}{3}\mu(G_{\mathbf{m}})\geqslant\limsup_{i\to\infty}\mu(F_{\mathbf{m}^{(i)}})/\sqrt{\operatorname{disc}(F_{\mathbf{m}^{(i)}})}$. Finally, Theorem 2.3 shows that the latter limit superior is equal to $\frac{1}{3}$. This gives $\nu(\xi_{\mathbf{m}})\geqslant\frac{1}{3}$ and, since $\xi_{\mathbf{m}}$ is not quadratic, we conclude that $\nu(\xi_{\mathbf{m}})=\frac{1}{3}$. □

6. Continued fraction expansions

In this section we define the notions of *reduced* and *balanced* extremal numbers and we describe the continued fraction expansions of the extremal numbers $\xi_{\mathbf{m}}$ introduced in §3. To begin, we first set some additional notation and recall some basic facts about continued fraction expansions.

Let $\mathcal{W}$ denote the monoid of words on the set $\{1,2,3,\dots\}$ of positive integers with the product given by concatenation of words. For any non-empty word $\mathbf{w}$ of $\mathcal{W}$ written either as a sequence $\mathbf{w}=(a_1,\dots,a_k)$ or as a string $\mathbf{w}=a_1\dots a_k$, we define

$$\varphi(\mathbf{w})=\begin{pmatrix}a_1&1\\1&0\end{pmatrix}\dots\begin{pmatrix}a_k&1\\1&0\end{pmatrix}\in\mathrm{GL}_2(\mathbb{Z}),$$

and for the empty word $\varnothing$, we set $\varphi(\varnothing)=I$. Then the map $\varphi:\mathcal{W}\to\mathrm{GL}_2(\mathbb{Z})$ is a morphism of monoids and so, using (2), we get an action of $\mathcal{W}$ on $\mathbb{R}\setminus\mathbb{Q}$ by which a word $\mathbf{w}$ sends a point ξ to $\varphi(\mathbf{w})\cdot\xi$. With our convention that the norm of a matrix is the maximum of the absolute values of its coefficients, we obtain the following estimates.

LEMMA 6.1. *For any* $\mathbf{w}_1,\mathbf{w}_2\in\mathcal{W}$, *we have*

$$\|\varphi(\mathbf{w}_1)\|\,\|\varphi(\mathbf{w}_2)\|\leqslant\|\varphi(\mathbf{w}_1\mathbf{w}_2)\|\leqslant 2\|\varphi(\mathbf{w}_1)\|\,\|\varphi(\mathbf{w}_2)\|.$$

Proof. This follows by observing that, for any non-empty word $\mathbf{w}\in\mathcal{W}$, the matrix $\varphi(\mathbf{w})$ takes the form

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

with $a\geqslant\max\{b,c\}$ and $\min\{b,c\}\geqslant d\geqslant 0$, and so $\|\varphi(\mathbf{w})\|=a$. □

We say that an irrational real quadratic number α is *reduced* if $0<\alpha<1$ and $\bar{\alpha}<-1$, where $\bar{\alpha}$ denotes the conjugate of α over $\mathbb{Q}$. Such a number is characterized as follows.

Lemma 6.2. *Let α be an irrational real quadratic number. Then α is reduced if and only if its continued fraction expansion takes the form $\alpha=[0,\Pi^\infty]=[0,\Pi,\Pi,...]$ for some non-empty word $\Pi=(a_1,...,a_k)$ in $\mathcal{W}$. When this happens the conjugate $\bar{\alpha}$ of α is given by $-\bar{\alpha}=[(\Pi^*)^\infty]=[\Pi^*,\Pi^*,...]$, where $\Pi^*=(a_k,...,a_1)$ is the reverse of Π. Moreover we have $\varphi(\Pi)\cdot(1/\alpha)=1/\alpha$ and $H(\alpha)\leqslant\|\varphi(\Pi)\|$.*

Conversely, if $0<\alpha<1$ and if $\varphi(\Pi)\cdot(1/\alpha)=1/\alpha$ for some non-empty word $\Pi\in\mathcal{W}$, then $\alpha=[0,\Pi^\infty]$, and so α is reduced.

Proof. The first two assertions are due to E. Galois [10]. The other two follow from the fact that the condition $\varphi(\Pi)\cdot(1/\alpha)=1/\alpha$ is equivalent to $1/\alpha=[\Pi,1/\alpha]$, which is in turn equivalent to $\alpha=[0,\Pi^\infty]$, while a short computation shows that it implies that $H(\alpha)\leqslant\|\varphi(\Pi)\|$. □

Since any extremal number comes with exactly two conjugates, it is natural to transpose the notion of reduced irrational real quadratic number to extremal numbers by stating the following.

Definition 6.3. An extremal number ξ is *reduced* if $0<\xi<1$ and if its conjugates ξ' and ξ'' satisfy $\xi'<-1$ and $\xi''<-1$.

Lemma 6.4. *Let $\xi=[a_0,a_1,a_2,...]$ be an extremal number in continued fraction form. For each sufficiently large index $i\geqslant 1$, the number $\xi_i:=[0,a_i,a_{i+1},a_{i+2},...]$ is a reduced extremal number in the $\mathrm{GL}_2(\mathbb{Z})$-equivalence class of ξ. Moreover, for any $i\geqslant 1$ for which ξ_i is reduced, the two conjugates of ξ_{i+1} belong to the open interval $(-a_i-1,-a_i)$.*

Proof. Let ξ' and ξ'' denote the conjugates of ξ. By Corollary 4.10, each ξ_i is extremal with conjugates ξ'_i and ξ''_i given recursively by

$$\xi'_1=\xi'-a_0,\quad \xi''_1=\xi''-a_0,\quad \xi'_{i+1}=\frac{1}{\xi'_i}-a_i,\quad \xi''_{i+1}=\frac{1}{\xi''_i}-a_i\quad (i\geqslant 1).$$

Moreover, since ξ' and ξ'' are distinct from ξ, they have different continued fraction expansions, and so there exists a smallest integer $k\geqslant 0$ such that $[a_0,...,a_k]$ is neither a convergent of ξ' nor one of ξ''. Then, for each index $i\geqslant k+3$, we have $\xi'_i<-1$ and $\xi''_i<-1$, and thus ξ_i is reduced. The last assertion is clear. □

In particular, each extremal number is equivalent to infinitely many reduced ones. We now show that this ambiguity disappears with the following stronger notion.

Definition 6.5. An extremal number is *balanced* if it is reduced and its conjugates have distinct integral parts.

PROPOSITION 6.6. *Any extremal number is equivalent to a unique balanced extremal number.*

Proof. Existence. Let ξ_1 be an extremal number with conjugates ξ_1' and ξ_1''. In order to show that ξ_1 is equivalent to a balanced extremal number, we may assume, in view of Lemma 6.4, that it is reduced. Then, we find continued fraction expansions of the form

$$\xi_1 = [0, a_1, a_2, a_3, \dots], \quad -\xi_1' = [a_0', a_{-1}', a_{-2}', \dots] \quad \text{and} \quad -\xi_1'' = [a_0'', a_{-1}'', a_{-2}'', \dots],$$

for sequences of positive integers $\{a_i\}_{i\geqslant 1}$, $\{a_i'\}_{i\leqslant 0}$ and $\{a_i''\}_{i\leqslant 0}$. If $a_0' \neq a_0''$, then ξ_1 is already balanced. Otherwise, since $\xi_1' \neq \xi_1''$, there exists a largest integer $k \leqslant -1$ such that $a_k' \neq a_k''$. For each $i=0, -1, \dots, k+1$, we put $a_i := a_i' = a_i''$ and define recursively

$$\xi_i := \frac{1}{a_i + \xi_{i+1}}, \quad \xi_i' := \frac{1}{a_i + \xi_{i+1}'} \quad \text{and} \quad \xi_i'' := \frac{1}{a_i + \xi_{i+1}''}.$$

For each of those i, we have

$$\xi_i = [0, a_i, a_{i+1}, a_{i+2}, \dots], \quad -\xi_i' = [a_{i-1}', a_{i-2}', \dots] \quad \text{and} \quad -\xi_i'' = [a_{i-1}'', a_{i-2}'', \dots],$$

and, by Corollary 4.10, the number ξ_i is extremal with conjugates ξ_i' and ξ_i''. In particular, ξ is equivalent to ξ_{k+1} which is balanced.

Uniqueness. Let ξ and η be equivalent balanced extremal numbers. In order to complete the proof of the proposition, it remains only to show that $\xi = \eta$. To this end, write $\xi = [0, a_1, a_2, \dots]$ and $\eta = [0, b_1, b_2, \dots]$. Since ξ and η are equivalent, it follows from Serret's theorem [18, Chapter I, Theorem 6B], that there exist integers $k, l \geqslant 1$ such that $a_{k+i} = b_{l+i}$ for each $i \geqslant 0$. Choose k minimal with this property and define

$$\zeta = [0, a_k, a_{k+1}, \dots] = [0, b_l, b_{l+1}, \dots].$$

If $k>1$, Lemma 6.4 shows that ζ has conjugates in the interval $(-a_{k-1}-1, -a_{k-1})$. Similarly, if $l>1$, it shows that these conjugates lie in the interval $(-b_{l-1}-1, -b_{l-1})$. If $k>1$ and $l>1$, this means that $a_{k-1} = b_{l-1}$, contradicting the choice of k. Thus, we must have $k=1$ or $l=1$, and so ζ is equal to ξ or η. In particular, ζ is balanced. In view of the above, this is possible only if $k=l=1$ which means that $\zeta = \xi = \eta$ as requested. □

The following simple fact is the only combinatorial property that we will need about the continued fraction expansion of general extremal numbers.

Proposition 6.7. *Let* $\xi=[0,a_1,a_2,a_3,\dots]$ *be the continued fraction expansion of an extremal real number from the interval* $(0,1)$. *There are finitely many finite words* $\Pi\in\mathcal{W}$ *whose cube is a prefix of* $P:=a_1a_2a_3\dots$.

Proof. Suppose that Π^3 is a prefix of P for some non-empty finite word $\Pi\in\mathcal{W}$, and consider the quadratic real number $\alpha:=[0,\Pi^\infty]$. By Lemma 6.2, we have $H(\alpha)\leqslant\varphi(\Pi)$. Moreover, since $[0,\Pi^3]$ is a common convergent of both ξ and α, and since its denominator is the largest coefficient $\|\varphi(\Pi^3)\|$ of $\varphi(\Pi^3)$, the theory of continued fractions gives

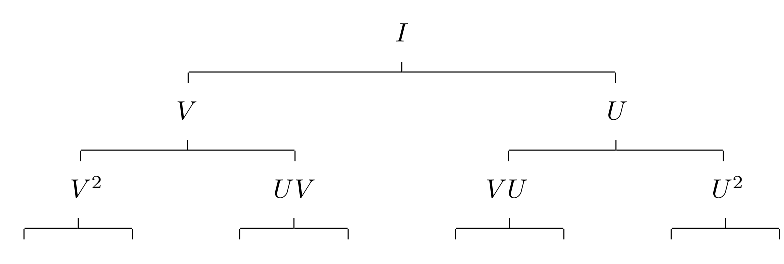
$$|\xi-\alpha|\leqslant|\xi-[0,\Pi^3]|+|\alpha-[0,\Pi^3]|\leqslant 2\|\varphi(\Pi^3)\|^{-2}.$$

By Lemma 6.1, we deduce from this that $|\xi-\alpha|\leqslant 2\,\|\varphi(\Pi)\|^{-6}\leqslant 2H(\alpha)^{-6}$. By Proposition 4.6, this holds only for finitely many quadratic numbers α. In turn, this means that $\|\varphi(\Pi)\|$ is bounded above, and so Π belongs to a finite set of prefixes of P. □

We now turn to a characterization of the continued fraction expansions of the extremal numbers $\xi_{\mathbf{m}}$. In view of the formulas (21), the first step is to describe the continued fraction expansion of the quadratic numbers $\alpha_{\mathbf{m}}$. For this, we denote by $\mathcal{W}_0$ the sub-monoid of $\mathcal{W}$ generated by the words $\mathbf{a}=(1,1)=1\,1$ and $\mathbf{b}=(2,2)=2\,2$. We let the endomorphims of $\mathcal{W}_0$ act on the right on $\mathcal{W}_0$, and denote by U and V the specific such endomorphisms determined by the conditions

$$\mathbf{a}^U=\mathbf{ab},\quad \mathbf{b}^U=\mathbf{b}\quad\text{and}\quad \mathbf{a}^V=\mathbf{a},\quad \mathbf{b}^V=\mathbf{ab},\tag{36}$$

as in [1, §3]. Building on these, we form a tree of endomorphisms of $\mathcal{W}_0$:



(37)

where each node ψ has successors $V\psi$ on the left and $U\psi$ on the right. For each node $\mathbf{m}$ of the Markoff tree (3), we denote by $\psi_{\mathbf{m}}$ the endomorphism of $\mathcal{W}_0$ which occupies the same position. This gives for example $\psi_{(5,1,2)}=I$ and $\psi_{(194,13,5)}=UV$.

LEMMA 6.8. *For each* $\mathbf{m}\in\Sigma$, *the quadratic number* $\alpha_{\mathbf{m}}$ *given by* (12) *is reduced and its continued fraction expansion is* $\alpha_{\mathbf{m}}=[0,\Pi_{\mathbf{m}}^{\infty}]$, *where*

$$\Pi_{\mathbf{m}}=\begin{cases}\mathbf{a}, & \text{if } \mathbf{m}=(1,1,1),\\ \mathbf{b}, & \text{if } \mathbf{m}=(2,1,1),\\ (\mathbf{ab})^{\psi_{\mathbf{m}}}, & \text{otherwise.}\end{cases}$$

Proof. The formulas (12) show that each $\alpha_{\mathbf{m}}$ is a reduced quadratic real number because, in the notation of (12), Proposition 2.1 gives $1\leqslant k\leqslant m\leqslant 2k$. Moreover, since $F_{\mathbf{m}}(1,\alpha_{\mathbf{m}})=0$, we find that $(\mathbf{x}_{\mathbf{m}}M)\cdot(1/\alpha_{\mathbf{m}})=1/\alpha_{\mathbf{m}}$. Thus, in view of Lemma 6.2, it remains simply to prove that $\mathbf{x}_{\mathbf{m}}M=\varphi(\Pi_{\mathbf{m}})$ for each $\mathbf{m}\in\Sigma$. This is a simple computation if $\mathbf{m}$ is one of the degenerate triples $(1,1,1)$ and $(2,1,1)$. For the remaining triples, we claim more precisely that the node $(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$ of (5) which occupies the same position as $\mathbf{m}$ in the Markoff tree (3) satisfies

$$\mathbf{x}M=\varphi((\mathbf{ab})^{\psi_{\mathbf{m}}}),\quad \mathbf{x}_1M=\varphi(\mathbf{a}^{\psi_{\mathbf{m}}})\quad\text{and}\quad \mathbf{x}_2M=\varphi(\mathbf{b}^{\psi_{\mathbf{m}}}). \tag{38}$$

Again, this is a quick computation for the root $(5,1,2)$ of the Markoff tree because, for that triple, we have $\psi_{\mathbf{m}}=I$ and we find that

$$\mathbf{x}M=\begin{pmatrix}12&5\\7&3\end{pmatrix}=\varphi(\mathbf{ab}),\quad \mathbf{x}_1M=\begin{pmatrix}2&1\\1&1\end{pmatrix}=\varphi(\mathbf{a})\quad\text{and}\quad \mathbf{x}_2M=\begin{pmatrix}5&2\\2&1\end{pmatrix}=\varphi(\mathbf{b}).$$

Assume that (38) holds for some node $\mathbf{m}$ of the Markoff tree. The left successor of $(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$ in (5) is $(\mathbf{x}_1M\mathbf{x},\mathbf{x}_1,\mathbf{x})$ and we find that

$$\begin{aligned}\mathbf{x}_1M\mathbf{x}M&=\varphi(\mathbf{a}^{\psi_{\mathbf{m}}})\varphi((\mathbf{ab})^{\psi_{\mathbf{m}}})=\varphi((\mathbf{aab})^{\psi_{\mathbf{m}}})=\varphi((\mathbf{ab})^{V\psi_{\mathbf{m}}}),\\ \mathbf{x}_1M&=\varphi(\mathbf{a}^{\psi_{\mathbf{m}}})=\varphi(\mathbf{a}^{V\psi_{\mathbf{m}}}),\\ \mathbf{x}M&=\varphi((\mathbf{ab})^{\psi_{\mathbf{m}}})=\varphi(\mathbf{b}^{V\psi_{\mathbf{m}}}),\end{aligned}$$

where $V\psi_{\mathbf{m}}$ is the left successor of $\psi_{\mathbf{m}}$ in (37). Similarly, we find that (38) holds with $(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$ replaced by its right successor $(\mathbf{x}M\mathbf{x}_2,\mathbf{x},\mathbf{x}_2)$ and $\psi_{\mathbf{m}}$ replaced by its right successor $U\psi_{\mathbf{m}}$. This proves our claim by induction on the level of $\mathbf{m}$ and therefore completes the proof of the lemma. □

THEOREM 6.9. *Let* $\xi=[0,a_1,a_2,a_3,...]$ *denote the continued fraction expansion of an irrational real number* ξ *with* $0<\xi<1$. *Then* ξ *belongs to the set* $\{\xi_{\mathbf{m}}:\mathbf{m}\in\Sigma^*\}$ *if and only if there exists a finite product* ψ *of* U *and* V *such that* $(\mathbf{ab})^{(VU)^i\psi}$ *is a prefix of* $P:=a_1a_2a_3...$ *for each* $i\geqslant 0$.

Proof. Suppose first that $\xi=\xi_{\mathbf{m}}$ for some $\mathbf{m}\in\Sigma^*$, and let $\{\mathbf{m}^{(i)}\}_{i\geqslant 1}$ denote the maximal zigzag in (4) starting with $\mathbf{m}^{(1)}=\mathbf{m}$. Define $\psi:=\psi_{\mathbf{m}^{(r)}}$, where

$$r=\begin{cases}1, & \text{if } m^{(2)} \text{ is the right successor of } \mathbf{m},\\ 2, & \text{otherwise.}\end{cases}$$

Then, for each $i\geqslant 0$, we have $\psi_{\mathbf{m}^{(2i+r)}}=(VU)^i\psi$ and Lemma 6.8 gives $\alpha_{\mathbf{m}^{(2i+r)}}=[0,\Pi_i^\infty]$ with $\Pi_i:=(\mathbf{ab})^{(VU)^i\psi}$. Since $\mathbf{ab}$ is a prefix of $(\mathbf{ab})^{VU}=\mathbf{ababb}$, we note that Π_i is a prefix of Π_{i+1} for each $i\geqslant 0$. Combining this with the fact that, by Theorem 3.6, the sequence $\{\alpha_{\mathbf{m}^{(2i+r)}}\}_{i\geqslant 0}$ converges to $\xi_{\mathbf{m}}$, we deduce that Π_i must be a prefix of P for each $i\geqslant 0$.

Conversely, suppose that there exists a finite product ψ of U and V such that $\Pi_i:=(\mathbf{ab})^{(VU)^i\psi}$ is a prefix of P for each $i\geqslant 0$. For each $i\geqslant 1$, denote by $\mathbf{m}^{(2i-1)}$ and $\mathbf{m}^{(2i)}$ the nodes of the Markoff tree (3) for which $(VU)^{i-1}\psi=\psi_{\mathbf{m}^{(2i-1)}}$ and $U(VU)^{i-1}\psi=\psi_{\mathbf{m}^{(2i)}}$. Then, by Lemma 6.8, we have $\xi=\lim_{i\to\infty}\alpha_{\mathbf{m}^{(2i-1)}}$ and, by construction, the sequence $\{\mathbf{m}^{(i)}\}_{i\geqslant 1}$ is a zigzag in the tree (4) with $\mathbf{m}^{(2)}$ being the right successor of $\mathbf{m}^{(1)}$. This zigzag is contained in a maximal one starting with some triple $\mathbf{m}\in\Sigma^*$. As Theorem 3.6 shows that $\xi_{\mathbf{m}}=\lim_{i\to\infty}\alpha_{\mathbf{m}^{(2i-1)}}$, we conclude that $\xi=\xi_{\mathbf{m}}$. □

7. Critical doubly infinite words

For each doubly infinite word

$$A=\dots a_{-2}a_{-1}a_0a_1a_2\dots$$

on the set of positive integers, we define

$$L(A)=\sup_{i\in\mathbb{Z}}([0,a_i,a_{i+1},\dots]+[a_{i-1},a_{i-2},\dots])\in[0,\infty]. \tag{39}$$

The relevance of this quantity to our problem is provided by the following key formula for the infimum of reduced real indefinite quadratic forms on $\mathbb{Z}^2\setminus\{(0,0)\}$ (see [5, Appendix 1] or [7, pp. 80–81]).

PROPOSITION 7.1. *Let ξ and η be irrational real numbers with $0<\xi<1$ and $\eta<-1$. Write*

$$\xi=[0,a_1,a_2,a_3,\dots] \quad \textit{and} \quad -\eta=[a_0,a_{-1},a_{-2},\dots].$$

Then the quadratic form $G(U,T)=(T-\xi U)(T-\eta U)\in\mathbb{R}[U,T]$ has

$$\frac{\mu(G)}{\sqrt{\operatorname{disc}(G)}}=L(\dots a_{-2}a_{-1}a_0a_1a_2\dots)^{-1}.$$

Our goal in this ultimate section is to show that any extremal number ξ with Lagrange constant $\nu(\xi)=\frac{1}{3}$ is equivalent to $\xi_{\mathbf{m}}$ for some $\mathbf{m}\in\Sigma^*$. In view of Proposition 6.6, we may restrict to balanced extremal numbers. Then, by combining the above proposition with Theorem 5.8, we obtain the following statement.

Corollary 7.2. *Let ξ be a balanced extremal number with $\nu(\xi)=\frac{1}{3}$. Denote by ξ' and ξ'' its conjugates and form the continued fraction expansions*

$$\xi=[0,a_1,a_2,a_3,\dots],\quad -\xi'=[a'_0,a'_{-1},a'_{-2},\dots]\quad\textit{and}\quad -\xi''=[a''_0,a''_{-1},a''_{-2},\dots].$$

Then, the infinite words $P:=a_1a_2a_3\dots$, $Q':=\dots a'_{-2}a'_{-1}a'_0$ and $Q'':=\dots a''_{-2}a''_{-1}a''_0$ satisfy $L(Q'P)=L(Q''P)=3$. Moreover, P is not ultimately periodic and we have $a'_0\neq a''_0$.

Proof. Let G' and G'' denote the real quadratic forms associated with ξ (see Definition 4.2). According to Proposition 7.1, we have

$$\frac{\mu(G')}{\sqrt{\operatorname{disc}(G')}}=L(Q'P)^{-1}\quad\text{and}\quad\frac{\mu(G'')}{\sqrt{\operatorname{disc}(G'')}}=L(Q''P)^{-1}.$$

Then Theorem 5.8 gives $L(Q'P)=L(Q''P)=\nu(\xi)^{-1}=3$. Finally, P is not ultimately periodic because ξ is not a quadratic number, and we have $a'_0\neq a''_0$ because ξ is balanced. □

In their presentations of Markoff's theory, both Dickson [7] and Bombieri [1] provide a combinatorial analysis of the doubly infinite words A with $L(A)\leqslant 3$. Those with $L(A)<3$ are well understood, they are exactly the purely periodic words with period $\mathbf{a}$, $\mathbf{b}$ or $(\mathbf{ab})^{\psi_{\mathbf{m}}}$ for some $\mathbf{m}$ in the Markoff tree (3) [1, Theorem 15], and so they form a countable set. By contrast, the doubly infinite words A with $L(A)=3$ form an uncountable set. Among these, some are *ultimately periodic* in the sense that they admit a periodic right infinite suffix such as the word $1^\infty\,2\,2\,1^\infty=\dots\,1\,1\,2\,2\,1\,1\,\dots$ (see [7, Theorem 63]). Putting these aside, we state the following.

Definition 7.3. A doubly infinite word A is *critical* if it has $L(A)=3$ and is not ultimately periodic.

In the context of Corollary 7.2, we are facing two critical words $Q'P$ and $Q''P$ with common suffix P. Our next goal is to provide a combinatorial analysis of this situation. Collecting results from the presentation of Bombieri in [1], we first make the following observation.

Lemma 7.4. *Let A be a critical word. There exist an integer $e\geqslant 1$ and a non-constant sequence $\{e_i\}_{i\in\mathbb{Z}}$ consisting of integers from the set $\{e,e+1\}$ such that A factors as*

$$\dots\mathbf{ab}^{e_{-1}}\mathbf{ab}^{e_0}\mathbf{ab}^{e_1}\dots\ (\textit{type I})\quad\textit{or}\quad\dots\mathbf{ba}^{e_{-1}}\mathbf{ba}^{e_0}\mathbf{ba}^{e_1}\dots\ (\textit{type II}).\qquad(40)$$

Moreover, if A is of type I (resp. type II), there exists a unique doubly infinite product B of the words $\mathbf{a}$ *and* $\mathbf{b}$ *such that* $A{=}B^{U^e}$ *(resp.* $A{=}B^{V^e}$*), and B is critical of type II (resp. type I).*

Proof. Since A is not ultimately periodic, Lemma 11 of [1] shows that it can be written in one of the forms (40) for some non-constant sequence of positive integers $\{e_i\}_{i\in\mathbb{Z}}$. Suppose that A is of type I, and put $e{=}\min_{i\in\mathbb{Z}} e_i$. Then, we have $A{=}B^{U^e}$ with $B{=}\dots\mathbf{a}\mathbf{b}^{e_{-1}-e}\mathbf{a}\mathbf{b}^{e_0-e}\mathbf{a}\mathbf{b}^{e_1-e}\dots$. Like A, this word B is not ultimately periodic and Lemma 14 of [1] gives $L(A){=}L(B){=}3$, and thus B is a critical word. Upon choosing an index i such that $e_i{=}e$, we find that B contains the subword $\mathbf{a}\mathbf{b}^{e_i-e}\mathbf{a}{=}\mathbf{a}\mathbf{a}$, and thus B is of type II. From this it follows that each difference e_j-e is equal to 0 or 1, and thus $e_j\in\{e,e+1\}$. The case where A is of type II is similar. □

The second preliminary result given below is connected with the fact that, for each $\mathbf{m}$ in the Markoff tree (3), the matrices $\mathbf{x_m}$ of §2 are symmetric and satisfy

$$\mathbf{x_m} M = \varphi((\mathbf{ab})^{\psi_\mathbf{m}})$$

(for this last relation see the proof of Lemma 6.8).

LEMMA 7.5. *For any finite product ψ of U and V, the word $(\mathbf{ab})^\psi$ admits a factorization of the form* $\mathbf{apb}$, *where* $\mathbf{p}{=}\mathbf{p}^*$ *is a palindrome in* $\mathcal{W}_0$.

The combinatorial argument given below is extracted from the proof of Theorem 15 of [1].

Proof. We proceed by induction on the length of ψ as a product of U and V. If this length is 0, we have $(\mathbf{ab})^\psi{=}\mathbf{apb}$, where $\mathbf{p}{=}\varnothing$ is the empty word. Otherwise, ψ takes one of the forms $\psi'U$ or $\psi'V$ for some product ψ' of U and V of smaller length. By hypothesis, we have $(\mathbf{ab})^{\psi'}{=}\mathbf{ap'b}$ for some palindrome $\mathbf{p'}\in\mathcal{W}_0$. Then $(\mathbf{ab})^\psi$ is either equal to $(\mathbf{ap'b})^U$ or $(\mathbf{ap'b})^V$, and so it takes the form $\mathbf{apb}$, where $\mathbf{p}$ is either $\mathbf{b}(\mathbf{p'})^U$ or $(\mathbf{p'})^V\mathbf{a}$. As $\mathbf{p'}$ is a palindrome, the formulas (7) of [1] show that, in both cases $\mathbf{p}$ is a palindrome. □

THEOREM 7.6. *Let $P{=}a_1a_2a_3\dots$ be a right infinite word which is not ultimately periodic. The following conditions are equivalent*:

(1) *there exist infinite words $Q'{=}\dots a'_{-2}a'_{-1}a'_0$ and $Q''{=}\dots a''_{-2}a''_{-1}a''_0$, with $a'_0\neq a''_0$, such that $L(Q'P){=}L(Q''P){=}3$;*

(2) *there exists a sequence of positive integers $\{n_i\}_{i\geqslant 1}$ such that, upon defining recursively*

$$\psi_1 = U^{n_1-1}, \quad \psi_i = \begin{cases} V^{n_i}\psi_{i-1}, & \text{if } i\geqslant 2 \text{ is even,} \\ U^{n_i}\psi_{i-1}, & \text{if } i\geqslant 3 \text{ is odd,} \end{cases} \tag{41}$$

the word $\mathbf{a}^{\psi_i}$ *is a prefix of* $\mathbf{a}P$ *for each* $i \geqslant 1$.

Moreover, when condition (1) *is fulfilled, one of the words* Q' *or* Q'' *is* $P^*\mathbf{ab}$ *and the other is* $P^*\mathbf{ba}$, *where* P^* *denotes the reciprocal of* P.

In the sequel, we only use the implication (1) $\Rightarrow$ (2). However the reverse implication shows in particular that there are uncountably many right infinite words P satisfying (1).

Proof. Suppose first that the condition (1) is fulfilled. Then, the words $A' := Q'P$ and $A'' := Q''P$ are both critical and, as they admit P as a common suffix, they are products of $\mathbf{a}$ and $\mathbf{b}$ of the same type (see Lemma 7.4). By permuting the words Q' and Q'' if necessary, we may assume without loss of generality that Q' ends with 1 and that Q'' ends with 2.

Suppose first that A' and A'' are of type I. Then there exist sequences of positive integers $\{e'_i\}_{i\in\mathbb{Z}}$ and $\{e''_i\}_{i\in\mathbb{Z}}$ such that

$$A' = \dots \mathbf{ab}^{e'_{-1}}\mathbf{ab}^{e'_0}\mathbf{ab}^{e'_1} \dots \quad \text{and} \quad A'' = \dots \mathbf{ab}^{e''_{-1}}\mathbf{ab}^{e''_0}\mathbf{ab}^{e''_1} \dots .$$

Since A' and A'' admit P as a common suffix, these two sequences coincide from some point on. By shifting the indexation, we may assume that $e'_0 \neq e''_0$ and that $e'_i = e''_i$ for each $i \geqslant 1$. As P is not ultimately periodic, the integers $e_i := e'_i = e''_i$ with $i \geqslant 1$ are not all equal to each other. Then, according to Lemma 7.4, the sequences $\{e'_i\}_{i\in\mathbb{Z}}$, $\{e''_i\}_{i\in\mathbb{Z}}$ and $\{e_i\}_{i\geqslant 1}$ take values in the same set $\{e, e+1\}$ for some integer $e \geqslant 1$. Since the suffix P is preceded by 1 in A' and by 2 in A'', we deduce that $e'_0 = e$ and $e''_0 = e+1$, so that

$$Q' = \dots \mathbf{ab}^{e'_{-2}}\mathbf{ab}^{e'_{-1}}\mathbf{a}, \quad Q'' = \dots \mathbf{ab}^{e''_{-2}}\mathbf{ab}^{e''_{-1}}\mathbf{ab} \quad \text{and} \quad P = \mathbf{b}^{e}\mathbf{ab}^{e_1}\mathbf{ab}^{e_2} \dots, \tag{42}$$

and therefore

$$A' = (Q'_1 P_1)^{U^e} \quad \text{and} \quad A'' = (Q''_1 P_1)^{U^e}$$

for some left infinite words Q'_1 with suffix $\mathbf{a}$ and Q''_1 with suffix $\mathbf{ab}$, and some right infinite word P_1 such that

$$\mathbf{a}P = (\mathbf{a}P_1)^{U^e}. \tag{43}$$

By Lemma 7.4, the words $A'_1 := Q'_1 P_1$ and $A''_1 := Q''_1 P_1$ are both critical of type II.

As the suffix P_1 is preceded by 1 in A'_1 and by 2 in A''_1, the same argument based on Lemma 7.4 shows that there exist an integer $f \geqslant 1$ and sequences $\{f'_i\}_{i<0}$, $\{f''_i\}_{i<0}$ and $\{f_i\}_{i>0}$ taking values in $\{f, f+1\}$ such that

$$Q'_1 = \dots \mathbf{ba}^{f'_{-2}}\mathbf{ba}^{f'_{-1}}\mathbf{ba}, \quad Q''_1 = \dots \mathbf{ba}^{f''_{-2}}\mathbf{ba}^{f''_{-1}}\mathbf{b} \quad \text{and} \quad P_1 = \mathbf{a}^{f}\mathbf{ba}^{f_1}\mathbf{ba}^{f_2} \dots . \tag{44}$$

From this, we deduce that

$$A'_1 = (Q'_2 P_2)^{V^f} \quad \text{and} \quad A''_1 = (Q''_2 P_2)^{V^f}$$

for some left infinite words Q_2' with suffix **ba** and Q_2'' with suffix **b**, and some right infinite word P_2 such that

$$\mathbf{a}P_1 = \mathbf{a}P_2^{V^f} = (\mathbf{a}P_2)^{V^f}. \tag{45}$$

Then, by Lemma 7.4, the words $A_2':=Q_2'P_2$ and $A_2'':=Q_2''P_2$ are both critical of type I.

Combining (43) and (45), we obtain

$$\mathbf{a}P = (\mathbf{a}P_1)^{U^e} = (\mathbf{a}P_2)^{V^f U^e}.$$

Moreover, (42) and (44) show that **ba** is a suffix of Q' and Q_1', while **ab** is a suffix of Q'' and Q_1''. Therefore, by iterating the above construction indefinitely, we obtain a sequence of positive integers $\{n_i\}_{i\geqslant 1}$ starting with $n_1=e+1$ and $n_2=f$, two sequences of left infinite words $\{Q_i'\}_{i\geqslant 1}$ and $\{Q_i''\}_{i\geqslant 1}$, and a sequence of right infinite words $\{P_i\}_{i\geqslant 1}$ with the following properties. For each $i\geqslant 1$, the word **ba** is a suffix of Q_i', the word **ab** is a suffix of Q_i'', and we have

$$A' = (Q_i'P_i)^{\psi_i}, \quad A'' = (Q_i''P_i)^{\psi_i} \quad \text{and} \quad \mathbf{a}P = (\mathbf{a}P_i)^{\psi_i} \tag{46}$$

for the sequence $\{\psi_i\}_{i\geqslant 1}$ defined by (41). If A' and A'' are of type II, we reach the same conclusion upon starting with $n_1=1$, $Q_1'=Q'$, $Q_1''=Q''$ and $P_1=P$. Then, in all cases, we deduce from the last equality in (46) that $\mathbf{a}^{\psi_i}$ is a prefix of $\mathbf{a}P$ for each $i\geqslant 1$, and this proves statement (2).

Lemma 7.5 shows that $(\mathbf{ab})^{\psi}=\mathbf{a}^{U\psi}=\mathbf{b}^{V\psi}$ takes the form $\mathbf{apb}$ with a palindrome $\mathbf{p}\in\mathcal{W}_0$ for any product ψ of U and V. Thus, for any integer $i\geqslant 1$, we can write

$$\mathbf{b}^{\psi_{2i}} = \mathbf{a}\mathbf{p}_{2i}\mathbf{b} \quad \text{and} \quad \mathbf{a}^{\psi_{2i+1}} = \mathbf{a}\mathbf{p}_{2i+1}\mathbf{b}$$

for some palindromes $\mathbf{p}_{2i}$ and $\mathbf{p}_{2i+1}$. Since $\psi_{2i+1}=U^{n_{2i+1}}\psi_{2i}$, we find that

$$(\mathbf{ab})^{\psi_{2i+1}} = \mathbf{a}^{\psi_{2i+1}}\mathbf{b}^{\psi_{2i}} = \mathbf{a}\mathbf{p}_{2i+1}\mathbf{ba}\mathbf{p}_{2i}\mathbf{b}.$$

Thus $\mathbf{p}_{2i+1}\mathbf{ba}\mathbf{p}_{2i}$ is a palindrome, and so

$$\mathbf{p}_{2i+1}\mathbf{ba}\mathbf{p}_{2i} = \mathbf{p}_{2i}\mathbf{ab}\mathbf{p}_{2i+1}. \tag{47}$$

This shows in particular that $\mathbf{p}_{2i}$ is a prefix of $\mathbf{p}_{2i+1}$ because, since $\mathbf{b}^{\psi_{2i}}$ is a proper suffix of $\mathbf{a}^{\psi_{2i+1}}=(\mathbf{ab}^{n_{2i+1}})^{\psi_{2i}}$, the length of $\mathbf{p}_{2i}$ as a product of **a** and **b** is shorter than the length of $\mathbf{p}_{2i+1}$.

Fix any index $i\geqslant 1$. By (46), we have $\mathbf{a}P=(\mathbf{a}P_{2i+1})^{\psi_{2i+1}}$, and thus

$$P = \mathbf{p}_{2i+1}\mathbf{b}P_{2i+1}^{\psi_{2i+1}}. \tag{48}$$

In particular, $\mathbf{p}_{2i+1}$ is a prefix of P and so $\mathbf{p}_{2i}$ is also a prefix of P. As $\mathbf{ab}$ is a suffix of Q''_{2i+1}, we deduce from (46) that A'' admits the suffix

$$\begin{aligned}(\mathbf{ab}P_{2i+1})^{\psi_{2i+1}} &= \mathbf{ap}_{2i+1}\mathbf{bap}_{2i}\mathbf{b}P_{2i+1}^{\psi_{2i+1}} \\ &= \mathbf{ap}_{2i}\mathbf{abp}_{2i+1}\mathbf{b}P_{2i+1}^{\psi_{2i+1}} && \text{by (47)}, \\ &= \mathbf{ap}_{2i}\mathbf{ab}P && \text{by (48)}.\end{aligned}$$

Thus, $\mathbf{p}_{2i}\mathbf{ab}$ is a common suffix of Q'' and $P^*\mathbf{ab}$. Similarly, since $\mathbf{ba}$ is a suffix of Q'_{2i}, the formulas (46) show that A' admits the suffix

$$(\mathbf{ba}P_{2i})^{\psi_{2i}} = \mathbf{b}^{\psi_{2i}}\mathbf{a}P = \mathbf{ap}_{2i}\mathbf{ba}P,$$

and thus $\mathbf{p}_{2i}\mathbf{ba}$ is a common suffix of Q' and $P^*\mathbf{ba}$. Letting i tend to infinity, we deduce that $Q''=P^*\mathbf{ab}$ and that $Q'=P^*\mathbf{ba}$.

Conversely, assume that P satisfies condition (2) of the theorem. To complete the proof, it remains only to show that $L(P^*\mathbf{ab}P)=L(P^*\mathbf{ba}P)=3$. Since $P^*\mathbf{ab}P$ is the reverse of $P^*\mathbf{ba}P$, Lemma 5 of [1] reduces this task to showing that $L(P^*\mathbf{ba}P)=3$. As the palindrome $\mathbf{p}_{2i+1}$ is a prefix of P whose length tends to infinity with i, any finite subword of $P^*\mathbf{ba}P$ is contained in $\mathbf{p}_{2i+1}\mathbf{bap}_{2i+1}$ for some $i\geqslant 1$, and so is contained in the purely periodic word $\dots\Pi_{2i+1}\Pi_{2i+1}\Pi_{2i+1}\dots$ with period $\Pi_{2i+1}=\mathbf{a}^{\psi_{2i+1}}=\mathbf{ap}_{2i+1}\mathbf{b}$. By Theorem 15 of [1], this word has $L(\dots\Pi_{2i+1}\Pi_{2i+1}\dots)<3$ (because $\Pi_{2i+1}=(\mathbf{ab})^{\psi}$ with $\psi=U^{n_{2i+1}-1}\psi_{2i}$). By continuity, this implies that $L(P^*\mathbf{ba}P)\leqslant 3$. Since P is not ultimately periodic, this must be an equality [1, Theorem 15]. □

We can now complete the proof of our main result which reads as follows.

THEOREM 7.7. *The set* $\{\xi_{\mathbf{m}}:\mathbf{m}\in\Sigma^*\}$ *constitute a system of representatives of the* $\mathrm{GL}_2(\mathbb{Z})$*-equivalence classes of extremal numbers* ξ *with* $\nu(\xi)=\frac{1}{3}$.

Proof. According to Theorem 3.6, the extremal numbers $\xi_{\mathbf{m}}$ with $\mathbf{m}\in\Sigma^*$ are pairwise inequivalent and, by Corollary 5.10, their Lagrange constant is $\frac{1}{3}$. It remains to show that any extremal number ξ with $\nu(\xi)=\frac{1}{3}$ is equivalent to one of these. As mentioned at the beginning of this section, in order to show this, we may assume, by Proposition 6.6, that ξ is balanced. Then Corollary 7.2 shows that its continued fraction expansion takes the form $\xi=[0,P]$, where P is a right infinite word on the positive integers which is not ultimately periodic and satisfies the condition (1) of Theorem 7.6. Let $\{n_i\}_{i\geqslant 1}$ be the sequence of positive integers such that, for the corresponding sequence $\{\psi_i\}_{i\geqslant 1}$ of endomorphisms of $\mathcal{W}_0$ given by (41), the word $\mathbf{a}^{\psi_i}$ is a prefix of $\mathbf{a}P$ for each $i\geqslant 1$. Define

$$\mathbf{v}_i = \begin{cases} \mathbf{a}^{\psi_i}, & \text{if } i\geqslant 1 \text{ is odd}, \\ \mathbf{b}^{\psi_i}, & \text{if } i\geqslant 2 \text{ is even}. \end{cases}$$

The recurrence relations (41) translate into

$$\mathbf{v}_{2i+1} = \mathbf{a}^{\psi_{2i+1}} = (\mathbf{a}\mathbf{b}^{n_{2i+1}})^{\psi_{2i}} = \mathbf{v}_{2i-1}\mathbf{v}_{2i}^{n_{2i+1}}, \tag{49}$$

$$\mathbf{v}_{2i+2} = \mathbf{b}^{\psi_{2i+2}} = (\mathbf{a}^{n_{2i+2}}\mathbf{b})^{\psi_{2i+1}} = \mathbf{v}_{2i+1}^{n_{2i+2}}\mathbf{v}_{2i}. \tag{50}$$

We know that $\mathbf{v}_{2i+1}$ is a prefix of $\mathbf{a}P$ for each $i\geqslant 1$. We claim that the reverse $\mathbf{v}_{2i}^*$ of $\mathbf{v}_{2i}$ is a prefix of $\mathbf{b}P$ for each $i\geqslant 1$. To prove this, we note, as in the proof of Theorem 7.6, that $\mathbf{v}_{2i+1}$ is the image of $\mathbf{ab}$ by $U^{n_{2i+1}-1}\psi_{2i}$ and so, by Lemma 7.5, it takes the form $\mathbf{v}_{2i+1}=\mathbf{a}\mathbf{p}_{2i+1}\mathbf{b}$ for some palindrome $\mathbf{p}_{2i+1}$. Then, $\mathbf{p}_{2i+1}$ is a prefix of P. Moreover, formula (49) implies that $\mathbf{v}_{2i}$ is a suffix of $\mathbf{p}_{2i+1}\mathbf{b}$. Thus, $\mathbf{v}_{2i}^*$ is a prefix of $\mathbf{b}\mathbf{p}_{2i+1}$, and so is a prefix of $\mathbf{b}P$.

Using (49) and (50), we also note that, for each $i\geqslant 2$, the word

$$\mathbf{v}_{2i+1} = \mathbf{v}_{2i-1}\mathbf{v}_{2i}^{n_{2i+1}} = \mathbf{v}_{2i-1}(\mathbf{v}_{2i-1}^{n_{2i}}\mathbf{v}_{2i-2})^{n_{2i+1}}$$

admits $\mathbf{v}_{2i-1}^{n_{2i}+1}$ as a prefix, while the word

$$\mathbf{v}_{2i}^* = (\mathbf{v}_{2i-1}^{n_{2i}}\mathbf{v}_{2i-2})^* = ((\mathbf{v}_{2i-3}\mathbf{v}_{2i-2}^{n_{2i-1}})^{n_{2i}}\mathbf{v}_{2i-2})^*$$

admits $(\mathbf{v}_{2i-2}^*)^{n_{2i-1}+1}$ as a prefix. Therefore, $\mathbf{v}_{2i-1}^{n_{2i}+1}$ is a prefix of $\mathbf{a}P$ and $(\mathbf{v}_{2i-2}^*)^{n_{2i-1}+1}$ is a prefix of $\mathbf{b}P$ for each $i\geqslant 2$. Since $[0,\mathbf{a}P]$ and $[0,\mathbf{b}P]$ are the continued fraction expansions of fixed extremal numbers (in the equivalence class of ξ), we deduce from Proposition 6.7 that $n_{2i}=n_{2i+1}=1$ for each sufficiently large integer i, say for $i\geqslant i_0$. Then, upon putting $\psi_0=\psi_{2i_0}$, we obtain

$$\psi_{2i+1} = U(VU)^{i-i_0}\psi_0$$

for each $i\geqslant i_0$, and so

$$\mathbf{a}^{\psi_{2i+1}} = (\mathbf{ab})^{(VU)^{i-i_0}\psi_0}$$

is a prefix of $\mathbf{a}P$ for each $i\geqslant i_0$. By Theorem 6.9, this implies that $[0,\mathbf{a}P]=\xi_{\mathbf{m}}$ for some $\mathbf{m}\in\Sigma^*$. □

We conclude with the following result which provides an additional link between extremal numbers and Markoff's theory.

Corollary 7.8. *Let ξ be an extremal number and let $\{\alpha_i\}_{i\geqslant 1}$ be a sequence of best quadratic approximations to ξ in the sense of Definition* 4.7. *Then the following assertions are equivalent*:

(1) $\nu(\xi)=\frac{1}{3}$;
(2) $\nu(\alpha_i)>\frac{1}{3}$ *for each sufficiently large* i;
(3) $\nu(\alpha_i)>\frac{1}{3}$ *for infinitely many* i.

Proof. Suppose first that $\nu(\xi)=\frac{1}{3}$. Then, by the preceding theorem, ξ is equivalent to $\xi_{\mathbf{m}}$ for some $\mathbf{m}\in\Sigma^*$ and so, by Lemma 4.8, each α_i with i sufficiently large is equivalent to $\alpha_{\mathbf{n}}$ or $\bar{\alpha}_{\mathbf{n}}$ for some $\mathbf{n}\in\Sigma^*$. According to Markoff's Theorem 2.3, these quadratic numbers have $\nu(\alpha_{\mathbf{n}})=\nu(\bar{\alpha}_{\mathbf{n}})>\frac{1}{3}$. This means that $\nu(\alpha_i)>\frac{1}{3}$ for each sufficiently large i, and a fortiori for infinitely many values of i.

Conversely, suppose that $\nu(\alpha_{i_j})>\frac{1}{3}$ for a strictly increasing sequence of positive integers $\{i_j\}_{j\geqslant 1}$. Without loss of generality, we may assume that these integers i_j all have the same parity. Then, by Proposition 4.9, the sequence $\{\bar{\alpha}_{i_j}\}_{j\geqslant 1}$ converges to some conjugate ξ' of ξ and so, upon defining

$$F_j(U,T):=(T-\alpha_{i_j}U)(T-\bar{\alpha}_{i_j}U) \quad \text{and} \quad G'(U,T):=(T-\xi U)(T-\xi' U),$$

we obtain $G'(U,T)/\sqrt{\operatorname{disc}(G')}=\lim_{j\to\infty} F_j(U,T)/\sqrt{\operatorname{disc}(F_j)}$, and thus

$$\nu(\xi)=\frac{\mu(G')}{\sqrt{\operatorname{disc}(G')}}\geqslant \limsup_{j\to\infty}\frac{\mu(F_j)}{\sqrt{\operatorname{disc}(F_j)}},$$

where the equality comes from Theorem 5.8. By Markoff's Theorem 2.3, the above limit superior is equal to $\frac{1}{3}$. This gives $\nu(\xi)\geqslant\frac{1}{3}$, and we conclude that $\nu(\xi)=\frac{1}{3}$ since ξ is not a quadratic number. □

Final remark. For each $\xi\in\mathbb{R}$, denote by $\hat{\lambda}_2(\xi)$ the supremum of all real numbers $\lambda>0$ such that the inequalities

$$|x_0|\leqslant X, \quad |x_0\xi-x_1|\leqslant X^{-\lambda} \quad \text{and} \quad |x_0\xi^2-x_2|\leqslant X^{-\lambda}$$

admit a non-zero solution $(x_0,x_1,x_2)\in\mathbb{Z}^3$ for each sufficiently large value of X. By [16], we know that the values taken by $\hat{\lambda}_2$ on the set of non-quadratic irrational real numbers are dense in the interval $\left[\frac{1}{2},1/\gamma\right]$. It would be interesting to know what happens if instead we consider the values taken by $\hat{\lambda}_2$ on the set of irrational numbers ξ with $\nu(\xi)=\frac{1}{3}$. By looking at Sturmian continued fractions, Y. Bugeaud and M. Laurent showed in [2, Theorem 3.1] that, for each bounded sequence of positive integers $\{s_i\}_{i\geqslant 1}$, there exists a real number ξ with $\hat{\lambda}_2(\xi)=(1+\sigma)/(2+\sigma)$, where $\sigma=\liminf_{k\to\infty}[0,s_k,s_{k-1},,...,s_1]$. I think that, by considering appropriate paths in the Markoff tree (4) like in §3, one should be able to produce real numbers ξ with the same exponents $\hat{\lambda}_2$ and with $\nu(\xi)=\frac{1}{3}$. By analogy with work of S. Fischler in [8], it is possible that this exhausts the set of all possible values taken by $\hat{\lambda}_2$ on the real numbers ξ with $\nu(\xi)=\frac{1}{3}$.

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