

Unitary Conditions for Lamé and Heun Differential Operators

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Abstract

In this paper, we explore the connections between the so-called “accessory parameter” of the Heun Equation and the properties of its monodromy groups. In particular, we investigate which numerical values of the accessory parameter yield unitary monodromy groups (i.e., those that preserve a Hermitian inner product). To this end, we employ both analytical and computational methods, extending previous work on the Lamé Equation. In particular, for a large class of Heun Equations (generalizing the Lamé Equation), we prove a connection between unitarity and the traces of certain monodromy matrices. We exploit this theorem to create an algorithm that finds accessory parameters that yield unitary monodromy groups. Using this algorithm, we calculate and report the values of the accessory parameter that give rise to unitary monodromy groups. We also draw convergence maps, demonstrating the convergence and overall robustness of our algorithm. Finally, we derive an asymptotic formula for the desired accessory parameters which agrees with our numerical results.

Keywords— Monodromy, Heun Equation, Lamé Equation, Darboux Equation, Analytic Langlands Correspondence

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Contents

1	Introduction	3
1.1	Context and Pertinent Surrounding Literature	4
1.2	Main Results	4
1.3	Organization	4
2	Background on Monodromy	5
2.1	Monodromy and Local Exponents	5
2.2	Unitarity	6
3	Unitarity conditions for the Lamé Equation	6
4	Unitarity conditions for the Heun Equation	8
4.1	Numerical Results and Figures	11
5	Spectrum of the Real-Analytic Heun Operator	13
6	Asymptotic Analysis	13
7	Code	14
8	Acknowledgements	15
9	Appendix: Additional Convergence Results for Other Parameters	17

1 Introduction

Consider the complex Fuchsian¹ differential equation $Lf = Bf$, where L is a second-order differential operator and $B \in \mathbb{C}$ is the “accessory parameter” of the equation. We say its monodromy group G is **unitary** if there exists some 2×2 nondegenerate Hermitian matrix H which is invariant under the action² $H \rightarrow g^\dagger H g$ for all $g \in G$. This paper focuses on the *Accessory Parameter Problem* for the Heun and Lamé differential equations, which reads as follows:

Question (Accessory Parameter Problem). *For which values B does a complex Fuchsian differential equation have a unitary monodromy group?*

We consider this question for several related Fuchsian differential equations. The simplest of these is the classical Lamé differential equation, which comes from the work of Lamé [15] in 1837 and is written in an elliptic form as

$$\frac{d^2 y}{dx^2} - (B + m_0(m_0 + 1)\wp(x))y = 0, \quad (1.1)$$

where m_0 and B are fixed parameters, and \wp is the Weierstrass Elliptic Function with a lattice of periods $\Lambda \subset \mathbb{C}$.

We are also interested in answering Question 1 for the Heun Equation [11]. It is written as

$$\frac{d^2 y}{dx^2} + \left(\frac{\gamma}{x} + \frac{\delta}{x-1} + \frac{\varepsilon}{x-a} \right) \frac{dy}{dx} + \frac{\alpha\beta x - \frac{B}{4}}{x(x-1)(x-a)} y = 0, \quad (1.2)$$

where $y^2 = 4x(x-1)(x-a)$ defines the Weierstrass function \wp of our original lattice Λ . Above, the parameters $\gamma, \delta, \varepsilon, \alpha$, and β are free to vary, subject only to the restriction that $\gamma + \delta + \varepsilon = 1 + \alpha + \beta$.

The Heun Equation is equivalent to an equation called the Darboux Equation through a change of variable defined in [19]. In particular, define e_1, e_2, e_3 satisfying

$$e_2 = \frac{a-2}{a+1}e_1, \quad e_3 = \frac{1-2a}{a+1}e_1.$$

Now, let $\wp(z)$ be the Weierstrass elliptic function with half-periods ω_1, ω_2 and $\omega_3 = \omega_1 + \omega_2$ such that

$$\wp(\omega_i) = e_i.$$

We substitute $\wp(z) = e_1 + (e_2 - e_1)x$. Finally, let $m_1 = \frac{1-\gamma}{2}$, $m_2 = \frac{1-\delta}{2}$, and $m_3 = \frac{1-\varepsilon}{2}$. With this change of variable, we convert Equation (1.2) into the Darboux Equation:

$$\frac{d^2 u}{dz^2} - \left(\sum_{i=0}^3 m_i(m_i + 1)\wp(x - \omega_i) \right) u = Bu. \quad (1.3)$$

Now, based on the local exponents of the Lamé Equation outlined in [2], the Lamé Equation (1.1) can be written as a specific case of the Heun Equation (1.2):

$$\frac{d^2 y}{dx^2} + \frac{1}{2} \left(\frac{1}{x} + \frac{1}{x-1} + \frac{1}{x-a} \right) \frac{dy}{dx} + \frac{\frac{x}{4} - B}{4x(x-1)(x-a)} y = 0. \quad (1.4)$$

This corresponds to a change of variables of (1.1); for more information on alternate forms of these equations, see [19].

To answer Question 1, we employ both analytical and computational methods. Analytically, we find theoretical conditions for unitarity based on the properties of the monodromy matrices and the parameters of the differential equation—in particular, concerning Theorem 3.1 and Theorem 4.1 below. We exploit our analytical results to design a computational method to find numerical values of the accessory parameter for which the Heun and Lamé Equations admit a unitary monodromy group. We observe that the square roots of these numerical values form a distorted version of our lattice Λ (See Theorem 6.1).

¹A *Fuchsian* differential equation is one in which every singularity is regular.

² $g^\dagger = \bar{g}^T$

1.1 Context and Pertinent Surrounding Literature

Monodromy of the Heun Equation has historically been studied in the context of isomonodromic deformations, tracing back to Paul Painlevé in the early 20th Century. Specifically, Painlevé’s *sixth equation* characterizes the isomonodromic deformations of the Heun Equation [20]. The accessory parameter has been studied as well—for instance, Nehari [16] examined the impact of the accessory parameter upon the Schwarz map generated by the ratio of two independent solutions to a Fuchsian differential equation. Additionally, Keen, Rauch, and Vasquez [13] have studied the accessory parameter’s potential as a parameter relating different covering maps of the punctured torus. More recently, Beukers [1] has also studied the accessory parameter’s impact on the p -adic radius of convergence for solutions to these differential equations.

The particular topic of the Accessory Parameter Problem (Question 1) was first explored by Beukers for the Lamé Equation [2]. He found asymptotic approximations for the possible values of the accessory parameter B . Additionally, using the unitary conditions for the monodromy group of the Lamé Equation, he derived a computational descent-based algorithm for approximating B .

The Accessory Parameter Problem has several important applications in mathematics. For instance, it was recently shown that the Accessory Parameter Problem for Darboux operators (which, by [19], are equivalent to Heun operators by a change of variable) is closely connected to the analytic Langlands correspondence [7], which is a key motivation for our study of the Heun Equation.

1.2 Main Results

In this paper, we seek to extend the method of Beukers [2] to answer Question 1. While Beukers restricted to the case of the Lamé Equation (1.4), we extend his analytical and computational results to the general Heun Equation (1.2), which contains the Lamé Equation as a specific case. As mentioned above, we propose and prove a theorem (Theorem 4.1) which characterizes the unitarity of the monodromy group by easily verifiable conditions. This allows us to extend Beukers’ algorithm to the much larger class of Heun Equations where at least two of the monodromy matrices are reflections.

To analyze our algorithm, we build another program to draw “convergence maps” displaying regions of convergence in the complex plane and identifying all accessory parameters satisfying Question 1. This allows us to gather accurate values of accessory parameters that yield unitary monodromy groups for this class of equations. Furthermore, in the general case of Heun Equations not covered by Theorem 4.1, we show that our algorithm still highly restricts the values of B that could *potentially* yield unitary monodromy groups. We believe that this may help elucidate the behavior of the accessory parameter in cases not covered analytically here, and hopefully lead to a better understanding of the Accessory Parameter Problem in the most general case.

Additionally, we cite a proposition from [2] that can be applied to illuminate properties the spectrum of the real-analytic Heun operator. We further propose a direct corollary connecting this proposition and Theorem 4.1 that connects the monodromy matrices of the Heun equation to the spectrum. Finally, we propose and prove an asymptotic formula for the desired accessory parameters.

1.3 Organization

In the following sections, we provide necessary background on monodromy and the unitary condition (Section 2), as well as the prior work of Beukers [2] on the Lamé Equation (Section 3). Within Section 3, we cover the construction of Beukers’s [2] computational algorithm in the case of the Lamé Equation (1.4). Section 4 presents the application of our methods on the general Heun Equation (1.2). Within Section 4, we propose and prove a novel theorem (Theorem 4.1), which allows for the application of this algorithm to the Heun Equation. We then present the numerical results of our algorithm on multiple Heun Equations including the Lamé equation. Section 5 presents some important properties regarding the spectrum of the real-analytic Heun operator. Section 6 presents an asymptotic formula for finding desired eigenvalues of the Heun

operator. Section 7 links to a GitHub repository with all of the code constituting our algorithm and instructions for its use.

2 Background on Monodromy

2.1 Monodromy and Local Exponents

In this section, we introduce monodromy groups and their correspondence to local exponents, which form a key part of our later analysis of the Heun Equation (see Section 4).

Take a differential equation

$$\frac{d^2y}{dx^2} + P(x)\frac{dy}{dx} + Q(x)y = 0$$

where $P(x)$ and $Q(x)$ are rational complex functions. Let the poles of this equation (i.e., those of $P(x)$ and $Q(x)$ collectively) be z_0, z_1, \dots, z_n , including ∞ if appropriate. Let $\Gamma_0, \Gamma_1, \dots, \Gamma_n$ be closed, simple, counter-clockwise loops about each pole that do not contain any other poles, starting at a common point $p \neq z_i$ for all integers i such that $0 \leq i \leq n$.

Let y_1 and y_2 be two independent solutions of the differential equation defined in a neighborhood of p . We can analytically continue y_1 and y_2 around Γ_k for some integer k such that $0 \leq k \leq n$, resulting in the two different functions \tilde{y}_1 and \tilde{y}_2 , respectively. Since \tilde{y}_1 and \tilde{y}_2 must also be two independent solutions of the above equation at p , there exists an invertible 2×2 matrix M_k for which we can write

$$M_k \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} \tilde{y}_1 \\ \tilde{y}_2 \end{pmatrix}.$$

We refer to this act of analytically continuing around a pole as *monodromy* and the matrix M_k as the *monodromy matrix* around Γ_k .

Let G be the matrix group generated by M_0, M_1, \dots, M_n (we call G the *monodromy group* of the differential equation), and let Γ be the group generated by the elements $\Gamma_0, \Gamma_1, \dots, \Gamma_n$ modulo $\prod_{i=0}^n \Gamma_{\sigma(i)}$ for any permutation σ ; note that this is the fundamental group of $P_1(\mathbb{C}) \setminus \{z_0, z_1, \dots, z_n\}$ with base point p . The mapping $f : \Gamma \rightarrow G$, where $f(\Gamma_k) = M_k$, is a group homomorphism.

The asymptotic behavior of the solutions of a differential equation near its singularities has a close connection with the monodromy matrices. Take a basis of two independent solutions y_1 and y_2 to the differential equation; generically, in a neighborhood of the singular point, we can write $y_1 = z^a u_1$ and $y_2 = z^b u_2$, where u_1 and u_2 are nonzero, analytic functions. We refer to a and b as the *local exponents* of this differential equation at the singularity.

Given the local exponents (a, b) at a singularity, the monodromy matrix around that singularity must have eigenvalues

$$e^{2\pi ia}, e^{2\pi ib}.$$

When $a \not\equiv b \pmod{\mathbb{Z}}$, this matrix can be diagonalized into

$$\begin{pmatrix} e^{2\pi ia} & 0 \\ 0 & e^{2\pi ib} \end{pmatrix}.$$

From [22], we see that the local exponents of the Heun Equation (1.2) are

$$\begin{aligned} \text{At } z = 0, & \quad (0, 1 - \gamma) \\ \text{At } z = 1, & \quad (0, 1 - \delta) \\ \text{At } z = a, & \quad (0, 1 - \varepsilon) \\ \text{At } z = \infty, & \quad (\alpha, \beta). \end{aligned}$$

2.2 Unitarity

Given a nondegenerate Hermitian matrix H , we define (as in [2]) the *unitary group corresponding to H* to be the group

$$U(H) = \{g \in GL(2, \mathbb{C}) \mid g^\dagger H g = H\}.$$

Note that for $h \in GL(2, \mathbb{C})$,

$$h^{-1}U(H)h = U(h^\dagger H h).$$

The following proposition is well known and fairly straightforward to prove:

Proposition 2.1 ([2]). *Let $H_0 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$. The unitary group $U(H_0)$ is the group generated by $SL(2, \mathbb{R})$ ($SL(2, \mathbb{R})$ is the group of 2×2 real matrices with determinant 1) and the diagonal matrices³ λI_2 .*

With this proposition, if we can show that a monodromy group is conjugate to a subgroup of the group generated by $SL(2, \mathbb{R})$ and the diagonal matrices λI_2 , we can prove this monodromy group admits an invariant nondegenerate Hermitian matrix and is therefore unitary. In particular, we can ensure that this Hermitian matrix is equal to H_0 .

3 Unitarity conditions for the Lamé Equation

In this section, we review Beukers's method of finding accessory parameters B such that the monodromy group of the Lamé Equation (1.4) is unitary [2]. In short, after we integrate the Lamé Equation to calculate monodromy matrices, we use these matrices to identify accessory parameters for which the equation's monodromy group is unitary. This provides the foundation for our later generalization of this algorithm in Section 4.

To utilize this method, we must first cite [2, Proposition 2] as a theorem. Note that this theorem holds whenever P , Q , and R are all reflections; from Section 2 we can see that this already applies to a larger class of equations ($\gamma, \delta, \varepsilon \in \mathbb{Z} + \frac{1}{2}$) than the Lamé Equation ($\gamma, \delta, \varepsilon = 1/2$).

Theorem 3.1 ([2]). *Let $P, Q, R \in GL(2, \mathbb{C})$ be reflections (i.e., they have eigenvalues $1, -1$), and suppose that PQR is parabolic with trace $\pm 2i$. Let G be the group generated by P, Q, R . Then, the following statements are equivalent:*

1. G is unitary.
2. The traces of PQ , QR , and PR are real.
3. The traces of PQ and QR are real and satisfy $(\text{tr}(PQ)^2 - 4)(\text{tr}(QR)^2 - 4) \geq 16$.

With Theorem 3.1, we have a powerful tool to identify unitary monodromy groups. Specifically, if we can ensure that the traces of two pairs of monodromy matrix products are all real, then we ensure that the monodromy group is unitary. This is central to the algorithm of [2]; using a gradient-descent-type method, we can iteratively find values of B for which two of the traces $\text{tr}(PQ)$, $\text{tr}(QR)$, $\text{tr}(PR)$ converge to real numbers, thereby guaranteeing unitarity.

In this section, we assume that $\gamma = \delta = \varepsilon = \frac{1}{2}$ so that the Heun Equation is equivalent to the Lamé Equation. We also set the singularities of our Heun equation to be at $-1, 0, 1$ so that it corresponds to a Darboux Equation (1.3) with a scaled integer lattice $\Lambda_0 = 2.622\mathbb{Z}[i]$, equivalent to that used in [2]. The algorithm works as follows:

1. Using the value of our accessory parameter B , we calculate the monodromy matrices M_1 , M_2 , and M_3 around our three poles a_1 , a_2 , and a_3 (the poles we use for the Heun Equation (1.2) are $0, 1$, and $a = -1$). This is done by analytically continuing two functions y and its derivative $\partial_x y$ about three paths, starting at a common point P , circling one of the poles, and returning to P . We use a Runge-Kutta method to integrate the Lamé Equation and thus analytically continue y and $\partial_x y$ around this path. The specific way that we find the monodromy matrices is as follows:

³Here, $\lambda \in \mathbb{C}$, $|\lambda| = 1$, and I_2 is the 2×2 identity matrix

- (i) Take the initial values $y_0 = 0, \partial_x y_0 = 1$ and then $y_0 = 1, \partial_x y_0 = 0$.
- (ii) Integrate as described above to find the final values $y_1, \partial_x y_1$ and $y_2, \partial_x y_2$.
- (iii) Calculate the monodromy matrix $M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ using the equations

$$M \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} y_1 \\ \partial_x y_1 \end{pmatrix}, \quad M \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} y_2 \\ \partial_x y_2 \end{pmatrix}.$$

The paths taken in our algorithm are shown in more detail in Figure 1.

2. Here, we utilize Beukers's gradient-descent algorithm [2]. After solving for the three monodromy matrices $M_1, M_2,$ and M_3 about each of the three poles, we can find the traces of $M_1 M_2$ and $M_2 M_3$, denoted t_{12} and t_{23} respectively. Note that t_{12} and t_{23} are analytic functions of B , and so we can take an approximation of their derivative with respect to B . We select a value ϵ such that $B + \epsilon$ is a better approximation of the accessory parameter such that the resulting monodromy group is unitary. We recompute the traces at $B + \epsilon$ and approximate our derivatives as

$$\lambda = \frac{t_{12}(B + \epsilon) - t_{12}(B)}{\epsilon}, \quad \mu = \frac{t_{23}(B + \epsilon) - t_{23}(B)}{\epsilon}.$$

3. We iterate B as $B \mapsto B + \epsilon$, where ϵ is given by

$$\text{Im}(t_{12}(B) + \lambda\epsilon) = 0, \quad \text{Im}(t_{23}(B) + \mu\epsilon) = 0,$$

as in [2]. This corresponds to Newton's method for finding roots of $\text{Im}(t_{12})$ and $\text{Im}(t_{23})$ from Theorem 3.1. This corresponds in turn to an accessory parameter with unitary monodromy group. Solving these linear equations for ϵ gives us

$$\epsilon = \frac{\bar{\mu}\text{Im}(t_{12}(B)) - \bar{\lambda}\text{Im}(t_{23}(B))}{\bar{\lambda}\mu}.$$

This allows us to calculate a better approximation of B using $B + \epsilon$. We then update B and repeat these steps as necessary until the monodromies and values of B have converged to an appropriate number of decimal places.

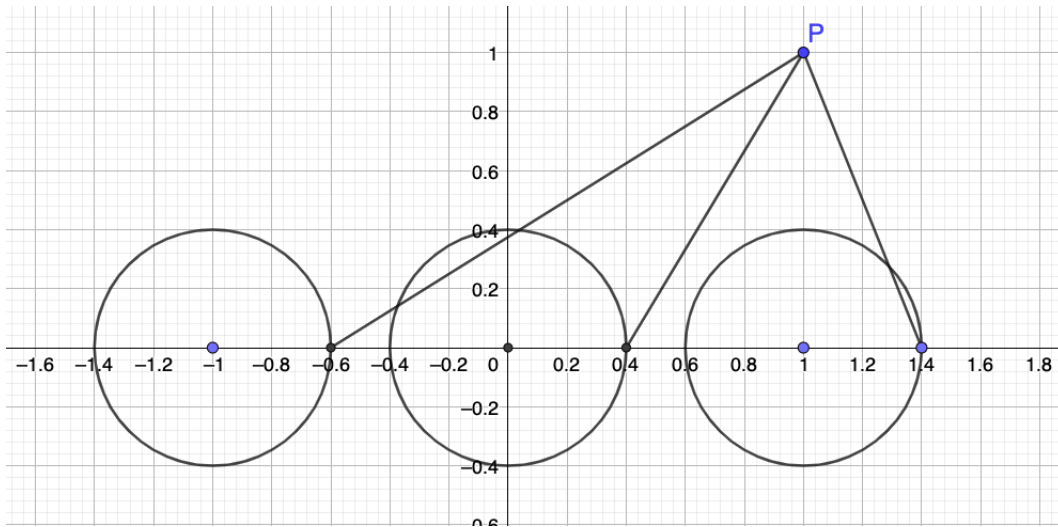


Figure 1: The paths we use to simulate monodromy. All paths start at the point $P = (1, 1)$, though any non-singular point would suffice. They go in a straight line to the rightmost point on a circle of radius 0.4 surrounding each pole. They then traverse the circle in a counterclockwise direction before returning on the same straight line back to the point P . In the case of the $n = \frac{1}{2}$ Lamé Equation, our poles are at $-1, 0, 1$. Note that we do not need to simulate the pole about ∞ because we have the identity $M_1 M_2 M_3 M_\infty = I_2$.

4 Unitarity conditions for the Heun Equation

In this section, we discuss our extension of the above methods into the general Heun Equation (1.2). We first give the following theorem. This is an extension of Theorem 3.1 to the Heun Equation:

Theorem 4.1. *Let G be the monodromy group generated by the matrices $P, Q, R \in GL(2, \mathbb{C})$, and assume that PQR is parabolic. Then, for the statements*

1. G is unitary,
2. For $\lambda_P = e^{-\pi i \gamma}$, $\lambda_Q = e^{-\pi i \delta}$, $\lambda_R = e^{-\pi i \varepsilon}$, we have

$$\frac{\operatorname{tr}(PQ)}{\lambda_P \lambda_Q}, \frac{\operatorname{tr}(QR)}{\lambda_Q \lambda_R}, \frac{\operatorname{tr}(PR)}{\lambda_P \lambda_R} \in \mathbb{R},$$

(1) \implies (2) in general and (2) \implies (1) when two of P, Q, R are reflections.

Key to the proof of this theorem is [2, Lemma 2], restated below.

Lemma 4.2 ([2]). *Let $P, Q, R \in GL(2, \mathbb{C})$ be reflections. Then, we must have*

$$\operatorname{tr}(PQ)^2 + \operatorname{tr}(QR)^2 + \operatorname{tr}(PR)^2 - \operatorname{tr}(PQ) \operatorname{tr}(QR) \operatorname{tr}(PR) = 2 + \operatorname{tr}((PQR)^2). \quad (4.1)$$

Furthermore, if PQR is parabolic with trace $\pm 2i$ and $\operatorname{tr}(PQ), \operatorname{tr}(QR), \operatorname{tr}(PR) \in \mathbb{R}$, then we also have that $\min(|\operatorname{tr}(PQ)|, |\operatorname{tr}(QR)|, |\operatorname{tr}(PR)|) > 2$.

Proof of Theorem 4.1. We first prove (1) \implies (2) in the general case.

From the fact that PQR is parabolic (as in [2]), we know that the Hermitian matrix which G preserves must have signature (1, 1) (i.e., this matrix has one positive and one negative eigenvalue). We can therefore conjugate the monodromy group G as detailed in Section 2.2 to make the Hermitian form equal to $H_0 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$.

From there, we utilize Proposition 2.1 to put P, Q, R in the form

$$\begin{aligned} P &= \lambda_P P_0, \\ Q &= \lambda_Q Q_0, \\ R &= \lambda_R R_0, \end{aligned}$$

where $\lambda_P, \lambda_Q, \lambda_R \in \mathbb{C}$ all have magnitude 1, and $P_0, Q_0, R_0 \in SL(2, \mathbb{R})$. Then, we see that

$$\begin{aligned} \operatorname{tr}(PQ) &= \operatorname{tr}(\lambda_P \lambda_Q P_0 Q_0) = \lambda_P \lambda_Q \operatorname{tr}(P_0 Q_0), \\ \operatorname{tr}(QR) &= \operatorname{tr}(\lambda_Q \lambda_R Q_0 R_0) = \lambda_Q \lambda_R \operatorname{tr}(Q_0 R_0), \\ \operatorname{tr}(PR) &= \operatorname{tr}(\lambda_P \lambda_R P_0 R_0) = \lambda_P \lambda_R \operatorname{tr}(P_0 R_0). \end{aligned}$$

Since P_0, Q_0 , and R_0 are all real matrices, we know that the traces of $P_0 Q_0, Q_0 R_0$, and $P_0 R_0$ are all real. Thus, rearranging the above expressions, we get

$$\frac{\operatorname{tr}(PQ)}{\lambda_P \lambda_Q}, \frac{\operatorname{tr}(QR)}{\lambda_Q \lambda_R}, \frac{\operatorname{tr}(PR)}{\lambda_P \lambda_R} \in \mathbb{R},$$

as desired.

Now, we assume without loss of generality that P and Q are reflections. We seek to prove that (2) \implies (1). We initially follow Beukers's proof before deviating from it to account for R not being a reflection [2]. By our assumption, we know that the eigenvalues of P are 1 and -1 . Therefore, we can conjugate the group G such that

$$P = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}.$$

Now, because Q is a reflection, we can write it as

$$Q = \begin{pmatrix} p & q \\ r & -p \end{pmatrix}.$$

Choose $a, b \in \mathbb{C}$ with $-2ab + a^2q - b^2r \neq \pm i$ such that $a^2 + b^2 = 1$ and $(a^2 - b^2)p + ab(q + r) = 0$.

Then, we conjugate by $M = \begin{pmatrix} a & b \\ -b & a \end{pmatrix}$, leaving P fixed and changing Q into

$$MQM^{-1} = \begin{pmatrix} 0 & -2abp + a^2q - b^2r \\ -2abp - b^2q + a^2r & 0 \end{pmatrix}.$$

Then, because $\det(Q) = -1$, we know that $(-2abp + a^2q - b^2r)(-2abp - b^2q + a^2r) = 1$, so with this conjugation, we can write $Q = \begin{pmatrix} 0 & q' \\ r' & 0 \end{pmatrix}$, where $q'r' = 1$. Now, we see that $\text{tr}(PQ) = i(q' - r') \in \mathbb{R}$. Let $q' = ik$ for some $k \in \mathbb{C}$. From $q'r' = 1$, we have $r' = -i/k$. Then, we have $i(q' - r') = k + 1/k \in \mathbb{R}$. Note that $k \neq \pm 1$ by our restrictions.

Lemma 4.3. *With P and Q as defined, we have $|\text{tr}(PQ)| > 2$.*

Proof. Define a new matrix R' such that, after the two conjugations detailed above,

$$R' = \begin{pmatrix} -\frac{2ik}{k^2-1} & b \\ \frac{4k^2+8k^4+4k^6}{4bk^2(k^2-1)^2} & \frac{2ik}{k^2-1} \end{pmatrix},$$

where $b \in \mathbb{C} \setminus \{0\}$. Now, this form of R' must exist by our requirement that $k \neq \pm 1$ and the fact that $k \neq 0$ by definition. This form satisfies the conditions that R' is a reflection and PQR' has eigenvalues both equivalent to i .

From here, there are two possibilities. Either PQR' is parabolic and therefore not diagonalizable or $PQR' = i\mathbb{1}$. We consider the two cases separately.

Case 1: PQR' is parabolic. In this case, we can apply Lemma 4.2, with P, Q , and R' all being complex reflections and PQR' being parabolic with trace $2i$. We directly get that $|\text{tr}(PQ)| > 2$, as desired.

Case 2: $PQR' = i\mathbb{1}$. In this case, we can slightly modify R' to get PQR' in a parabolic form. Since R' has two distinct eigenvalues by its definition, we know it is diagonalizable. We can therefore write

$$R' = UDU^{-1},$$

where D is some diagonal matrix and U is some invertible matrix. By this definition, we see that

$$PQR' = PQUDU^{-1} = i\mathbb{1},$$

meaning that

$$PQUD = iU.$$

Now, consider the matrix

$$\tilde{R} = UD \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} U^{-1}.$$

Note that \tilde{R} is a reflection since its eigenvalues are preserved as ± 1 . We also see that

$$PQ\tilde{R} = PQUD \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} U^{-1} = iU \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} U^{-1}$$

has its eigenvalues both equivalent to i . Furthermore, we can clearly see that $PQ\tilde{R}$ is not diagonalizable and therefore parabolic. Then, we can apply Lemma 4.2 to P, Q , and \tilde{R} to get that $|\text{tr}(PQ)| > 2$, as desired. \square

Now, $|\frac{1}{k} + k| = |\text{tr}(PQ)| > 2$ and $\frac{1}{k} + k \in \mathbb{R}$. Therefore, we must have $k \in \mathbb{R}$. With this knowledge, we let $R = \begin{pmatrix} p & q \\ r & s \end{pmatrix}$. We get immediately that $\text{tr}(PR) = i(r - q)$ and $\text{tr}(QR) = i(kr - \frac{q}{k})$. Let $r_{PR} = \frac{\text{tr}(PR)}{\lambda_P \lambda_r}$ and $r_{QR} = \frac{\text{tr}(QR)}{\lambda_Q \lambda_R}$. Then, solving for q and r , we get

$$q = \lambda_R \frac{-r_{PR}k + r_{QR}}{k - k^{-1}}, \quad r = \lambda_R \frac{-r_{PR}k^{-1} + r_{QR}}{k - k^{-1}}.$$

Note that we have expressed q and r as real multiples of λ_R . Similarly, we can solve for p and s using the restrictions that $\text{tr}(R) = 1 + \lambda_R^2$ and $\text{tr}(PQR) = -2\lambda_R$. Indeed, we see that these two restrictions correspond to, respectively,

$$\begin{aligned} p + s &= 1 + \lambda_R^2, \\ \frac{p}{k} + sk &= -2\lambda_R. \end{aligned}$$

Solving these two equations, we get

$$p = \frac{k^2 \lambda_R^2 + k^2 + 2k\lambda_R}{k^2 - 1}, \quad s = -\frac{\lambda_R^2 + 2k\lambda_R + 1}{k^2 - 1}.$$

Now, because $|\lambda_R| = 1$ by definition, we know that $\frac{1 + \lambda_R^2}{\lambda_R} = 2 + 2\cos(2\arg(\lambda_R)) \in \mathbb{R}$. Thus, we see that we can rewrite p and s as real multiples of λ_R :

$$p = \lambda_R \frac{k^2(2 + 2\cos(2\arg(\lambda_R))) + 2k}{k^2 - 1} \quad s = -\lambda_R \frac{2 + 2\cos(2\arg(\lambda_R)) + 2k}{k^2 - 1}.$$

Thus, for some real matrix $R_0 = \begin{pmatrix} p_0 & q_0 \\ r_0 & s_0 \end{pmatrix}$, we have

$$R = \lambda_R R_0.$$

Now, by definition, we know that $\det(R) = \lambda_R^2$, so $\det(R_0) = 1$. We see that, therefore, for some real matrices $P_0, Q_0, R_0 \in SL(2, \mathbb{R})$, P, Q, R can be expressed as $P = \lambda_P P_0$, $Q = \lambda_Q Q_0$, and $R = \lambda_R R_0$. Thus, by Proposition 2.1, G is unitary, as desired. \square

Importantly, this theorem allows us to extend Beukers's algorithm (described in Section 3 in its original form). Previously, our algorithm was restricted by the hypothesis of Theorem 3.1, so its results were only guaranteed to be accurate for the specific case of the Heun Equations where all monodromies are reflections. This theorem allows us to extend the algorithm to an infinite class of Heun Equations, where any one of the parameters is free to vary.

Leveraging Theorem 4.1, we can force the monodromy group to be unitary using the approximated derivatives of the traces of pairwise matrix products. To this end, the steps of our extended algorithm are described below. Sourcecode for our own implementation of this algorithm is available in Section 7.

1. Using the value of our accessory parameter B , we calculate the monodromy matrices, P, Q, R with the same method as detailed in Section 3.
2. Calculate the traces of PQ and QR . Denote these with the functions $t_{12}(B)$ and $t_{23}(B)$, as before. Choose some value B as a guess and let $B + \epsilon$ be a better approximation of the accessory parameter that will yield a unitary monodromy group.
3. We approximate the derivatives of t_{12} and t_{23} as before:

$$\lambda = \frac{t_{12}(B + \epsilon) - t_{12}(B)}{\epsilon} \quad \text{and} \quad \mu = \frac{t_{23}(B + \epsilon) - t_{23}(B)}{\epsilon}.$$

4. We want to ensure that $\frac{t_{12}(B + \epsilon)}{\lambda_P \lambda_Q}, \frac{t_{23}(B + \epsilon)}{\lambda_Q \lambda_R} \in \mathbb{R}$. We rewrite this as

$$\text{Im} \left(\frac{t_{12}(B) + \lambda\epsilon}{\lambda_P \lambda_Q} \right) = 0, \quad \text{Im} \left(\frac{t_{23}(B) + \mu\epsilon}{\lambda_Q \lambda_R} \right) = 0.$$

Solving these, we can calculate ϵ as

$$\epsilon = \frac{\frac{\overline{\mu}}{\lambda_Q \lambda_R} \operatorname{Im}\left(\frac{t_{12}(B)}{\lambda_P \lambda_Q}\right) - \frac{\overline{\lambda}}{\lambda_P \lambda_Q} \operatorname{Im}\left(\frac{t_{23}(B)}{\lambda_P \lambda_Q}\right)}{\frac{\operatorname{Im}(\overline{\lambda\mu})}{\lambda_P \lambda_Q \lambda_Q \lambda_R}}.$$

Then, we iterate B as $B \mapsto B + \epsilon$. We repeat this algorithm as necessary to eventually converge to an appropriate number of decimal places.

Note that although our algorithm only guarantees that two of the three terms in statement 2 of Theorem 4.1 are real, we can prove analytically that this leads to the third term being real using asymptotic analysis similar to that in [2, Section 5]. In particular, one can prove that only one unique unitary accessory parameter exists within a neighborhood of size $O(1/|z|)$ of each Gaussian integer lattice point z ; if only one point in this region gives rise to two real terms of Statement 2, then all three such terms must be real. Additionally, from our algorithm, we see that at each of our found accessory parameters, the third term descends to a real value within around 0.1–1% relative error.

4.1 Numerical Results and Figures

By Theorem 4.1, for the Lamé Equation (where all three monodromies are reflections) and for Heun Equations where two of the monodromies are reflections, the convergent values of this algorithm are guaranteed to yield unitary monodromy groups, since (1) \iff (2). However, in other cases, we still have (1) \implies (2) in Theorem 4.1, so the algorithm's values still yield candidate unitary monodromy groups. In particular, one such value of B must exist near each (squared) lattice point by Theorem 6.1, giving an additional guarantee of unitarity.

We run our algorithm on several sets of parameters. For all of these parameters, we set the singularities of our Heun equation to be at $-1, 0, 1$, so that it corresponds to a Darboux equation with lattice Λ_0 . First, as a verification that our modified algorithm functions properly, we test it on the parameters $\gamma = \delta = \varepsilon = \frac{1}{2}$ (i.e., the Lamé Equation). In the following diagram position of each pixel represents the starting guess value of B , and its color/brightness represents the eventual convergent value after 20 repetitions of the algorithm⁴.

Figure 2(a) shows several regions of solid color, where all of the initial guesses in that area converge to a single value of the accessory parameter that yields a unitary monodromy group. These convergent values are the values of the accessory parameter we desire. Along with this convergence map, 2(b) shows a plot of the outputs of our algorithm as it converges.

Taking the square roots of these convergent values, we obtain a distorted version of our lattice Λ_0 . We plot this distorted lattice in Figure 2(c). This is consistent with the findings of Beukers in his formula for approximating accessory parameters [2]. We observe heightened distortion for values of z where $\operatorname{Re}(z) > 5$ that we believe is due to numerical error in our algorithm.

The square roots of the Convergence Maps of the Lamé equation and the $\varepsilon = \frac{1}{8}$ and $\varepsilon = \frac{5}{8}$ Heun equations can be found in the Appendix 9.

⁴We color our map using the standard HSV domain coloring of the complex plane, as implemented by `Color.hsva` in Pygame.

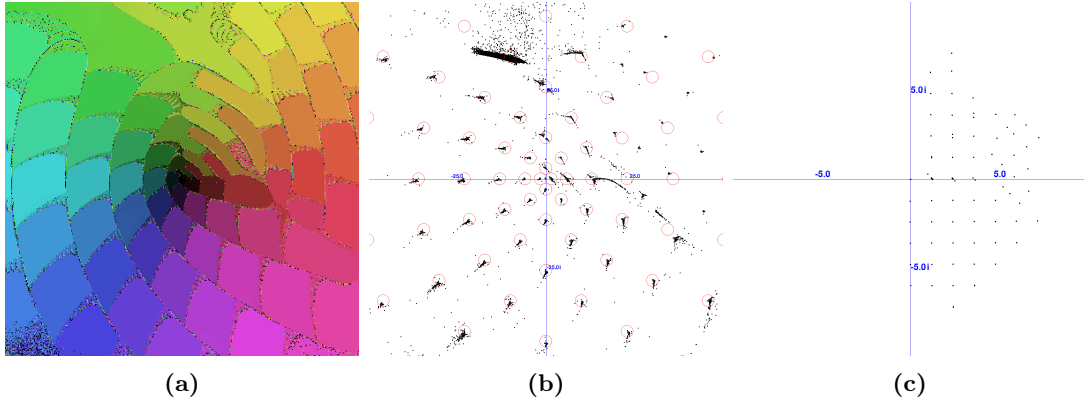


Figure 2: (a) This is the “convergence map” for the Lamé Equation depicting the complex plane with real axis ranging between -50 and 50 and the imaginary axis ranging between $-50i$ and $50i$ with resolution of 16 pixels per square unit. The position of each pixel represents the initial guess value of B . Using a standard HSV color transform, we display the final value of B after 20 repetitions through our algorithm.

(b) This figure displays the output values of B from our algorithm in black plotted on the complex plane. The clumping of the black points indicates the convergence of our algorithm. The centers of the red circles are the numerical values calculated by [2].

(c) This is the distorted lattice we obtain from taking the square root of the accessory parameters. We can see that it very closely emulates the lattice of Gaussian integers with slight distortion. We believe that the extreme distortion for $\text{Re}(z) > 5$ is due to numerical error, associated with large values of the approximated derivatives.

Then, following Theorem 4.1, we vary ε while keeping γ and δ fixed as $\frac{1}{2}$. In Figure 3(a), we see the convergence map and the plot of the outputs of the algorithm with $\varepsilon = \frac{1}{8}$. We have compiled the same images for $\varepsilon = \frac{5}{8}$ in Figure 4 which has been placed in the Appendix 9.

Additionally, we compiled the convergence map and plot of the algorithm outputs for an equation outside the class of equations that Theorem 4.1 guarantees our algorithm to work on. This map for $\gamma = \frac{1}{2}$, $\delta = \frac{3}{4}$, and $\varepsilon = \frac{1}{4}$ is shown in the Appendix 9.

Additionally, we notice that if we take the square roots of our calculated accessory parameters, the resulting values resemble a distorted lattice of integers. These patterns are displayed for our varying values of ε as shown in Figures 2(c), 3(c), and 8.

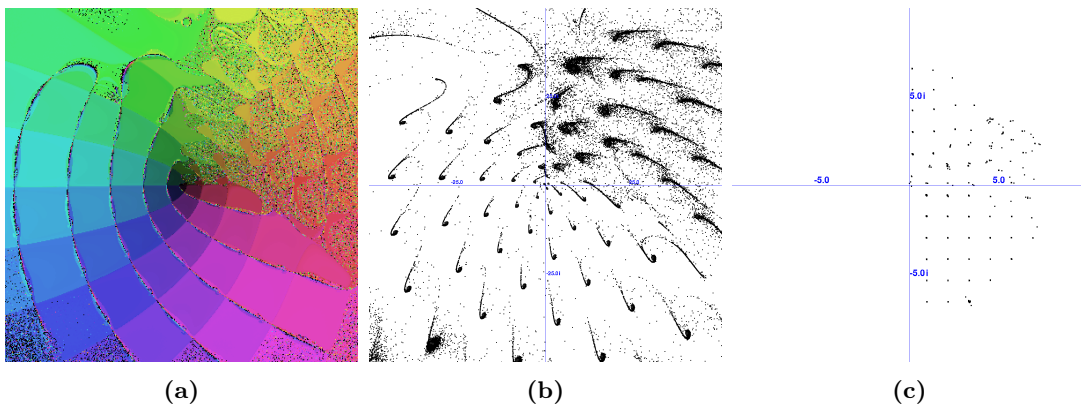


Figure 3: (a) This is the convergence map for the Heun Equation with $\gamma = \delta = \frac{1}{2}$, and $\varepsilon = \frac{1}{8}$. The map covers the complex plane, with real axis ranging from -50 to 50 and imaginary axis ranging from $-50i$ to $50i$ coloring it with the same method we use in Figure 2.

(b) Here, we plot the output values of our algorithm as they converge. We see the black points clumping up as the algorithm converges to accessory parameters.

(c) This is the distorted lattice we obtain from taking square roots of the accessory parameters we calculated for the Heun Equation with $\varepsilon = 0.125$.

5 Spectrum of the Real-Analytic Heun Operator

Following Beukers [2], we can translate the Accessory Parameter Question (Question 1) into a question regarding the spectrum of the real-analytic Heun Operator. In this section, we put forward two important propositions to our understanding of this translation. The first is Proposition 4 in [2].

Proposition 5.1 ([2], Prop. 4). *Let G be the monodromy group of the linear second order differential equation $y'' + py' + qy = 0$, where $p, q \in \mathbb{C}(z)$. Then G is unitary if and only if there exists a nontrivial C^2 function f on $\mathbb{C} \setminus \{0, 1, a\}$ which is a real-analytic solution of the Heun Equation. Furthermore, f is uniquely determined up to a constant factor.*

Note that the Heun equation is in the form of the linear second order differential equation specified above. We have also quantified values of the accessory parameter B for which the Heun equation (1.2) is unitary in Theorem 4.1, allowing us to deduce the following corollary:

Corollary 5.2. *Let the monodromy group of the Heun equation be generated by the matrices $P, Q, R \in GL(2, \mathbb{C})$ with PQR parabolic. Let $\lambda_P = e^{-\pi i \gamma}$, $\lambda_Q = e^{-\pi i \delta}$, $\lambda_R = e^{-\pi i \varepsilon}$, where γ, δ , and ε are as defined in Heun equation. Suppose that two of P, Q, R are reflections and satisfy*

$$\frac{\operatorname{tr}(PQ)}{\lambda_P \lambda_Q}, \frac{\operatorname{tr}(QR)}{\lambda_Q \lambda_R}, \frac{\operatorname{tr}(PR)}{\lambda_P \lambda_R} \in \mathbb{R}.$$

Then, the Heun equation must possess a real-analytic solution f , unique up to scaling.

Thus, rewriting the Heun equation in the form

$$Ly = By,$$

where L is the Heun operator and B is the accessory parameter, Corollary 5.2 provides us with the full spectrum of the real-analytic Heun operator. Similarly, if we remove the assumption that any of P, Q, R are reflections, then using the general statement that (1) \implies (2) in Theorem 4.1, Corollary 5.2 still provides us with significant restrictions on what the spectrum of the real-analytic Heun operator can be.

6 Asymptotic Analysis

Now, as [2] did, we create an asymptotic formula for finding accessory parameters for the Heun Equation (1.2). First, however, we convert the Heun Equation into the Darboux Equation through the change of variable defined in [19].

For this equation, we propose the following theorem, modified from [2, Conjecture 1]:

Theorem 6.1. *Let $\bar{\Lambda}$ be the lattice generated by $\overline{\omega_1}$ and $\overline{\omega_2}$, and let Δ be the area of the fundamental parallelogram of the lattice $\bar{\Lambda}$. Let $l_0 \in \frac{\pi}{\Delta} \bar{\Lambda}$. Furthermore, let ζ be the Weierstrass Zeta Function and define $\eta_i = \zeta(z + \omega_i) - \zeta(z)$ to be the quasi-periods of the Weierstrass Zeta Function. Then, up to order $\frac{1}{|l_0|}$, the accessory parameters B which solve the Accessory Parameter Problem 1 are given by*

$$B = l_0^2 - \left(\sum_{i=0}^3 m_i(m_i + 1) \right) \left(\frac{\eta_1 \overline{\omega_2} - \eta_2 \overline{\omega_1}}{2i\Delta} + \frac{\pi l_0}{\Delta \overline{l_0}} \right) + \mathcal{O}\left(\frac{1}{|l_0|}\right).$$

*Additionally, solutions u must be both real-valued and even.*⁵

Proof. As in [2], we let $u = e^{lz + \beta(z)}$, for some function $\beta(z)$. We have $\lim_{|l| \rightarrow \infty} \frac{B}{l^2} = 1$. From the fact that u solves Equation (1.3), we have $\beta'' + (\beta')^2 + 2l\beta' - \left(\sum_{i=0}^3 m_i(m_i + 1) \wp(x - \omega_i) \right) \wp(z) = 0$. We asymptotically expand β to

$$\beta(z) = \frac{\beta_1(z)}{l} + \frac{\beta_2(z)}{l^2} + \dots$$

⁵The proof for this fact can be found in [2, Section 4].

From this expansion, we have

$$2\beta'_1 - \left(\sum_{i=0}^3 m_i(m_i + 1)\wp(x - \omega_i) \right) \wp = 0.$$

Since we are considering u asymptotically up to order $\frac{1}{l_0}$, we take the approximation $\beta(z) = \frac{\beta_1(z)}{l}$. Now, as $\zeta'(z) = -\wp(z)$, we can solve the above equation to obtain

$$\beta_1(z) = - \left(\sum_{i=0}^3 m_i(m_i + 1)\wp(x - \omega_i) \right) \frac{\zeta(z)}{2}.$$

Now, let's take the solution $u = \exp \left(lz + \beta(z) - \overline{lz + \beta(z)} \right) + cc.$ to the equation, where $cc.$ denotes the complex conjugate of the first term. Taking the first-order approximation, we get this in the form

$$u = \exp \left[lz - \overline{lz} - \left(\sum_{i=0}^3 m_i(m_i + 1)\zeta(z - \omega_i)/2l \right) + \overline{\left(\sum_{i=0}^3 m_i(m_i + 1)\zeta(z - \omega_i)/2\overline{l} \right)} \right] + cc.$$

Now, u is doubly-periodic because it solves the Darboux Equation, which contains several doubly-periodic Weierstrass elliptic functions. We can exploit this periodicity to infer that, for some $n_1, n_2 \in \mathbb{Z}$, we have

$$l\omega_1 - \overline{l\omega_1} - \left(\sum_{i=0}^3 m_i(m_i + 1) \right) \frac{\eta_1}{2l} + \overline{\left(\sum_{i=0}^3 m_i(m_i + 1) \right) \frac{\eta_1}{2\overline{l}}} = -2\pi in_2 + \mathcal{O}(1/|l|^2),$$

$$l\omega_2 - \overline{l\omega_2} - \left(\sum_{i=0}^3 m_i(m_i + 1) \right) \frac{\eta_2}{2l} + \overline{\left(\sum_{i=0}^3 m_i(m_i + 1) \right) \frac{\eta_2}{2\overline{l}}} = 2\pi in_1 + \mathcal{O}(1/|l|^2).$$

Note that we can combine all of the separate Weierstrass Zeta Functions into single η terms because $\zeta(z - \omega_i + \omega_j) - \zeta(z - \omega_i) = \zeta(z + \omega_j) - \zeta(z) = \eta_j$.

Let's now consider a lattice point $l_0 = \frac{\pi(m_2\overline{\omega_2} + m_1\overline{\omega_1})}{\Delta}$. Let $l = l_0 + \epsilon$. Then, from the above, we have

$$\epsilon\omega_1 - \overline{\epsilon\omega_1} = \left(\sum_{i=0}^3 m_i(m_i + 1) \right) \frac{\eta_1}{2l_0} - \overline{\left(\sum_{i=0}^3 m_i(m_i + 1) \right) \frac{\eta_1}{l_0}},$$

$$\epsilon\omega_2 - \overline{\epsilon\omega_2} = \left(\sum_{i=0}^3 m_i(m_i + 1) \right) \frac{\eta_2}{2l_0} - \overline{\left(\sum_{i=0}^3 m_i(m_i + 1) \right) \frac{\eta_2}{l_0}}.$$

Then, solving for ϵ and plugging into $l = l_0 + \epsilon$, we have

$$l = l_0 - \frac{\left(\sum_{i=0}^3 m_i(m_i + 1) \right)}{2i\Delta} \left(\frac{\eta_1\overline{\omega_2} - \eta_2\overline{\omega_1}}{l_0} + \frac{\overline{\eta_2\omega_1} - \overline{\eta_1\omega_2}}{\overline{l_0}} \right) + \mathcal{O}(1/|l_0|^2).$$

By Legendre's Relation, we see that $\overline{\eta_2\omega_1} - \overline{\eta_1\omega_2} = 2\pi i$. Therefore, we have

$$B = l^2 = l_0^2 - \frac{\left(\sum_{i=0}^3 m_i(m_i + 1) \right)}{2i\Delta} \left(\eta_1\overline{\omega_2} - \eta_2\overline{\omega_1} + 2\pi i \frac{l_0}{l_0} \right) + \mathcal{O}(1/|l_0|),$$

as desired. \square

7 Code

In the interest of replicability, we have published the multiple Python code files we use to find accessory parameters B as well as instructions for their use on a GitHub repository. This code can be found at this link: <https://github.com/ericc2023/HeunSimulation>.

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9 Appendix: Additional Convergence Results for Other Parameters

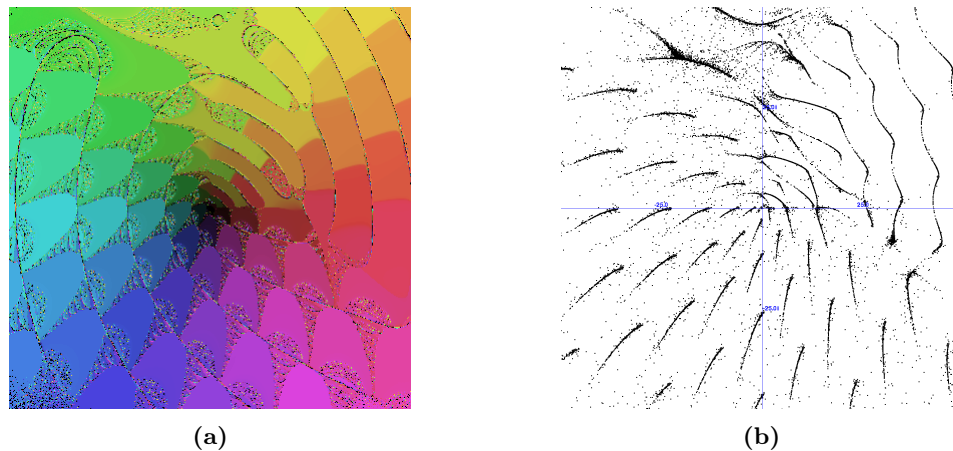


Figure 4: (a) This is the convergence map for the Heun Equation with $\gamma = \delta = \frac{1}{2}$, and $\varepsilon = \frac{5}{8}$. The map has real axis ranging from -50 to 50 and imaginary axis ranging from $-50i$ to $50i$ coloring it with the same method we use in Figure 2.

(b) Here, we plot the output values of our algorithm as they converge. We see the black points clumping up as the algorithm converges to accessory parameters. The long lines in the top right indicate that our algorithm is not converging very well in those areas.

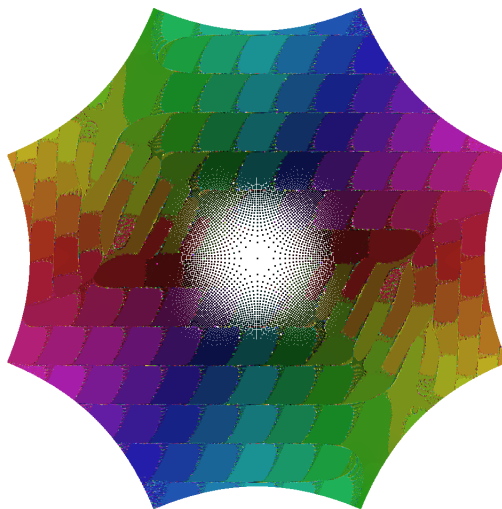


Figure 5: The complex square roots of the values in the Lamé equation Convergence Map in Figure 2(a)

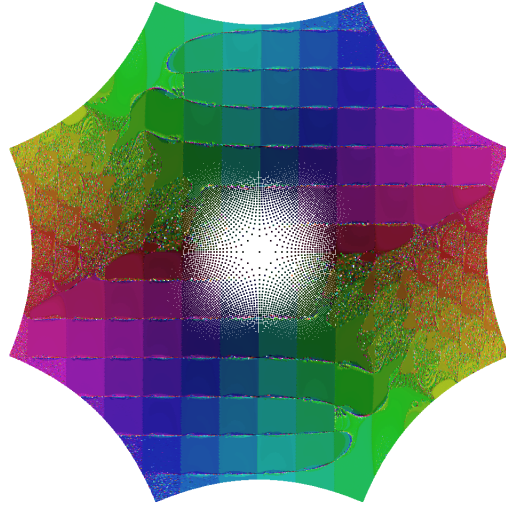


Figure 6: The complex square roots of the values in the $\varepsilon = 0.125$ Heun Equation Convergence Map in Figure 3(a)

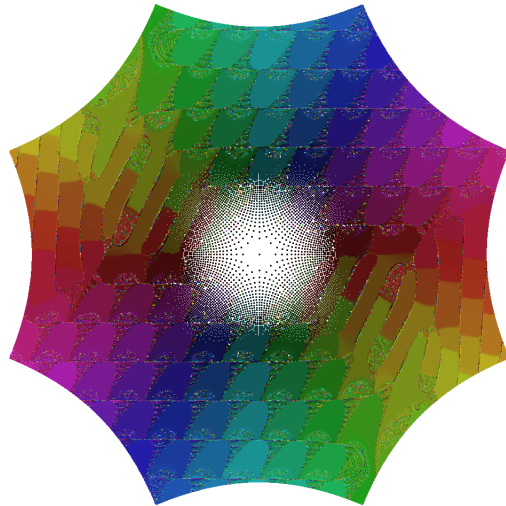


Figure 7: The complex square roots of the values in the $\varepsilon = 0.625$ Heun Equation Convergence Map in Figure 4(a)

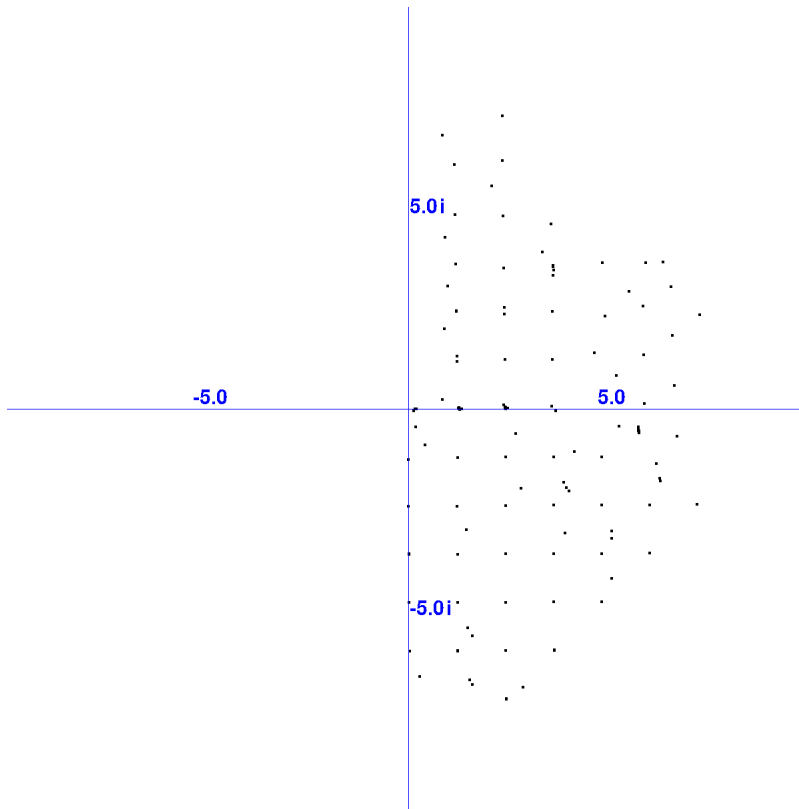
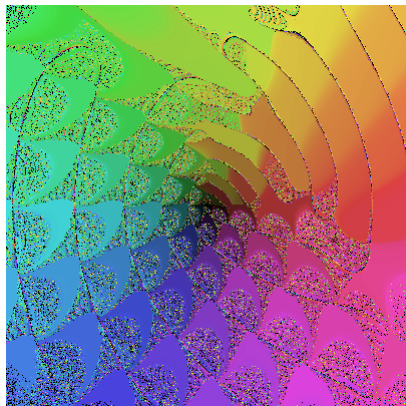
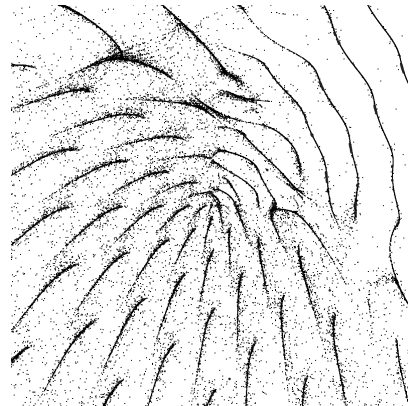


Figure 8: The distorted lattice obtained from square rooting our calculated accessory parameters for the Heun Equation with $\varepsilon = 0.625$.



(a)



(b)

Figure 9: (a) This is the convergence map for the Heun Equation with $\gamma = \frac{1}{2}$, $\delta = \frac{3}{4}$ and $\varepsilon = \frac{1}{4}$ and defined on the lattice Λ_0 . The map has real axis ranging from -50 to 50 and imaginary axis ranging from $-50i$ to $50i$ coloring it with the same method we use in Figure 2.

(b) Here, we plot the output values of our algorithm as they converge. We see the black points clumping up as the algorithm converges to accessory parameters. The top right also shows long lines of black points, which means our algorithm is not converging quickly or at all for those values.