

# Sign choices in the AGM for genus two theta constants Jean Kieffer

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## Sign choices in the AGM for genus two theta constants

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#### Abstract

Existing algorithms to compute genus 2 theta constants in quasi-linear time use Borchardt sequences, an analogue of the arithmetic-geometric mean for four complex numbers. In this paper, we show that these Borchardt sequences are only given by good choices of square roots, as in the genus 1 case. This removes the sign indeterminacies when computing genus 2 theta constants without relying on numerical integration.

#### Résumé

Les algorithmes existants pour le calcul de thêta-constantes en genre 2 en temps quasilinéaire utilisent des suites de Borchardt, un analogue de la moyenne arithmético-géométrique pour quatre nombres complexes. Dans cet article, nous montrons que ces suites de Borchardt sont constituées uniquement de bons choix de signes, comme c'est le cas en genre 1. Ce résultat permet de lever les indéterminations de signes lors du calcul de thêta-constantes en genre 2 sans recours à l'intégration numérique.

Keywords: Theta functions, Genus 2, Algorithms, Borchardt mean Subject classification (2010): 11Y35; 11Y16; 11F41; 11F27

#### 1 Introduction

Denote by  $\mathcal{H}_g$  the Siegel half space of principally polarized abelian varieties of dimension g, consisting of all matrices  $\tau \in M_g(\mathbb{C})$  such that  $\tau$  is symmetric and  $\operatorname{Im}(\tau)$  is positive definite; for instance,  $\mathcal{H}_1$  is the usual upper half plane. The theta constants are the holomorphic functions on  $\mathcal{H}_g$  defined by

$$\theta_{a,b}(\tau) = \sum_{m \in \mathbb{Z}^g} \exp\left(i\pi \left(\left(m + \frac{a}{2}\right)^t \tau \left(m + \frac{a}{2}\right) + \left(m + \frac{a}{2}\right)^t b\right)\right), \quad (1)$$

where a and b run through  $\{0,1\}^g$  (by convention, vectors in formula (1) are written vertically). Theta constants have a fundamental importance in the

theory of Siegel modular forms, as every scalar-valued Siegel modular function of any weight on  $\mathcal{H}_g$  has an expression in terms of quotients of theta constants [15, Thm. 9 p. 222]. Moreover, for  $1 \leq g \leq 3$ , then the stronger result that every Siegel modular form is a polynomial in the theta constants holds [13, 14, 9].

In numerical algorithms manipulating modular forms, the following operations are therefore very common: first, given (quotients of) theta constants at a given  $\tau \in \mathcal{H}_g$ , compute  $\tau$ ; second, given  $\tau \in \mathcal{H}_g$ , compute the theta constants  $\theta_{a,b}(\tau)$ . For instance, these operations are important building blocks in algorithms computing modular polynomials [7, 20, 21] or Hilbert class polynomials [6, 8, 25] via complex approximations.

The arithmetic-geometric mean (AGM) [1, 3, 2, 16] gives an algorithm to find  $\tau$  given its theta constants. This algorithm is quasi-linear in terms of the required precision. In order to compute theta constants in quasi-linear time as well, a well-studied strategy is to combine the AGM with Newton iterations. This strategy was first described in [5] in the genus 1 case, in [4] in the genus 2 case, and later extended to theta functions, in opposition to theta constants, in [18, 19]. These references also outline extensions to higher genus.

The genus 1 case. Let us detail the genus 1 case to convey the general idea. After reducing the argument  $\tau \in \mathcal{H}_1$  using Gauss's algorithm [25, §6.1], we can assume that  $\tau$  belongs to the classical fundamental domain under the action of  $\mathrm{SL}_2(\mathbb{Z})$ , denoted by  $\mathcal{F}_1$ .

First assume that theta quotients at  $\tau \in \mathcal{F}_1$  are given. Then the sequence

$$B(\tau) = \left(\frac{\theta_{0,0}^2(2^n \tau)}{\theta_{0,0}^2(\tau)}, \frac{\theta_{0,1}^2(2^n \tau)}{\theta_{0,0}^2(\tau)}\right)_{n > 0}$$

is an AGM sequence, meaning that each term is obtained from the previous one by means of the transformation

$$(x,y) \mapsto \left(\frac{x+y}{2}, \sqrt{x}\sqrt{y}\right)$$

for some choice of the square roots. This is a consequence of the duplication formula [23, p. 221], the correct square roots being the theta quotients themselves. In the algorithm, the sign ambiguity is easily removed using the fact that  $\sqrt{x}$  and  $\sqrt{y}$  should lie in a common open quarter plane [5, Thm. 2]: we say that the sequence  $B(\tau)$  is given by good sign choices. It converges quadratically to  $1/\theta_{0,0}^2(\tau)$ , as the series expansion (1) shows.

It turns out that the sequence  $B(-1/\tau)$  is also an AGM sequence with good sign choices [5, Prop. 7]. Its first term can be computed from theta quotients at  $\tau$  using the transformation formulas for theta constants under  $\mathrm{SL}_2(\mathbb{Z})$ . The limit of  $B(-1/\tau)$  is  $1/\theta_{0,0}^2(-1/\tau)$ . Finally, we can recover  $\tau$  using the formula

$$\theta_{0,0}^2 \left( \frac{-1}{\tau} \right) = -i\tau \theta_{0,0}^2(\tau). \tag{2}$$

Since AGM sequences with good sign choices converge quadratically, this gives an algorithm to *invert* theta functions on  $\mathcal{F}_1$  with quasi-linear complexity in the output precision, at least for fixed  $\tau$ . This method was already known to Gauss [10, X.1, pp. 184–206], and we recommend [3, §3C] for a historical exposition of Gauss's works on the AGM and elliptic functions.

In order to compute theta functions at a given  $\tau \in \mathcal{F}_1$ , the most efficient known method is to build a Newton scheme [5], using the AGM method to invert theta constants. This yields a quasi-linear algorithm to compute genus 1 theta constants, whose complexity can be made uniform in  $\tau \in \mathcal{F}_1$  [5, Thm. 5].

The genus 2 case. A similar strategy can be applied to theta functions in genus 2, using Borchardt sequences, a generalization of AGM sequences for four complex numbers [1, 2, 16]. Let us refer to §2 for the definition of Borchardt sequences, the numbering of genus 2 theta constants, and the definition of the matrices  $\gamma_k \in \operatorname{Sp}_4(\mathbb{Z})$  for  $0 \le k \le 3$ . The Borchardt sequences we consider are the sequences  $B(\gamma_k \tau)$  for  $0 \le k \le 3$ , where

$$B(\tau) = \left(\frac{\theta_0^2(2^n\tau)}{\theta_0^2(\tau)}, \, \frac{\theta_1^2(2^n\tau)}{\theta_0^2(\tau)}, \, \frac{\theta_2^2(2^n\tau)}{\theta_0^2(\tau)}, \, \frac{\theta_3^2(2^n\tau)}{\theta_0^2(\tau)}\right)_{n \geq 0}$$

for every  $\tau \in \mathcal{H}_2$ . Their first terms are given by different combinations of theta quotients at  $\tau$  (see Corollary 3.3). It is known that for a given  $\tau$ , all but a finite number of sign choices in these Borchardt sequences are good, and the other sign choices can be determined using certified computations of hyperelliptic integrals at relatively low precision: see the discussion before Prop. 3.3 in [19], and [22] for an algorithm that provides this input. However, the required precision and the cost of the numerical integration algorithms depend heavily on  $\tau$ .

Actually, when  $\tau$  belongs to the usual fundamental domain  $\mathcal{F}_2$  under the action of  $\mathrm{Sp}_4(\mathbb{Z})$ , practical experiments suggest that *all* sign choices are good in the genus 2 algorithm as well [4, Conj. 9.1], [8, Conj. 9]. The goal of this paper is to prove this fact. More precisely, we define in §2 a subset  $\mathcal{F}' \subset \mathcal{H}_2$  containing  $\mathcal{F}_2$ , and prove the following result.

**Theorem 1.1.** For every  $\tau \in \mathcal{F}'$ , every  $0 \le k \le 3$  and every  $n \ge 0$ , the theta constants

$$\theta_i(2^n \gamma_k \tau)$$
 for  $0 < i < 3$ 

are contained in a common open quarter plane.

Dupont [4, Prop. 9.1] proved this result in the particular case of  $\gamma_0 = I_4$ .

As a consequence, we can invert genus 2 theta constants in quasi-linear time by using only Borchardt sequences with good sign choices. On the practical side, this result reduces the effort needed to invert genus 2 theta constants with controlled precision losses; see for instance [4, §7.4.2] for an analysis of precision losses when computing limits of Borchardt sequences. On the theoretical side, we hope that our result can be a first step towards removing other heuristic assumptions when computing genus 2 theta constants (in particular, the assumption [4, §10.2] that the function used in the Newton scheme is analytic

with invertible Jacobian), and obtaining algorithms with uniform complexity in  $\tau \in \mathcal{F}_2$ .

This document is organized as follows. In Section 2, we introduce our notational conventions. In Section 3, we use the action of the symplectic group to bring the matrices  $2^n \gamma_k \tau \in \mathcal{H}_2$  closer to the cusp at infinity: this is critical to obtain accurate information from the series expansion (1). We give estimates on genus 2 theta constants in Section 4, and we finish the proof of the main theorem in Section 5.

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### 2 Theta constants and Borchardt sequences

We define a Borchardt sequence to be a sequence of complex numbers

$$(s_b^{(n)})_{b \in (\mathbb{Z}/2\mathbb{Z})^2, n \ge 0}$$

with the following property: for every  $n \geq 0$ , there exist  $t_b^{(n)}$  for  $b \in (\mathbb{Z}/2\mathbb{Z})^2$  such that  $t_b^{(n)}$  is a square root of  $s_b^{(n)}$ , and

$$s_b^{(n+1)} = \frac{1}{4} \sum_{b_1 + b_2 = b} t_{b_1}^{(n)} t_{b_2}^{(n)} \quad \text{for each } b \in (\mathbb{Z}/2\mathbb{Z})^2.$$

The duplication formula [23, p. 221] states that for every  $\tau \in \mathcal{H}_2$ , the sequence

$$B(\tau) = \left(\theta_{0,b}^2(2^n \tau)\right)_{b \in \{0,1\}^2, n \ge 0}$$

is a Borchardt sequence; the choice of square roots at each step is given by the theta constants  $\theta_{0,b}(2^n\tau)$  themselves. By the series expansion (1), we have

$$\theta_{0,b}(2^n\tau) = \sum_{m \in \mathbb{Z}^2} \exp\left(-2^n \pi m^t \operatorname{Im}(\tau) m\right) \exp\left(i\pi \left(2^n m^t \operatorname{Re}(\tau) m + m^t b\right)\right).$$

When n tends to infinity, all the terms except m=0 converge rapidly to zero, because  $\text{Im}(\tau)$  is positive definite. Therefore the Borchardt sequence  $B(\tau)$  converges to (1,1,1,1).

We say that a set of complex numbers is  $in\ good\ position$  when it is included in an open quarter plane seen from the origin, i.e. a set of the form

$$\{r \exp(i(\alpha_0 + \alpha)) \mid r > 0 \text{ and } 0 < \alpha < \pi/2\}$$

for some  $\alpha_0 \in \mathbb{R}$ . The property of being in good position is invariant by nonzero complex scaling. A Borchardt sequence is given by *good sign choices* if for every  $n \geq 0$ , the complex numbers  $t_h^{(n)}$  for  $b \in (\mathbb{Z}/2\mathbb{Z})^2$  are in good position.

Let us now detail the algorithm to recover  $\tau \in \mathcal{H}_2$  from its theta quotients. We first introduce the matrices  $\gamma_k \in \operatorname{Sp}_4(\mathbb{Z})$  alluded to in the introduction. Let

$$S_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, S_2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, S_3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

and define the matrix  $\gamma_k \in \operatorname{Sp}_4(\mathbb{Z})$  for  $0 \le k \le 3$  by

$$\gamma_0 = I_4$$
, and  $\gamma_k = \begin{pmatrix} -I_2 & -S_k \\ S_k & -I + S_k^2 \end{pmatrix}$  for  $1 \le k \le 3$ .

For convenience, we also introduce a numbering of theta constants [4, §6.2]:

$$\theta_{(a_0,a_1),(b_0,b_1)} =: \theta_j \text{ where } j = b_0 + 2b_1 + 4a_0 + 8a_1 \in [0,15].$$

Assuming that the choices of square roots in the sequences  $B(\gamma_k \tau)$  can be determined, we can compute  $\tau \in \mathcal{F}_2$  from its theta quotients as follows.

**Algorithm 2.1** ([4, §9.2.3]).

**Input:** The projective vector of squares of theta constants  $\theta_j^2(\tau)$  for  $j \in [0, 15]$ , for some  $\tau \in \mathcal{H}_2$ .

**Output:** The matrix  $\tau$ .

- 1. For each  $0 \le k \le 3$ , compute the first term of the sequence  $B(\gamma_k \tau)/\theta_0^2(\gamma_k \tau)$  using the transformation formulas for theta constants under  $\mathrm{Sp}_4(\mathbb{Z})$  (see Igusa [15, Thm. 2 p. 175 and Cor. p. 176], or Corollary 3.3);
- 2. For each  $0 \le k \le 3$ , compute  $1/\theta_0^2(\gamma_k \tau)$  as the limit of the Borchardt sequence  $B(\gamma_k \tau)/\theta_0^2(\gamma_k \tau)$ ;
- 3. Use the input and the newly computed  $\theta_0^2(\gamma_0\tau) = \theta_0^2(\tau)$  to compute all squares of theta constants at  $\tau$ ;
- 4. Recover  $\tau = \begin{pmatrix} z_1 & z_3 \\ z_3 & z_2 \end{pmatrix}$  using the relations given in [4, §6.3.1]:

$$\theta_0^2(\gamma_1 \tau) = -iz_1 \theta_4^2(\tau), \quad \theta_0^2(\gamma_2 \tau) = -iz_2 \theta_8^2(\tau), \quad \theta_0^2(\gamma_3 \tau) = -\det(\tau) \theta_0^2(\tau).$$

In the sequel, we use the following notational conventions. For  $\tau \in \mathcal{H}_2$ , we write

$$\tau = \begin{pmatrix} z_1(\tau) & z_3(\tau) \\ z_3(\tau) & z_2(\tau) \end{pmatrix} \quad \text{and} \quad \begin{cases} x_j(\tau) = \operatorname{Re} z_j(\tau) \\ y_j(\tau) = \operatorname{Im} z_j(\tau) \end{cases} \quad \text{for } 1 \le j \le 3.$$

For  $1 \le j \le 3$ , we also write

$$q_j(\tau) = \exp(-\pi y_j(\tau)).$$

We denote by  $\lambda_1(\tau)$  the smallest eigenvalue of  $\text{Im}(\tau)$ , and define

$$r(\tau) = \min \left\{ \lambda_1(\tau), \frac{y_1(\tau)}{2}, \frac{y_2(\tau)}{2} \right\}.$$

We often omit the argument  $\tau$  to ease notation. We define  $\mathcal{F}'$  to be the set of all  $\tau \in \mathcal{H}_2$  such that the following conditions are satisfied:

$$|x_{j}(\tau)| \leq \frac{1}{2} \quad \text{for each } 1 \leq j \leq 3,$$

$$2|y_{3}(\tau)| \leq y_{1}(\tau) \leq y_{2}(\tau),$$

$$y_{1}(\tau) \geq \frac{\sqrt{3}}{2},$$

$$|z_{j}(\tau)| \geq 1 \quad \text{for } j \in \{1, 2\}.$$

$$(3)$$

The domain  $\mathcal{F}'$  contains the classical fundamental domain  $\mathcal{F}_2$  for the action of  $\operatorname{Sp}_4(\mathbb{Z})$  on  $\mathcal{H}_2$  [17, Prop. 3 p. 33]. Assumptions similar to (3) are usual when giving analytic estimates on theta constants: for instance, the domain  $\mathcal{B}$  in [25] is defined by the first three inequalities of (3).

Finally, for each  $\tau \in \mathcal{H}_2$ , we write

$$\xi_{4,6}(\tau) = 2 \exp\left(i\pi \frac{z_{1}(\tau)}{4}\right), 
\xi_{8,9}(\tau) = 2 \exp\left(i\pi \frac{z_{2}(\tau)}{4}\right), 
\xi_{0}(\tau) = 1 + 2 \exp(i\pi z_{1}(\tau)) + 2 \exp(i\pi z_{2}(\tau)), 
\xi_{0,2}(\tau) = 1 + 2 \exp(i\pi z_{1}(\tau)), 
\xi_{0,1}(\tau) = 1 + 2 \exp(i\pi z_{2}(\tau)), \text{ and} 
\xi_{12}(\tau) = \exp\left(i\pi \frac{z_{1}(\tau) + z_{2}(\tau)}{4}\right) \left(\exp\left(i\pi \frac{z_{3}(\tau)}{2}\right) + \exp\left(-i\pi \frac{z_{3}(\tau)}{2}\right)\right).$$

These complex numbers correspond to the first term(s) of the series defining theta constants at  $\tau$ . For instance,  $\xi_{4,6}(\tau)$  approximates both  $\theta_4(\tau)$  and  $\theta_6(\tau)$ . We will recall the definitions (4) before using them in the computations of §4.

## 3 Other expressions for theta constants at $2^n \gamma_k \tau$

For every  $n \geq 0$ , we define

$$\eta_1^{(n)} = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 2^n & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \eta_2^{(n)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 2^n \end{pmatrix},$$

$$\eta_3^{(n)} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 2^n & 0 \\ 1 & 0 & 0 & 2^n \end{pmatrix}, \quad \text{and} \quad \eta_4^{(n)} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \eta_3^{(n)}.$$

Lemma 3.1. Let  $n \geq 0$ .

1. For every  $1 \le k \le 4$ , the matrix  $\eta_k^{(n)}$  belongs to  $\operatorname{Sp}_4(\mathbb{Z})$ .

2. For every 
$$\tau = \begin{pmatrix} z_1 & z_3 \\ z_3 & z_2 \end{pmatrix} \in \mathcal{H}_2$$
, we have
$$\tau_1^{(n)} := \eta_1^{(n)} (2^n \gamma_1 \tau) = \begin{pmatrix} 2^{-n} z_1 & z_3 \\ z_3 & 2^n z_2 \end{pmatrix},$$

$$\tau_2^{(n)} := \eta_2^{(n)} (2^n \gamma_2 \tau) = \begin{pmatrix} 2^n z_1 & z_3 \\ z_3 & 2^{-n} z_2 \end{pmatrix},$$

$$\tau_3^{(n)} := \eta_3^{(n)} (2^n \gamma_3 \tau) = 2^{-n} \tau, \quad and$$

$$\tau_4^{(n)} := \eta_4^{(n)} (2^n \gamma_3 \tau) = \begin{pmatrix} -2^n / z_1 & -z_3 / z_1 \\ -z_3 / z_1 & 2^{-n} (z_2 - z_3^2 / z_1) \end{pmatrix}.$$
(5)

*Proof.* 1. The lines of each  $\eta_k^{(n)}$  define a symplectic basis of  $\mathbb{Z}^4$ .

2. The action of  $\mathrm{Sp}_4(\mathbb{Z})$  on  $\mathcal{H}_2$  extends to an action of the larger group

$$\mathrm{GSp}_4(\mathbb{Q}) = \left\{ \gamma \in \mathrm{GL}_4(\mathbb{Q}) \mid \exists \mu \in \mathbb{Q}^\times, \gamma^t \begin{pmatrix} 0 & I_2 \\ -I_2 & 0 \end{pmatrix} \gamma = \mu \begin{pmatrix} 0 & I_2 \\ -I_2 & 0 \end{pmatrix} \right\}.$$

The matrix  $2^n \gamma_k \tau$  is the image of  $\tau$  under

$$\begin{pmatrix} -2^n I_2 & -2^n S_k \\ S_k & -I + S_i^2 \end{pmatrix} \in \mathrm{GSp}_4(\mathbb{Q}).$$

When we multiply this matrix by  $\eta_k^{(n)}$  on the left, we obtain

Diag
$$(-1, -2^n, -2^n, -1)$$
 for  $k = 1$ ,  
Diag $(-2^n, -1, -1, -2^n)$  for  $k = 2$ , and  
Diag $(-1, -1, -2^n, -2^n)$  for  $k = 3$ .

We recall the transformation formulas for theta constants in genus 2. For a square matrix m, we denote by  $m_0$  the column vector containing the diagonal of m.

**Proposition 3.2** ([15, Thm. 2 p. 175 and Cor. p. 176]). Let  $a, b \in \{0, 1\}^2$ , and let

$$\gamma = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in \operatorname{Sp}_4(\mathbb{Z}).$$

Define

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \gamma^t \begin{pmatrix} a - (CD^t)_0 \\ b - (AB^t)_0 \end{pmatrix}.$$

Then, for every  $\tau \in \mathcal{H}_2$ , we have

$$\theta_{a,b}(\gamma \tau) = \kappa(\gamma) \, \zeta_8^{\varepsilon(\gamma,a,b)} \det(C\tau + D)^{1/2} \, \theta_{a',b'}(\tau)$$

where

$$\zeta_8 = e^{i\pi/4}, \qquad \binom{a'}{b'} = \binom{\alpha}{\beta} \mod 2,$$

$$\varepsilon(\gamma, a, b) = 2(B\alpha)^t (C\beta) - (D\alpha)^t (B\alpha) - (C\beta)^t (A\beta) + 2((AB^t)_0)^t (D\alpha - C\beta),$$

and  $\kappa(\gamma)$  is an eighth root of unity depending only on  $\gamma$ , with a sign ambiguity coming from the choice of a holomorphic square root of  $\det(C\tau + D)$ .

**Corollary 3.3.** For every  $\tau \in \mathcal{H}_2$ , we have the following equalities of projective tuples:

$$(\theta_{j}(2^{n}\gamma_{1}\tau))_{0 \leq j \leq 3} = \begin{cases} (\theta_{4}(\tau):\theta_{0}(\tau):\theta_{6}(\tau):\theta_{2}(\tau)) & \text{if } n = 0, \\ (\theta_{0}(\tau_{1}^{(n)}):\theta_{4}(\tau_{1}^{(n)}):\theta_{2}(\tau_{1}^{(n)}):\theta_{6}(\tau_{1}^{(n)})) & \text{if } n \geq 1, \end{cases}$$

$$(\theta_{j}(2^{n}\gamma_{2}\tau))_{0 \leq j \leq 3} = \begin{cases} (\theta_{8}(\tau):\theta_{9}(\tau):\theta_{0}(\tau):\theta_{1}(\tau)) & \text{if } n = 0, \\ (\theta_{0}(\tau_{2}^{(n)}):\theta_{1}(\tau_{2}^{(n)}):\theta_{8}(\tau_{2}^{(n)}):\theta_{9}(\tau_{2}^{(n)})) & \text{if } n \geq 1, \end{cases}$$

$$(\theta_{j}(2^{n}\gamma_{3}\tau))_{0 \leq j \leq 3} = (\theta_{0}(\tau_{3}^{(n)}):\theta_{8}(\tau_{3}^{(n)}):\theta_{4}(\tau_{3}^{(n)}):\theta_{12}(\tau_{3}^{(n)})) & \text{for every } n \geq 0,$$

$$(\theta_{j}(2^{n}\gamma_{3}\tau))_{0 \leq j \leq 3} = (\theta_{0}(\tau_{4}^{(n)}):\theta_{8}(\tau_{4}^{(n)}):\theta_{1}(\tau_{4}^{(n)}):\theta_{9}(\tau_{4}^{(n)})) & \text{for every } n \geq 0, \end{cases}$$

$$where the \ \tau_{i}^{(n)} \ are \ defined \ as \ in \ (5).$$

*Proof.* Apply Proposition 3.2 to the matrices  $\eta_i^{(n)}$ .

When  $\tau \in \mathcal{F}'$ , the real and imaginary parts of  $\tau_k^{(n)}$  for  $1 \le k \le 3$  are easy to study: for instance, from the second inequality in (3) we always have

$$y_3(\tau_k^{(n)})^2 \le \frac{1}{4}y_1(\tau_k^{(n)})y_2(\tau_k^{(n)}).$$

Such estimates are less obvious for the matrices  $\tau_4^{(n)}$ .

**Lemma 3.4.** Let  $\tau \in \mathcal{F}'$ . Then, for every  $n \geq 0$ , we have

$$\begin{aligned} \left| y_3(\tau_4^{(n)}) \right| &\leq \frac{3}{2^{n+2}} y_1(\tau_4^{(n)}), \\ y_3(\tau_4^{(n)})^2 &\leq \frac{3}{7} y_1(\tau_4^{(n)}) y_2(\tau_4^{(n)}), \quad and \\ \left| x_2(\tau_4^{(n)}) \right| &\leq \frac{9}{2^{n+3}}. \end{aligned}$$

*Proof.* Write  $z_1$  for  $z_1(\tau)$ , etc. We have

$$y_3(\tau_4^{(n)}) = \operatorname{Im}(-z_3/z_1) = \frac{1}{|z_1|^2}(x_3y_1 - y_3x_1),$$

so

$$|y_3(\tau_4^{(n)})| \le \frac{3y_1}{4|z_1|^2} = \frac{3}{2^{n+2}}y_1(\tau_4^{(n)}),$$

since  $y_1(\tau_4^{(n)}) = 2^n y_1/|z_1|^2$  by (5). For the second inequality, we have

$$\operatorname{Im}(\tau_4^{(n)}) = \begin{pmatrix} 2^{-n}z_1 & -2^{-n}z_3 \\ 0 & 1 \end{pmatrix}^{-t} (2^{-n}\operatorname{Im}\tau) \begin{pmatrix} 2^{-n}\overline{z}_1 & -2^{-n}\overline{z}_3 \\ 0 & 1 \end{pmatrix}^{-1}$$

so

$$\det \operatorname{Im}(\tau_4^{(n)}) = \frac{1}{|z_1|^2} \det \operatorname{Im} \tau.$$

Moreover det Im  $\tau \geq \frac{3}{4}y_1^2$ , so

$$\frac{y_3(\tau_4^{(n)})^2}{y_1(\tau_4^{(n)})y_2(\tau_4^{(n)})} \le \frac{y_3(\tau_4^{(n)})^2}{y_3(\tau_4^{(n)})^2 + \frac{3y_1^2}{4\|z_1\|^2}} \le \frac{1}{1 + \frac{4}{3}|z_1|^2} \le \frac{3}{7}.$$

For the last inequality, we compute

$$2^{n}x_{2}(\tau_{4}^{(n)}) = x_{2} - \frac{1}{|z_{1}|^{2}}((x_{3}^{2} - y_{3}^{2})x_{1} + 2x_{3}y_{3}y_{1})$$

and

$$\left| \frac{1}{|z_1|^2} (x_3^2 - y_3^2) x_1 \right| \le \frac{1}{2} \max\{x_3^2, \frac{y_3^2}{|z_1|^2}\} \le \frac{1}{8},$$

so

$$\left|2^{n}x_{2}(\tau_{4}^{(n)})\right| \le \frac{1}{2} + \frac{1}{8} + \frac{1}{2} = \frac{9}{8}.$$

#### 4 Bounds on theta constants

Typically, when  $\tau \in \mathcal{H}_2$  is close enough to the cusp at infinity (more precisely when  $\operatorname{Im} z_1(\tau), \operatorname{Im} z_2(\tau)$ , and  $\operatorname{det} \operatorname{Im}(\tau)$  are large), useful information on theta constants at  $\tau$  can be obtained from the series expansion (1). Our computations are similar in spirit to those found in [17, pp. 116–117], [4, §6.2], [11, §5.1]. All our estimates are based on the following key lemma.

**Lemma 4.1.** Let  $f: \mathbb{N} \to \mathbb{R}$  be a strictly increasing function, and assume that  $f(k+2) - f(k+1) \ge f(k+1) - f(k)$  for every  $k \ge 0$ . Let 0 < q < 1. Then

$$\sum_{k=0}^{\infty} q^{f(k)} \le \frac{q^{f(0)}}{1 - q^{f(1) - f(0)}}.$$

*Proof.* Use that  $f(k) \geq f(0) + k(f(1) - f(0))$  for all k.

**Lemma 4.2.** Let  $k \geq 1$ , and let  $\tau \in \mathcal{H}_2$  such that

$$y_3(\tau)^2 \le \frac{1}{4}y_1(\tau)y_2(\tau)$$
 and  $k|y_3(\tau)| \le y_2(\tau)$ .

Define

$$\xi_{4,6}(\tau) = 2\exp\left(i\pi\frac{z_1(\tau)}{4}\right)$$

and

$$\rho_{4,6}^{(k)}(q_1, q_2) = \frac{q_1^2}{1 - q_1^4} + \frac{q_2^{1 - \frac{1}{k}}}{1 - q_2^{3 - \frac{1}{k}}} + \frac{q_2^{1 + \frac{1}{k}}}{1 - q_2^{3 + \frac{1}{k}}} + \frac{q_1^{1/2}}{1 - q_2^{2/2}} + \frac{q_1^{1/2} q_2^{2/2}}{(1 - q_2^{3/2})(1 - q_1^2)} + \frac{q_1^{25/8} q_2^{3/2}}{(1 - q_2^{9/2})(1 - q_1^6)}.$$

Then for  $j \in \{4,6\}$ , we have

$$\left| \frac{\theta_j(\tau)}{\xi_{4,6}(\tau)} - 1 \right| \le \rho_{4,6}^{(k)} (q_1(\tau), q_2(\tau)).$$

*Proof.* Write  $u = \binom{1/2}{0}$ . Using the definition, we obtain

$$\left| \frac{\theta_j(\tau)}{\xi_{4,6}(\tau)} - 1 \right| \le \frac{1}{2} q_1^{-1/4} \sum_{\substack{m \in \mathbb{Z}^2 \\ m \ne \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \end{pmatrix}}} \exp\left(-\pi (m+u)^t \operatorname{Im}(\tau)(m+u)\right).$$

We split this sum in two parts, according to whether the second coordinate of m is zero or not. The first part gives

$$q_1^{-1/4} \sum_{m \in \mathbb{N} + \frac{3}{2}} q_1^{m^2} \le q_1^{-1/4} \frac{q_1^{9/4}}{1 - q_1^4} = \frac{q_1^2}{1 - q_1^4}$$

by Lemma 4.1. The second part is

$$q_1^{-1/4} \sum_{m_1 \in \mathbb{N} + \frac{1}{2}} \sum_{m_2 \ge 1} q_1^{m_1^2} q_2^{m_2^2} \cdot 2 \cosh(2\pi y_3 m_1 m_2).$$

We use the fact that for every  $(m_1, m_2) \in \mathbb{R}^2_+$ ,

$$\left|2y_3m_1m_2\right| \le \frac{y_1}{2}m_1^2 + \frac{y_2}{2}m_2^2.$$

When  $m_1 = 1/2$ , we use the following bound instead:

$$\left| 2y_3 m_1 m_2 \right| = |y_3 m_2| \le \frac{y_2 m_2}{k}.$$

Therefore the total contribution of the second part is bounded by

$$\begin{split} q_1^{-1/4} & \sum_{m_2 \ge 1} q_1^{1/4} q_2^{m_2^2} \cdot 2 \cosh\left(\pi \frac{y_2}{k} m_2\right) \\ & + q_1^{-1/4} \sum_{m_1 \in \mathbb{N} + \frac{3}{2}} \sum_{m_2 \ge 1} q_1^{m_1^2} q_2^{m_2^2} \cdot 2 \cosh\left(\pi \left(\frac{y_1}{2} m_1^2 + \frac{y_2}{2} m_2^2\right)\right) \\ & \le \frac{q_2^{1 - \frac{1}{k}}}{1 - q_2^{3 - \frac{1}{k}}} + \frac{q_2^{1 + \frac{1}{k}}}{1 - q_2^{3 + \frac{1}{k}}} + \frac{q_1^{7/8} q_2^{1/2}}{(1 - q_2^{3/2})(1 - q_1^2)} + \frac{q_1^{25/8} q_2^{3/2}}{(1 - q_2^{9/2})(1 - q_1^6)} \end{split}$$

by other applications of Lemma 4.1.

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**Lemma 4.3.** Let  $k \geq 1$ , and let  $\tau \in \mathcal{H}_2$  such that

$$y_3(\tau)^2 \le \frac{1}{4}y_1(\tau)y_2(\tau)$$
 and  $k|y_3(\tau)| \le y_1(\tau)$ .

Define

$$\xi_{8,9}(\tau) = 2\exp\left(i\pi \frac{z_2(\tau)}{4}\right),\,$$

and

$$\begin{split} \rho_{8,9}^{(k)}(q_1,q_2) &= \frac{q_2^2}{1 - q_2^4} + \frac{q_1^{1 - \frac{1}{k}}}{1 - q_1^{3 - \frac{1}{k}}} + \frac{q_1^{1 + \frac{1}{k}}}{1 - q_1^{3 + \frac{1}{k}}} \\ &\quad + \frac{q_2^{7/8} q_1^{1/2}}{(1 - q_1^{3/2})(1 - q_2^2)} + \frac{q_2^{25/8} q_1^{3/2}}{(1 - q_1^{9/2})(1 - q_2^6)}. \end{split}$$

Then for  $j \in \{8, 9\}$ , we have

$$\left| \frac{\theta_j(\tau)}{\xi_{8,9}(\tau)} - 1 \right| \le \rho_{8,9}^{(k)} (q_1(\tau), q_2(\tau)).$$

*Proof.* We proceed in a similar fashion as in the proof of Lemma 4.2 by switching the roles of  $q_1$  and  $q_2$ .

**Lemma 4.4.** Let  $\tau \in \mathcal{H}_2$  such that

$$y_3(\tau)^2 \le \frac{1}{4}y_1(\tau)y_2(\tau).$$

Define

$$\begin{split} \xi_0(\tau) &= 1 + 2 \exp(i\pi z_1(\tau)) + 2 \exp(i\pi z_2(\tau)), \\ \xi_{0,2}(\tau) &= 1 + 2 \exp(i\pi z_1(\tau)), \\ \xi_{0,1}(\tau) &= 1 + 2 \exp(i\pi z_2(\tau)), \end{split}$$

and

$$\rho_0(q_1, q_2) = \frac{2q_1^4}{1 - q_1^5} + \frac{2q_2^4}{1 - q_2^5} + \frac{2q_1^{1/2}q_2^{1/2}}{(1 - q_1^{3/2})(1 - q_2^{3/2})} + \frac{2q_1^{3/2}q_2^{3/2}}{(1 - q_1^{9/2})(1 - q_2^{9/2})}.$$

Then we have

$$\begin{aligned} |\theta_{0}(\tau) - \xi_{0}(\tau)| &\leq \rho_{0}(q_{1}(\tau), q_{2}(\tau)), \\ |\theta_{j}(\tau) - \xi_{0,2}(\tau)| &\leq \rho_{0}(q_{1}(\tau), q_{2}(\tau)) + 2q_{2}(\tau) & for \ j \in \{0, 2\}, \\ |\theta_{j}(\tau) - \xi_{0,1}(\tau)| &\leq \rho_{0}(q_{1}(\tau), q_{2}(\tau)) + 2q_{1}(\tau) & for \ j \in \{0, 1\}, \ and \\ |\theta_{j}(\tau) - 1| &\leq \rho_{0}(q_{1}(\tau), q_{2}(\tau)) + 2q_{1}(\tau) + 2q_{2}(\tau) & for \ 0 \leq j \leq 3. \end{aligned}$$

*Proof.* We proceed again in a similar fashion as in the proof of Lemma 4.2. The terms of  $\rho_0(q_1, q_2)$  are obtained by considering the following subsets of indices  $m \in \mathbb{Z}^2$ :

$$\{\binom{m_1}{0} \mid |m_1| \ge 2\}, \quad \{\binom{0}{m_2} \mid |m_2| \ge 2\},$$

and

$$\{\binom{m_1}{m_2} \mid |m_1| \ge 1, |m_2| \ge 1\}.$$

**Lemma 4.5.** Let  $\tau \in \mathcal{H}_2$  such that

$$|x_3(\tau)| \le \frac{1}{2}$$
 and  $2|y_3(\tau)| \le \min\{y_1(\tau), y_2(\tau)\}.$ 

Write

$$\xi_{12}(\tau) = \exp\left(i\pi \frac{z_1(\tau) + z_2(\tau)}{4}\right) \left(\exp\left(i\pi \frac{z_3(\tau)}{2}\right) + \exp\left(-i\pi \frac{z_3(\tau)}{2}\right)\right),$$

and

$$\begin{split} \rho_{12}(q_1,q_2) &= \frac{q_1^{3/2}}{1-q_1^{7/2}} + \frac{q_1^{5/2}}{1-q_1^{9/2}} + \frac{q_2^{3/2}}{1-q_2^{7/2}} + \frac{q_2^{5/2}}{1-q_2^{9/2}} \\ &\quad + \frac{q_1^{7/8}q_2^{7/8}}{(1-q_1^2)(1-q_2^2)} + \frac{q_1^{25/8}q_2^{25/8}}{(1-q_1^6)(1-q_2^6)}. \end{split}$$

Then we have

$$\left|\frac{\theta_{12}(\tau)}{\xi_{12}(\tau)} - 1\right| \le \rho_{12}(q_1(\tau), q_2(\tau)).$$

*Proof.* By (1), we have

$$\theta_{12}(\tau) = 2 \sum_{m_1 \in \mathbb{N} + \frac{1}{2}} \sum_{m_2 \in \mathbb{N} + \frac{1}{2}} \exp(i\pi(m_1^2 z_1 + m_2^2 z_2)) \cdot (\exp(2\pi i m_1 m_2 z_3) + \exp(-2\pi i m_1 m_2 z_3)).$$

We leave the term corresponding to  $(m_1, m_2) = (\frac{1}{2}, \frac{1}{2})$  aside, and write

$$\left| \frac{\theta_{12}(\tau)}{2 \exp(i\pi(z_1 + z_2)/4)} - (\exp(i\pi z_3/2) + \exp(-i\pi z_3/2)) \right|$$

$$\leq \sum_{\substack{(m_1, m_2) \in (\mathbb{N} + \frac{1}{2})^2 \\ (m_1, m_2) \neq (\frac{1}{2}, \frac{1}{2})}} q_1^{m_1^2 - \frac{1}{4}} q_2^{m_2^2 - \frac{1}{4}} \cdot 2 \cosh(2\pi m_1 m_2 y_3).$$

Since  $|x_3| \leq \frac{1}{2}$ , the absolute value of the argument of  $\exp(i\pi z_3/2)$  is at most  $\pi/4$ . Therefore,

$$\left| \exp(i\pi z_3/2) + \exp(-i\pi z_3/2) \right| \ge \exp(\pi |y_3|/2).$$

We obtain

$$\left| \frac{\theta_{12}(\tau)}{\xi_{12}(\tau)} - 1 \right| \le \sum_{\substack{(m_1, m_2) \in (\mathbb{N} + \frac{1}{2})^2 \\ (m_1, m_2) \ne (\frac{1}{2}, \frac{1}{2})}} q_1^{m_1^2 - \frac{1}{4}} q_2^{m_2^2 - \frac{1}{4}} \cdot 2 \cosh\left(2\pi (m_1 m_2 - \frac{1}{4})y_3\right).$$

We separate the terms corresponding to  $m_2 = \frac{1}{2}$ . Since  $2|y_3| \leq y_1$ , their contribution is bounded by

$$\sum_{m_1 \in \mathbb{N} + \frac{3}{2}} \left( q_1^{m_1^2 - \frac{1}{2}m_1} + q_1^{m_1^2 + \frac{1}{2}m_1 - \frac{1}{2}} \right) \le \frac{q_1^{3/2}}{1 - q_1^{7/2}} + \frac{q_1^{5/2}}{1 - q_1^{9/2}}.$$

Similarly, the contribution from the terms with  $m_1 = 1/2$  is bounded by

$$\frac{q_2^{3/2}}{1 - q_2^{7/2}} + \frac{q_2^{5/2}}{1 - q_2^{9/2}}.$$

For the remaining terms, we use the majoration

$$\left|2\pi(m_1m_2 - \frac{1}{4})y_3\right| \le \left|2\pi m_1m_2y_3\right| \le \pi \left|y_3\right| (m_1^2 + m_2^2) \le \frac{\pi}{2}(m_1^2y_1 + m_2^2y_2).$$

Thus, the rest of the sum is bounded by

$$\sum_{m_1, m_2 \in \mathbb{N} + \frac{3}{2}} q_1^{m_1^2 - \frac{1}{4}} q_2^{m_2^2 - \frac{1}{4}} \cdot 2 \cosh\left(\frac{\pi}{2} (m_1^2 y_1 + m_2^2 y_2)\right)$$

$$\leq \sum_{m_1, m_2 \in \mathbb{N} + \frac{3}{2}} \left(q_1^{\frac{1}{2} m_1^2 - \frac{1}{4}} q_2^{\frac{1}{2} m_2^2 - \frac{1}{4}} + q_1^{\frac{3}{2} m_1^2 - \frac{1}{4}} q_2^{\frac{3}{2} m_2^2 - \frac{1}{4}}\right)$$

$$\leq \frac{q_1^{7/8} q_2^{7/8}}{(1 - q_1^2)(1 - q_2^2)} + \frac{q_1^{25/8} q_2^{25/8}}{(1 - q_1^6)(1 - q_2^6)}.$$

We give another version of these estimates that we will use for  $\tau_4^{(n)}$ .

**Lemma 4.6.** Let  $k \geq 2$ , and let  $\tau \in \mathcal{H}_2$  such that

$$y_3(\tau)^2 \le \frac{3}{7} y_1(\tau) y_2(\tau)$$
 and  $k |y_3(\tau)| \le y_1(\tau)$ .

Let  $\alpha = \sqrt{3/7}$ . Define

$$\rho_{0,1}^{\prime(k)}(q_1, q_2) = \frac{2q_2^4}{1 - q_2^5} + \frac{2q_1}{1 - q_1^3} + \frac{2q_1^{1 - \frac{2}{k}}q_2}{1 - q_1^{3 - \frac{2}{k}}} + \frac{2q_1^{1 + \frac{2}{k}}q_2}{1 - q_1^{3 + \frac{2}{k}}} + \frac{2q_1^{1 + \alpha}q_2^{4(1 + \alpha)}}{(1 - q_1^{3(1 - \alpha)})(1 - q_2^{5(1 - \alpha)})} + \frac{2q_1^{1 + \alpha}q_2^{4(1 + \alpha)}}{(1 - q_1^{3(1 + \alpha)})(1 - q_2^{5(1 + \alpha)})}$$

and

$$\rho_{8,9}^{\prime(k)}(q_1, q_2) = \frac{q_2^2}{1 - q_2^4} + \frac{q_1^{1 - \frac{1}{k}}}{1 - q_1^{3 - \frac{1}{k}}} + \frac{q_1^{1 + \frac{1}{k}}}{1 - q_1^{3 + \frac{1}{k}}} + \frac{q_1^{2 + \frac{1}{k}}}{1 - q_1^{3 + \frac{1}{k}}} + \frac{q_2^{2 + \frac{9}{4}\alpha}q_1^{1 + \alpha}}{(1 - q_2^{4(1 - \alpha)})(1 - q_1^{3(1 - \alpha)})} + \frac{q_2^{2 + \frac{9}{4}\alpha}q_1^{1 + \alpha}}{(1 - q_2^{4(1 + \alpha)})(1 - q_1^{3(1 + \alpha)})}.$$

Then we have

$$|\theta_j(\tau) - \xi_{0,1}(\tau)| \le \rho'_{0,1}(\tau) \quad \text{for } j \in \{0,1\}$$

and

$$\left| \frac{\theta_j(\tau)}{\xi_{8,9}(\tau)} - 1 \right| \le \rho'_{8,9}(\tau) \quad \text{for } j \in \{8,9\}.$$

*Proof.* We bound the cross-product terms by

$$|2y_3m_1m_2| \le \alpha y_1m_1^2 + \alpha y_2m_2^2,$$
  
 $|2y_3m_1m_2| \le \frac{1}{k}y_1m_1$  if  $m_2 = \frac{1}{2}$ , and  
 $|2y_3m_1m_2| \le \frac{2}{k}y_1m_1$  if  $m_2 = 1$ .

For  $j \in \{0,1\}$ , we separate the terms with  $|m_2| \leq 1$  or  $m_1 = 0$ , and obtain

$$|\theta_{j}(\tau) - \xi_{0,1}(\tau)| \leq 2 \sum_{m_{2} \geq 2} q_{2}^{m_{2}^{2}} + 2 \sum_{m_{1} \geq 1} q_{1}^{m_{1}^{2}} + 2 \sum_{m_{2} \geq 1} q_{2} (q_{1}^{m_{1}^{2} - \frac{2}{k}m_{1}} + q_{1}^{m_{1}^{2} + \frac{2}{k}m_{1}})$$

$$+ 2 \sum_{m_{1} \geq 1} \sum_{m_{2} \geq 2} q_{1}^{m_{1}^{2}} q_{2}^{m_{2}^{2}} \cdot 2 \cosh\left(\alpha(y_{1}m_{1}^{2} + y_{2}m_{2}^{2})\right)$$

$$\leq \frac{2q_{2}^{4}}{1 - q_{2}^{5}} + \frac{2q_{1}}{1 - q_{1}^{3}} + \frac{2q_{1}^{1 - \frac{2}{k}}q_{2}}{1 - q_{1}^{3 - \frac{2}{k}}} + \frac{2q_{1}^{1 + \frac{2}{k}}q_{2}}{1 - q_{1}^{3 + \frac{2}{k}}}$$

$$+ \frac{2q_{1}^{1 - \alpha}q_{2}^{4(1 - \alpha)}}{(1 - q_{1}^{3(1 - \alpha)})(1 - q_{2}^{5(1 - \alpha)})} + \frac{2q_{1}^{1 + \alpha}q_{2}^{4(1 + \alpha)}}{(1 - q_{1}^{3(1 + \alpha)})(1 - q_{2}^{5(1 + \alpha)})}.$$

For  $j \in \{8,9\}$ , we separate the terms with  $|m_2| = \frac{1}{2}$  or  $m_1 = 0$ . We obtain

$$\left| \frac{\theta_{j}(\tau)}{\xi_{8,9}(\tau)} - 1 \right| \leq q_{2}^{-1/4} \sum_{m_{2} \in \mathbb{N} + \frac{3}{2}} q_{2}^{m_{2}^{2}} + \sum_{m_{1} \geq 1} \left( q_{1}^{m_{1}^{2} - \frac{1}{k}m_{1}} + q_{1}^{m_{1}^{2} + \frac{1}{k}m_{1}} \right)$$

$$+ q_{2}^{-1/4} \sum_{m_{2} \in \mathbb{N} + \frac{3}{2}} \sum_{m_{1} \geq 1} q_{2}^{m_{2}^{2}} q_{1}^{m_{2}^{2}} \cdot 2 \cosh\left(\alpha(y_{1}m_{1}^{2} + y_{2}m_{2}^{2})\right)$$

$$\leq \frac{q_{2}^{2}}{1 - q_{2}^{4}} + \frac{q_{1}^{1 - \frac{1}{k}}}{1 - q_{1}^{3 - \frac{1}{k}}} + \frac{q_{1}^{1 + \frac{1}{k}}}{1 - q_{1}^{3 + \frac{1}{k}}}$$

$$+ \frac{q_{2}^{2 - \frac{9}{4}\alpha} q_{1}^{1 - \alpha}}{(1 - q_{2}^{4(1 - \alpha)}(1 - q_{1}^{3(1 - \alpha)})} + \frac{q_{2}^{2 + \frac{9}{4}\alpha} q_{1}^{1 + \alpha}}{(1 - q_{2}^{4(1 + \alpha)})(1 - q_{1}^{3(1 + \alpha)})} \cdot \square$$

Finally, when n is large, we will show that the theta constants  $\theta_j(2^n\gamma_k\tau)$  for  $0 \le j \le 3$  are in good position using the following lemma. Recall the definition of  $r(\tau)$  and  $\lambda_1(\tau)$  from §2.

#### Lemma 4.7. Let $\tau \in \mathcal{H}_2$ .

- 1. If  $r(\tau) \geq 0.4$ , then the  $\theta_j(\tau)$  for  $0 \leq j \leq 3$  are in good position.
- 2. If  $\lambda_1(\tau) \geq 0.6$ , then the  $\theta_j(\tau)$  for  $0 \leq j \leq 3$  are in good position.

Proof. 1. Write

$$q = \exp(-\pi r(\tau)).$$

For  $0 \le j \le 3$ , we have

$$|\theta_{j}(\tau) - 1| \le 4q^{2} + \sum_{n \in \mathbb{Z}^{2}, \|n\|^{2} \ge 2} \exp(-\pi\lambda_{1}(\tau) \|n\|^{2})$$

$$\le 8q^{2} + 4q^{4} + 8q^{5} + 4q^{8} + 4\frac{1+q}{(1-q)^{2}}q^{9}.$$
(6)

In this inequality, the first term  $4q^2$  comes from the four vectors  $n \in \mathbb{Z}^2$  with ||n|| = 1. Then we separate the terms  $n = \binom{n_1}{n_2}$  such that  $|n_1| \geq 3$  and  $|n_2| \geq 3$ ; this accounts for the term  $4q^9(1+q)/(1-q)^2$ , as in the proof of [4, Prop. 6.1]. We leave the remaining terms as they are.

If  $q \leq 0.287$ , then the quantity on the right hand side of (6) is less than  $\sqrt{2}/2$ , and the  $\theta_j(\tau)$  are contained in a disk which is itself contained in a quarter plane. We have  $q \leq 0.287$  when  $r(\tau) \geq 0.4$ .

2. Write

$$q = \exp(-\pi\lambda_1(\tau)).$$

Then for  $0 \le j \le 3$ , we have

$$|\theta_j(\tau) - 1| \le 4q + 4q^2 + 4q^4 + 8q^5 + 4q^8 + 4\frac{1+q}{(1-q)^2}q^9.$$

This quantity is less than  $\sqrt{2}/2$  when  $\lambda_1(\tau) \geq 0.6$ .

We conclude this section with lower bounds on r or  $\lambda_1$  at  $\gamma_k \tau$  for  $\tau \in \mathcal{F}'$  and  $1 \leq k \leq 3$ .

**Lemma 4.8.** For every  $\tau \in \mathcal{F}'$ , we have

$$r(\gamma_1 \tau) \ge \frac{9 y_1(\tau)}{34 |z_1(\tau)|^2}, \quad r(\gamma_2 \tau) \ge \frac{9 y_2(\tau)}{34 |z_2(\tau)|^2}, \quad and \quad \lambda_1(\gamma_3 \tau) \ge \frac{9}{44 y_2(\tau)}.$$

Proof. We have

$$\operatorname{Im}(\gamma_1 \tau) = \begin{pmatrix} z_1 & z_3 \\ 0 & -1 \end{pmatrix}^{-t} \operatorname{Im}(\tau) \begin{pmatrix} \overline{z}_1 & \overline{z}_3 \\ 0 & -1 \end{pmatrix}^{-1} = \frac{1}{|z_1|^2} \begin{pmatrix} y_1 & \alpha \\ \alpha & \beta \end{pmatrix}$$

with  $\alpha = y_1 x_3 - y_3 x_1$ , so  $|\alpha| \le \frac{3}{4} y_1$ . Moreover,

$$\det \operatorname{Im}(\gamma_1 \tau) = \frac{1}{|z_1|^2} \det \operatorname{Im}(\tau)$$

and det  $Im(\tau) \ge 9/16$ , so

$$\beta \le \frac{|z_1|^2}{y_1} \det \operatorname{Im}(\tau) + \frac{9}{16} y_1 \quad \text{and} \quad \beta \ge \frac{|z_1|^2}{y_1} \det \operatorname{Im}(\tau) \ge \frac{9}{16} y_1.$$

Therefore,

$$\lambda_1(\gamma_1 \tau) \ge \frac{\det \operatorname{Im}(\gamma_1 \tau)}{\operatorname{Tr} \operatorname{Im}(\gamma_1 \tau)} \ge \frac{y_1}{|z_1|^2} \frac{1}{1 + \frac{25}{16} \frac{y_1^2}{|z_1|^2 \det \operatorname{Im}(\tau)}} \ge \frac{9y_1}{34 |z_1|^2}.$$

We did not use the property that  $y_1 \leq y_2$ , so the same proof works for  $\gamma_2 \tau$ . Finally, we consider  $\gamma_3 \tau$ . We have

$$\operatorname{Im}(\gamma_3 \tau) = \frac{1}{\left|\det \tau\right|^2} \begin{pmatrix} \beta_1 & \alpha \\ \alpha & \beta_2 \end{pmatrix}$$

with

$$\beta_1 = y_1 |z_3|^2 + y_2 |z_1|^2 - y_3 (z_1 \overline{z}_3 + z_3 \overline{z}_1),$$
  
$$\beta_2 = y_1 |z_2|^2 + y_2 |z_3|^2 - y_3 (z_2 \overline{z}_3 + z_3 \overline{z}_2).$$

We compute

$$|\det \tau|^2 \operatorname{Tr} \operatorname{Im}(\gamma_3 \tau) = \beta_1 + \beta_2 \le y_1 y_2^2 + y_1^2 y_2 + \frac{1}{2} (y_1 + y_2 + |y_3|) \le \frac{11}{3} y_1 y_2^2$$

because  $y_1y_2 \ge 3/4$ . Therefore,

$$\lambda_1(\gamma_3 \tau) \ge \frac{3 \det \operatorname{Im}(\tau)}{11 y_1 y_2^2} \ge \frac{9}{44 y_2}.$$

#### 5 Proof of the main theorem

In this final section, we prove Theorem 1.1 by separating different cases according to the value of n. If n is large enough, then Lemmas 4.7 and 4.8 are enough to conclude; if n is smaller, then we apply the theta transformation formula (Proposition 3.2) and the bounds on other theta constants given in §4.

In the proofs, we use numerical calculations, typically in order to show that a given angle  $\alpha(q)$  is smaller than  $\pi/2$  for certain values of q. Such calculations are easily certified using interval arithmetic, since the functions  $\alpha(q)$  we consider are simple: they are either increasing or convex functions of q.

In order to help the reader visualize the estimates, we created pictures using GeoGebra [12].

**Proposition 5.1.** Let  $\tau \in \mathcal{F}'$ . Then for every  $n \geq 0$ , the theta constants  $\theta_j(2^n\tau)$  for  $0 \leq j \leq 3$  are in good position.

*Proof.* For every  $n \geq 0$ , we have

$$r(2^n \tau) = 2^n r(\tau) \ge \sqrt{3}/4 \ge 0.4,$$

so the result follows from Lemma 4.7.

Lemma 5.2. Let  $\tau \in \mathcal{F}'$ .

1. For every  $n \ge 0$  such that  $2^n \le 8.77y_1(\tau)$ , the theta constants  $\theta_j(\tau_1^{(n)})$  for  $j \in \{0, 2, 4, 6\}$  are in good position.

2. For every  $n \ge 0$  such that  $2^n \le 8.77y_2(\tau)$ , the theta constants  $\theta_j(\tau_2^{(n)})$  for  $j \in \{0, 1, 8, 9\}$  are in good position.

*Proof.* We only prove the first statement, the second one being symmetric. We separate three cases: n = 0, n = 1, and  $n \ge 2$ .

Case 1: n = 0. Then  $\tau_1^{(n)} = \tau$ . By [24, Prop. 7.7], we have

$$|\theta_j(\tau) - 1| \le 0.405$$
 for  $j \in \{0, 1, 2, 3\}$ , and  $\left|\frac{\theta_j(\tau)}{\xi_{4,6}(\tau)} - 1\right| \le 0.348$  for  $j \in \{4, 6\}$ .

The absolure value of the argument of  $\xi_{4,6}(\tau)$  is at most  $\pi/8$ . Therefore the angle between any two  $\theta_j(\tau)$  for  $j \in \{0, 1, 2, 3, 4, 6\}$  is at most

$$\frac{\pi}{8} + \arcsin(0.348) + \arcsin(0.405) < \frac{\pi}{2}$$

Case 2: n = 1. We study the relative positions of  $\xi_{0,2}$  and  $\xi_{4,6}$  at  $\tau_1^{(1)}$ . Since  $|2^{-n}x_1(\tau)| \leq 1/4$ , the absolute value of the argument of  $\xi_{4,6}(\tau_1^{(1)})$  is bounded above by  $\pi/16$ . Moreover,

$$\left|\xi_{0,2}(\tau_1^{(1)})\right| \ge 1, \quad \left|\arg(\xi_{0,2}(\tau_1^{(1)}))\right| \le \arctan\left(\frac{2q_1\sin(\pi/4)}{1+2q_1\cos(\pi/4)}\right),$$

and the arguments of  $\xi_{0,2}$  and  $\xi_{4,6}$  have the same sign. Therefore the angle between any two  $\theta_j(\tau_1^{(1)})$  for  $j \in \{0, 2, 4, 6\}$  is at most

$$\max\left\{\frac{\pi}{16},\arctan\left(\frac{2q_1\sin(\pi/4)}{1+2q_1\cos(\pi/4)}\right)\right\}+\arcsin\rho_{4,6}^{(4)}(q_1,q_2)+\arcsin(\rho_0(q_1,q_2)+2q_2)$$

by Lemmas 4.2 and 4.4. This quantity is less than  $\pi/2$  because

$$q_2(\tau_1^{(1)}) \le \exp(-\pi\sqrt{3})$$
 and  $q_1(\tau_1^{(1)}) \le \exp(-\pi\sqrt{3}/8)$ .

Case 3:  $n \ge 2$ . We proceed as in Case 2, but we now have

$$q_2(\tau_1^{(n)}) \le \exp(-2\pi\sqrt{3}), \quad 8|y_3(\tau_1^{(n)})| \le y_2(\tau_1^{(n)}), \quad \text{and} \quad |x_1(\tau_1^{(n)})| \le \frac{1}{8}.$$

Therefore the angle between the  $\theta_j(\tau_1^{(n)})$  for  $j \in \{0, 2, 4, 6\}$  is bounded by

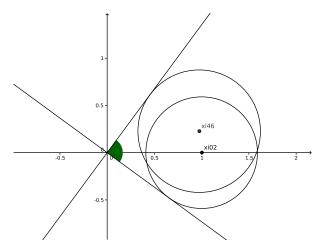
$$\max \left\{ \frac{\pi}{32}, \arctan\left(\frac{2q_1 \sin(\pi/8)}{1 + 2q_1 \cos(\pi/8)}\right) \right\}$$

$$+ \arcsin(\rho_0(q_1, \exp(-2\pi\sqrt{3})) + 2\exp(-2\pi\sqrt{3}))$$

$$+ \arcsin\rho_{4.6}^{(8)}(q_1, \exp(-2\pi\sqrt{3})).$$
(7)

This angle remains less that  $\pi/2$  when  $q_1(\tau_1^{(n)}) \leq 0.699$ . This is the case when  $2^n \geq 8.77 y_1(\tau)$ .

The geometric situation in Case 3 of Lemma 5.2 can be represented as follows.



In this picture, we take  $q_1=0.699$ , and represent two complex numbers  $\xi_{0,2}$  and  $\xi_{4,6}$  with modulus one, separated by an angle of

$$\max\left\{\frac{\pi}{32}, \arctan\left(\frac{2q_1\sin(\pi/8)}{1+2q_1\cos(\pi/8)}\right)\right\} \simeq 0.22.$$

Then we draw disks centered in  $\xi_{0,2}$  and  $\xi_{4,6}$  with radii  $\rho_0(q_1, \exp(-2\pi\sqrt{3}))$  and  $\rho_{4,6}^{(8)}(q_1, \exp(-2\sqrt{3}))$  respectively. Finally we represent the smallest angular sector seen from the origin containing these two disks. The green angle is equal to the quantity (7), and is indeed smaller than  $\pi/2$ .

Proposition 5.3. Let  $\tau \in \mathcal{F}'$ .

- 1. For every  $n \geq 0$ , the theta constants  $(\theta_j(2^n\gamma_1\tau))_{0\leq j\leq 3}$  are in good position.
- 2. For every  $n \ge 0$ , the theta constants  $(\theta_j(2^n\gamma_2\tau))_{0 \le j \le 3}$  are in good position.

*Proof.* By Lemma 4.8, we have

$$r(\gamma_1 \tau) \ge \frac{9 y_1}{34 |z_1|^2} \ge \frac{9 y_1}{34 (1/4 + y_1^2)} \ge \frac{0.205}{y_1(\tau)}$$

because  $y_1(\tau) \ge \sqrt{3}/2$ . By Lemma 4.7, the  $\theta_j(2^n\gamma_1\tau)$  for  $0 \le j \le 3$  are in good position when  $2^n r(\gamma_1\tau) \ge 0.4$ . This is the case when  $2^n \ge 1.96y_1$ . On the other hand, Lemma 5.2 applies when  $2^n \le 8.77y_1$ . The second statement is proved in the same way.

**Lemma 5.4.** Let  $\tau \in \mathcal{F}'$ . Then, for every  $n \geq 0$  such that  $2^n \leq 1.66y_1$ , the theta constants  $\theta_j(\tau_3^{(n)})$  for  $j \in \{0, 4, 8, 12\}$  are in good position.

*Proof.* Write  $q = q_1(\tau_3^{(n)})$  for short. We separate two cases:  $n \ge 1$ , and n = 0.

Case 1:  $n \ge 1$ . In this case, we have

$$|x_j(\tau_3^{(n)})| \le 1/4$$
 for each  $1 \le j \le 3$ .

Therefore, given the expressions of  $\xi_0$ ,  $\xi_{4,6}$ ,  $\xi_{8,9}$  and  $\xi_{12}$  (see (4)), and by Lemmas 4.2 to 4.5,

• The angle between  $\theta_4(\tau_3^{(n)})$  and  $\theta_8(\tau_3^{(n)})$  is bounded by

$$\frac{\pi}{8} + 2\arcsin \rho_{4,6}^{(2)}(q,q).$$

• The angle between  $\theta_4(\tau_3^{(n)})$  (or  $\theta_8$ ) and  $\theta_0(\tau_3^{(n)})$  is bounded by

$$\frac{\pi}{16} + \arcsin \rho_{4,6}^{(2)}(q,q) + 2q \sin(\pi/4) + \arcsin \rho_0(q,q).$$

• The angle between  $\theta_{12}(\tau_3^{(n)})$  and  $\theta_4(\tau_3^{(n)})$  (or  $\theta_8$ ) is bounded by

$$\frac{3\pi}{16} + \arcsin \rho_{12}(q,q) + \arcsin \rho_{4,6}^{(2)}(q,q).$$

 $\bullet$  The angle between  $\theta_{12}(\tau_3^{(n)})$  and  $\theta_0(\tau_3^{(n)})$  is bounded by

$$\frac{\pi}{4} + \arcsin \rho_{12}(q, q) + \arcsin \rho_0(q, q).$$

All these quantities remain less than  $\pi/2$  when  $q \leq 0.151$ . This is the case when  $2^n \leq 1.66y_1$ .

Case 2: n = 0. In this case, we have  $q \le \exp(-\pi\sqrt{3}/2)$ . Therefore,

• The angle between  $\theta_4$  and  $\theta_8$  is bounded by

$$\frac{\pi}{4} + 2\arcsin \rho_{4,6}^{(2)}(q,q) < \frac{\pi}{2}.$$

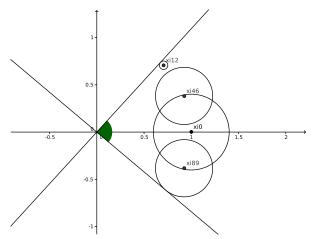
• The angle between  $\theta_4$  (or  $\theta_8$ ) and  $\theta_0$  is bounded by

$$\frac{\pi}{8} + \arcsin \rho_{4,6}^{(2)}(q,q) + \arcsin(\rho_0(q,q) + 4q) < \frac{\pi}{2}.$$

• The angle between  $\theta_{12}$  and  $\theta_4$  (or  $\theta_8$ ) is bounded by

$$\frac{3\pi}{8} + \arcsin \rho_{12}(q, q) + \arcsin \rho_{4,6}^{(2)}(q, q) < \frac{\pi}{2}.$$

These estimations can be represented as follows, with similar conventions as in the picture after Lemma 5.2:



We finally study the angle between  $\theta_{12}$  and  $\theta_0$ . The argument of  $\xi_{12}(\tau)$  is  $x_1/4 + x_2/4 + \beta$  with  $\beta = \arg(\exp(i\pi z_3/2) + \exp(-i\pi z_3/2))$ . Up to conjugating, we may assume that  $y_3 \geq 0$  and  $x_3 \geq 0$ . Then

$$\exp(i\pi z_3/2) + \exp(-i\pi z_3/2) = \exp(-i\pi z_3/2)(1 + \exp(i\pi z_3))$$

SO

$$\beta + \frac{\pi x_3}{2} \ge \arctan\left(\frac{q_3 \sin(\pi x_3)}{1 + q_3}\right) \ge \arctan\left(\frac{2x_3 q_3}{1 + q_3}\right).$$

In general, we have

$$|\beta| \le \frac{\pi}{4} - \arctan\left(\frac{q^{1/2}}{1 + q^{1/2}}\right).$$

On the other hand,

$$1 \le \operatorname{Re}(\xi_0(\tau)) \le 1 + 4q$$
,  $\operatorname{Im}(\xi_0(\tau)) = 2q_1 \sin(\pi x_1) + 2q_2 \sin(\pi x_2)$ .

We discuss two cases according to the signs of  $x_1$  and  $x_2$ :

• If  $x_1$  and  $x_2$  have opposite signs, then the angle between  $\theta_{12}$  and  $\theta_0$  is at most

$$\frac{3\pi}{8} + \arctan(2q) + \arcsin \rho_{12}(q,q) + \arcsin \rho_{0}(q,q).$$

• If  $x_1$  and  $x_2$  have the same sign, say positive, then

$$\frac{x_1 + x_2}{4} - \arg \xi_0(\tau) \le \frac{x_1 + x_2}{4}.$$

Therefore the angle between  $\theta_{12}$  and  $\theta_0$  is at most

$$\frac{\pi}{2} - \arctan\left(\frac{q^{1/2}}{1+q^{1/2}}\right) + \arcsin\rho_{12}(q,q) + \arcsin\rho_{0}(q,q).$$

This function of q is not increasing, but it is convex.

A numerical investigation shows that both quantities remain less than  $\pi/2$  when  $q \leq \exp(\sqrt{3}/2)$ .

**Lemma 5.5.** Let  $\tau \in \mathcal{F}'$ , and let  $n_0 \in \mathbb{N}$  such that  $2^{n_0} > 1.66y_1$ . Then, for every  $n \geq n_0$  such that  $2^n \leq 4.2y_2(\tau)$ , the theta constants  $\theta_j(\tau_4^{(n)})$  for  $j \in \{0, 1, 8, 9\}$  are in good position.

*Proof.* By assumption, we have  $y_1(\tau_4^{(n)}) \ge \frac{3}{4} \cdot 1.66 \ge 1.24$ , so  $q_1(\tau_4^{(n)}) \le 0.021$ . Moreover we must have  $n \ge 1$ , so by Lemma 3.4,  $|x_2(\tau_4^{(n)})| \le 9/16$ , and

$$|y_3(\tau_4^{(n)})| \le \frac{3}{8}y_1(\tau_4^{(n)}).$$

Therefore, we can apply Lemma 4.6 with k=8/3: we have

$$\left| \theta_{j}(\tau_{4}^{(n)}) - \xi_{0,1}(\tau_{4}^{(n)}) \right| \leq \rho_{0,1}^{(8/3)}(0.021, q_{2}(\tau_{4}^{n})) \quad \text{for } j \in \{0, 1\},$$

$$\left| \frac{\theta_{j}(\tau_{4}^{(n)})}{\xi_{8,9}(\tau_{4}^{(n)})} - 1 \right| \leq \rho_{8,9}^{(8/3)}(0.021, q_{2}(\tau_{4}^{(n)}) \quad \text{for } j \in \{8, 9\}.$$

Let us investigate the difference between the arguments of  $\xi_{8,9}(\tau_4^{(n)})$  and  $\xi_{0,1}(\tau_4^{(n)})$ . Both have the sign of  $x_2(\tau_4^{(n)})$ , which we may assume to be positive. If the argument of  $\xi_{8,9}$  is the largest, then the difference is bounded by

$$\arg \xi_{8,9}(\tau_4^{(n)}) \le \frac{9\pi}{64}.$$

If the argument of  $\xi_{0,1}$  is the largest, we distinguish two cases. If  $x_2(\tau_4^{(n)}) \geq \frac{3\pi}{8}$ , then

$$\arg \xi_{0,1}(\tau_4^{(n)}) - \arg \xi_{8,9}(\tau_4^{(n)}) \le \arctan\left(\frac{2q_2}{1 + 2q_2\cos(9\pi/16)}\right) - \frac{3\pi}{32}$$

On the other hand, if  $x_2(\tau) \leq 3\pi/8$ , then

$$\arg \xi_{0,1}(\tau_4^{(n)}) - \arg \xi_{8,9}(\tau_4^{(n)}) \le \arg \xi_{0,1}(\tau_4^{(n)}) \le \arctan\left(\frac{2q_2\sin(3\pi/8)}{1 + 2q_2\cos(3\pi/8)}\right)$$

Note that  $|\xi_{0,1}(\tau_4^{(n)})|$  is always greater than  $\cos(\pi/16)$ . Therefore the angle between the  $\theta_j(\tau_4^{(n)})$  for  $j \in \{0,1,8,9\}$  is at most

$$\max \left\{ \frac{9\pi}{64}, \arctan\left(\frac{2q_2}{1 + 2q_2\cos(9\pi/16)}\right) - \frac{3\pi}{32}, \arctan\left(\frac{2q_2\sin(3\pi/8)}{1 + 2q_2\cos(3\pi/8)}\right) \right\} + \arcsin \rho_{8,9}^{\prime(8/3)}(0.021, q_2) + \arcsin \frac{\rho_{0,1}^{\prime(8/3)}(0.021, q_2)}{\cos(\pi/16)}.$$

This quantity is less than  $\pi/2$  when  $q_2(\tau_4^{(n)}) \le 0.38$ . Since  $y_2(\tau_4^{(n)}) \ge \frac{3}{2^{n+2}}y_2(\tau)$  by Lemma 3.4, this is the case when  $2^n \le 2.43y_2(\tau)$ .

On the other hand, if  $2^n > 2.43y_2(\tau)$ , then we must have  $n \ge 2$ . Moreover,

$$y_1(\tau_4^{(n)}) > 2.43 \frac{y_1(\tau)y_2(\tau)}{|z_1(\tau)^2|} > 1.82,$$

so  $q_1(\tau_4^{(n)}) < 0.0033$ . Then, the angle bound improves to

$$\begin{split} \max \left\{ & \frac{9\pi}{128}, \arctan \left( \frac{2q_2 \sin(9\pi/32)}{1 + 2q_2 \cos(9\pi/32)} \right) \right\} \\ & + \arcsin \rho_{8,9}^{\prime (16/3)}(0.0033, q_2) + \arcsin \rho_{0,1}^{\prime (16/3)}(0.0033, q_2). \end{split}$$

This quantity is less than  $\pi/2$  when  $q_2(\tau_4^{(n)}) \leq 0.571$ , and the latter inequality holds when  $2^n \leq 4.2y_2(\tau)$ .

**Proposition 5.6.** Let  $\tau \in \mathcal{F}'$ . Then, for every  $n \geq 0$ , the theta constants  $\theta_j(2^n\gamma_3\tau)$  for  $0 \leq j \leq 3$  are in good position.

*Proof.* By Lemma 4.8, we have

$$\lambda_1(\gamma_3\tau) \ge \frac{9}{44y_2(\tau)}.$$

Therefore, by Lemma 4.7, the theta constants are in good position as soon as

$$2^n \frac{9}{44y_2(\tau)} \ge 0.6$$
, or  $2^n \ge 2.94y_2(\tau)$ .

When n is smaller, we use the transformation formulas. Lemma 5.4 applies when  $2^n \le 1.66y_1(\tau)$ , and Lemma 5.5 applies when  $1.66y_1(\tau) < 2^n \le 4.2y_2(\tau)$ .

Propositions 5.1, 5.3 and 5.6 together imply Theorem 1.1.

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