

Universal optimality of the E_8 and Leech lattices and interpolation formulas

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Abstract

We prove that the E_8 root lattice and the Leech lattice are universally optimal among point configurations in Euclidean spaces of dimensions 8 and 24, respectively. In other words, they minimize energy for every potential function that is a completely monotonic function of squared distance (for example, inverse power laws or Gaussians), which is a strong form of robustness not previously known for any configuration in more than one dimension. This theorem implies their recently shown optimality as sphere packings, and broadly generalizes it to allow for long-range interactions.

The proof uses sharp linear programming bounds for energy. To construct the optimal auxiliary functions used to attain these bounds, we prove a new interpolation theorem, which is of independent interest. It reconstructs a radial Schwartz function f from the values and radial derivatives of f and its Fourier transform \hat{f} at the radii $\sqrt{2n}$ for integers $n \geq 1$ in \mathbb{R}^8 and $n \geq 2$ in \mathbb{R}^{24} . To prove this theorem, we construct an interpolation basis using integral transforms of quasimodular forms, generalizing Viazovska's work on sphere packing and placing it in the context of a more conceptual theory.

Contents

1. Introduction	2
2. Preliminaries and background on modular forms	16
3. Functional equations and the group algebra $\mathbb{C}[\mathrm{PSL}_2(\mathbb{Z})]$	25
4. Solutions of functional equations and modular form kernels	40
5. Proof of the interpolation formula	59
6. Positivity of kernels and universal optimality	77
7. Generalizations and open questions	88
Acknowledgements	91
References	92

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1. Introduction

What is the best way to arrange a discrete set of points in \mathbb{R}^d ? Of course the answer depends on the objective: there are many different ways to measure the quality of a configuration for interpolation, quadrature, discretization, error correction, or other problems. A configuration that is optimal for one purpose will often be good for others, but usually not optimal for them as well. Those that optimize many different objectives simultaneously play a special role in mathematics. In this paper, we prove a broad optimality theorem for the E_8 and Leech lattices, via a new interpolation formula for radial Schwartz functions. Our results help characterize the exceptional nature of these lattices. (See [20] and [17] for their definitions and basic properties.)

1.1. *Potential energy minimization.* One particularly fruitful family of objectives to optimize is energy under different potential functions. Given a *potential function* $p: (0, \infty) \rightarrow \mathbb{R}$, we define the *potential energy* of a finite subset \mathcal{C} of \mathbb{R}^d to be

$$\sum_{\substack{x, y \in \mathcal{C} \\ x \neq y}} p(|x - y|),$$

where $|\cdot|$ is the Euclidean norm (we include each pair of points in both orders, which differs by a factor of 2 from the convention in physics). Our primary interest is in infinite sets \mathcal{C} , for which potential energy requires renormalization because the double sum typically diverges. Define a *point configuration*, or just *configuration*, \mathcal{C} to be a nonempty, discrete, closed subset of \mathbb{R}^d (i.e., every ball in \mathbb{R}^d contains only finitely many points of \mathcal{C}). We say \mathcal{C} has *density* ρ if

$$\lim_{r \rightarrow \infty} \frac{|\mathcal{C} \cap B_r^d(0)|}{\text{vol}(B_r^d(0))} = \rho,$$

where $B_r^d(0)$ denotes the closed ball of radius r about 0 in \mathbb{R}^d . For such a set, we can renormalize the energy by considering the average energy per particle, as follows.

Definition 1.1. Let $p: (0, \infty) \rightarrow \mathbb{R}$ be any function. The *lower p -energy* of a point configuration \mathcal{C} in \mathbb{R}^d is

$$E_p(\mathcal{C}) := \liminf_{r \rightarrow \infty} \frac{1}{|\mathcal{C} \cap B_r^d(0)|} \sum_{\substack{x, y \in \mathcal{C} \cap B_r^d(0) \\ x \neq y}} p(|x - y|).$$

If the limit of the above quantity exists, and not just its limit inferior, then we call $E_p(\mathcal{C})$ the *p -energy* of \mathcal{C} (and say that its p -energy exists). We allow the possibility that the energy may be $\pm\infty$.

The simplest case is when the configuration is a *lattice* Λ , i.e., the \mathbb{Z} -span of a basis of \mathbb{R}^d . In that case, it has density

$$\frac{1}{\text{vol}(\mathbb{R}^d/\Lambda)}$$

and p -energy

$$\sum_{x \in \Lambda \setminus \{0\}} p(|x|),$$

assuming this sum is absolutely convergent. More generally, a *periodic configuration* is the union of finitely many orbits under the translation action of a lattice, i.e., the union of pairwise disjoint translates $\Lambda + v_j$ of a lattice Λ , with $1 \leq j \leq N$. Such a configuration has density

$$\frac{N}{\text{vol}(\mathbb{R}^d/\Lambda)}$$

and p -energy

$$(1.1) \quad \frac{1}{N} \sum_{j,k=1}^N \sum_{x \in \Lambda \setminus \{v_k - v_j\}} p(|x + v_j - v_k|),$$

again assuming absolute convergence. Many important configurations are periodic, but others are not, and we do not assume periodicity in our main theorems.

Typically we take the potential function p to be decreasing, and we envision the points of \mathcal{C} as particles subject to a repulsive force. Our framework is purely classical and does not incorporate quantum effects; thus, we should not think of the particles as atoms. However, classical models have other applications [4], such as describing mesoscale materials. Our goal is then to arrange these particles so as to minimize their p -energy, subject to maintaining a fixed density.¹ More precisely, we compare with the lower p -energies of other configurations:

Definition 1.2. Let \mathcal{C} be a point configuration in \mathbb{R}^d with density ρ , where $\rho > 0$, and let $p: (0, \infty) \rightarrow \mathbb{R}$ be any function. We say that \mathcal{C} *minimizes energy*

¹Fixing the density prevents the particles from minimizing energy by receding to infinity. If fixing the density seems unphysical, we could instead impose a chemical potential that penalizes decreasing the density of the configuration, to account for exchange with the external environment. That turns out to be equivalent, in the sense that one can achieve any desired density by choosing an appropriate chemical potential. Specifically, the chemical potential is a Lagrange multiplier that converts the density-constrained optimization problem to an unconstrained problem. This approach is called the *grand canonical ensemble*, and it is typically set up for finite systems before taking a thermodynamic limit. See, for example, Section 1.2.1(c) and Theorem 3.4.6 in [38].

for p if its p -energy $E_p(\mathcal{C})$ exists and every configuration in \mathbb{R}^d of density ρ has lower p -energy at least $E_p(\mathcal{C})$. We also call \mathcal{C} a *ground state* for p .

In certain contrived cases it is easy to determine the minimal energy. For example, if p vanishes at the square roots of positive integers and is nonnegative elsewhere, then \mathbb{Z}^d clearly minimizes p -energy. However, rigorously determining ground states seems hopelessly difficult in general, because of the complexity of analyzing long-range interactions. This issue arises in physics and materials science as the *crystallization problem* [2, 43]: how can we understand why particles so often arrange themselves periodically at low temperatures? Even the simplest mathematical models of crystallization are enormously subtle, and surprisingly little has been proved about them.

Two important classes of potential functions are inverse power laws $r \mapsto 1/r^s$ with $s > 0$ and Gaussians $r \mapsto e^{-\alpha r^2}$ with $\alpha > 0$. Inverse power laws are special because they are homogeneous, which implies that their ground states are scale-free: if \mathcal{C} is a ground state in \mathbb{R}^d with density 1, then $\rho^{-1/d}\mathcal{C}$ is a ground state with density ρ . Gaussians lack this property, and the shape of their ground states may depend on density (see, for example, [15]). In applications, Gaussian potential functions are typically used to approximate effective potential functions for more complex materials. For example, for a dilute solution of polymer chains in an athermal solvent, Gaussians describe the effective interaction between the centers of mass of the polymers (see Sections 3.4 and 3.5 of [30]). Point particles with Gaussian interactions are known as the *Gaussian core model* in physics [45].

Both inverse power laws and Gaussians arise naturally in number theory (see, for example, [33] and [40]). Given a lattice Λ in \mathbb{R}^d , its *Epstein zeta function* is defined by

$$\zeta_\Lambda(s) = \sum_{x \in \Lambda \setminus \{0\}} \frac{1}{|x|^{2s}}$$

for $\operatorname{Re}(s) > d/2$ (and by analytic continuation for all s except for a pole at $s = d/2$), and its *theta series* is defined by

$$\Theta_\Lambda(z) = \sum_{x \in \Lambda} e^{\pi iz|x|^2}$$

for $\operatorname{Im}(z) > 0$. Then the energy of Λ under $r \mapsto 1/r^s$ is $\zeta_\Lambda(s/2)$ when $s > d$, while its energy under $r \mapsto e^{-\alpha r^2}$ is $\Theta_\Lambda(i\alpha/\pi) - 1$. In other words, minimizing energy among lattices amounts to seeking extreme values for number-theoretic special functions. The restriction to lattices makes this problem much more tractable than the crystallization problem, but it remains difficult. The answer is known in certain special cases, such as sufficiently large s when $d \leq 8$ (see [39]), but the only cases in which the answer was previously known for all s and α were one or two dimensions [33].

Energy minimization also generalizes the sphere packing problem in \mathbb{R}^d , in which we wish to maximize the minimal distance between neighboring particles while fixing the particle density. (Centering non-overlapping spheres at the particles then yields a densest sphere packing.) One simple way to see why is to pick a constant r_0 and use the potential function

$$p(r) = \begin{cases} 0 & \text{if } r \geq r_0, \text{ and} \\ 1 & \text{if } 0 < r < r_0. \end{cases}$$

Then the p -energy of a periodic configuration vanishes if and only if the configuration has minimal distance at least r_0 . More generally, we can use a steep potential function such as $r \mapsto 1/r^s$ with s large (or, similarly, $r \mapsto e^{-\alpha r^2}$ with α large). As $s \rightarrow \infty$, the contribution to energy from short distances becomes increasingly important, and in the limit minimizing energy requires maximizing the minimal distance. In many cases, the ground state will be slightly distorted at any finite s , compared with the limit as $s \rightarrow \infty$. For example, that seems to happen in five or seven dimensions [15]. However, the E_6 root lattice in \mathbb{R}^6 appears to minimize energy for all sufficiently large s , provably among lattices [39] and perhaps among all configurations [15].

1.2. *Universal optimality.* In contrast to the sphere packing problem, even one-dimensional energy minimization is not easy to analyze. Cohn and Kumar [13] proved that the integer lattice \mathbb{Z} in \mathbb{R} minimizes energy for every completely monotonic function of squared distance, i.e., every function of the form $r \mapsto g(r^2)$, where g is completely monotonic. Recall that a function $g: (0, \infty) \rightarrow \mathbb{R}$ is *completely monotonic* if it is infinitely differentiable and satisfies the inequalities $(-1)^k g^{(k)} \geq 0$ for all $k \geq 0$. In other words, g is nonnegative, weakly decreasing, convex, and so on. For example, inverse power laws are completely monotonic, as are decreasing exponential functions. By Bernstein's theorem [44, Theorem 9.16], every completely monotonic function $g: (0, \infty) \rightarrow \mathbb{R}$ can be written as a convergent integral

$$g(r) = \int e^{-\alpha r} d\mu(\alpha)$$

for some measure μ on $[0, \infty)$. Equivalently, the completely monotonic functions of squared distance are the cone spanned by the Gaussians and the constant function 1. For example, inverse power laws can be obtained via

$$\frac{1}{r^s} = \int_0^\infty e^{-\alpha r^2} \frac{\alpha^{s/2-1}}{\Gamma(s/2)} d\alpha.$$

It follows that if a periodic configuration is a ground state for every Gaussian, then the same is true for every completely monotonic function of squared distance (by monotone convergence, because the potential is an increasing limit

of weighted sums of finitely many Gaussians). Following Cohn and Kumar, we call such a configuration universally optimal:

Definition 1.3. Let \mathcal{C} be a point configuration in \mathbb{R}^d with density ρ , where $\rho > 0$. We say \mathcal{C} is *universally optimal* if it minimizes p -energy whenever $p: (0, \infty) \rightarrow \mathbb{R}$ is a completely monotonic function of squared distance.

Note that the role of density in this definition is purely bookkeeping. If \mathcal{C} is a universal optimum in \mathbb{R}^d with density 1, then $\rho^{-1/d}\mathcal{C}$ is a universal optimum with density ρ for any $\rho > 0$, because the set of completely monotonic functions is invariant under rescaling the input variable. We can also reformulate universal optimality by fixing a Gaussian and varying the density: a periodic configuration \mathcal{C} in \mathbb{R}^d with density 1 is universally optimal if and only if for every $\rho > 0$, $\rho^{-1/d}\mathcal{C}$ is a ground state for $r \mapsto e^{-\pi r^2}$. This perspective on the Gaussian core model is common in the physics literature, such as [45], because varying the density of particles governed by a fixed interaction is a common occurrence in physics, while changing how they interact is more exotic.

It might seem more natural to use completely monotonic functions of distance, rather than squared distance, but squared distance turns out to be a better choice (for example, in allowing Gaussians). One can check that every completely monotonic function of distance is also a completely monotonic function of squared distance; equivalently, if $r \mapsto g(r^2)$ is completely monotonic, then so is g itself.² Thus, using squared distance strengthens the definition.

When a configuration is universally optimal, it has an extraordinary degree of robustness: it remains optimal for a broad range of potential functions, rather than depending on the specific potential. Numerical studies of energy minimization indicate that universal optima are rare [15], and this special property highlights their importance across different fields.

Before the present paper, no examples of universal optima in \mathbb{R}^d with $d > 1$ had been rigorously proved. In fact, for $d > 1$ no proof was known of a ground state for any inverse power law or similarly natural repulsive potential function. The most noteworthy theorem we are aware of along these lines is a proof by Theil [46] of crystallization for certain Lennard-Jones-type potentials in \mathbb{R}^2 . However, the potentials analyzed by Theil are attractive at long distances, and the proof makes essential use of this attraction.

Despite the lack of proof, the A_2 root lattice (i.e., the hexagonal lattice) is almost certainly universally optimal in \mathbb{R}^2 . It is known to be universally optimal

²That is, if p is completely monotonic on $(0, \infty)$, then so is $r \mapsto p(r^{1/2})$. More generally, if p and q' are both completely monotonic functions, then so is the composition $p \circ q$. The reason is that if one computes the k -th derivative $(p \circ q)^{(k)}$, for example using Faà di Bruno's formula, then each term has sign $(-1)^k$, as desired.

among lattices [33], and proving its universal optimality in full generality is an important open problem.

The case of three dimensions is surprisingly tricky even to describe. For the potential function $r \mapsto e^{-\pi r^2}$, the appropriately scaled face-centered cubic lattice is widely conjectured to be optimal among lattices of density ρ as long as $\rho \leq 1$, while the body-centered cubic lattice is conjectured to be optimal when $\rho \geq 1$. At density 1, they have the same energy by Poisson summation, because they are dual to each other. However, one can sometimes lower the energy by moving beyond lattices: Stillinger [45] applied Maxwell's double tangent construction to obtain a small neighborhood around density 1, namely $(0.99899854\dots, 1.00100312\dots)$, in which phase coexistence between these lattices improves upon both of them by a small amount. Specifically, at density 1 phase coexistence lowers the energy by approximately 0.0004%, in a way that seemingly cannot be achieved exactly by any periodic configuration. Thus, the behavior of the Gaussian core model in three dimensions is more complex than one might expect from the case of lattices. Even guessing the ground states on the basis of simulations is far from straightforward, and proofs seem to be well beyond present-day mathematics.

In contrast, we completely resolve the cases of eight and twenty-four dimensions, as conjectured in [13]:

THEOREM 1.4. *The E_8 root lattice and the Leech lattice are universally optimal in \mathbb{R}^8 and \mathbb{R}^{24} , respectively. Furthermore, they are unique among periodic configurations, in the following sense. Let \mathcal{C} be E_8 or the Leech lattice, and let \mathcal{C}' be any periodic configuration in the same dimension with the same density. If there exists a completely monotonic function of squared distance p such that $E_p(\mathcal{C}') = E_p(\mathcal{C}) < \infty$, then \mathcal{C}' is isometric to \mathcal{C} .*

Of course, the uniqueness assertion cannot hold among all configurations, because removing a single particle changes neither the density nor the energy. Uniqueness also trivially fails when p decays slowly enough that $E_p(\mathcal{C}) = \infty$, because universal optimality then implies that $E_p(\mathcal{C}') = \infty$ for every \mathcal{C}' . One could attempt to renormalize a divergent potential (analogously to the analytic continuation of the Epstein zeta function), but we will not address that possibility. See [24] and [40] for more information about renormalization.

Even for lattices, Theorem 1.4 has numerous consequences, including extreme values of the theta and Epstein zeta functions. For another application, consider a flat torus $T = \mathbb{R}^d/\Lambda$, where Λ is a lattice in \mathbb{R}^d . The *height* of T is a regularization of $-\log \det \Delta_T$, where Δ_T is the Laplacian on T (see [5] or [40]). If T has volume 1, then the height is a constant depending only on d plus

$$\lim_{s \rightarrow d/2} \left(\pi^{-d/2} \Gamma(d/2) \zeta_\Lambda(s) - \frac{1}{s - d/2} \right),$$

by Theorem 2.3 in [5]. Thus, if Λ is universally optimal, then T minimizes height among all flat d -dimensional tori of fixed volume. The minimal height was previously known only when $d = 1$ (trivial), $d = 2$ (due to Osgood, Phillips, and Sarnak [36]), and $d = 3$ (due to Sarnak and Strömbergsson [40]), to which we can now add $d = 8$ and $d = 24$, as conjectured in [40]:

COROLLARY 1.5. *Let d be 8 or 24, and let Λ_d be E_8 or the Leech lattice, accordingly. Among all lattices Λ in \mathbb{R}^d with determinant 1, the minimum value of $\zeta_\Lambda(s)$ for each $s \in (0, \infty) \setminus \{d/2\}$ is achieved when $\Lambda = \Lambda_d$, as is the minimum value of $\Theta_\Lambda(it)$ for each $t > 0$. Furthermore, \mathbb{R}^d/Λ_d has the smallest height among all d -dimensional flat tori of volume 1. For each of these optimization problems, Λ_d is the unique optimal lattice with determinant 1, up to isometry.*

Optimality and uniqueness for $\zeta_\Lambda(s)$ with $s > d/2$ and for $\Theta_\Lambda(it)$ follow from Theorem 1.4, as does optimality for the height. To deal with $s < d/2$ and to prove uniqueness (as well as optimality) for the height, we can use formula

$$\begin{aligned} \pi^{-s}\Gamma(s)\zeta_\Lambda(s) &= \int_1^\infty (\Theta_\Lambda(it) - 1)t^{s-1} dt - \frac{1}{s} \\ &\quad + \int_1^\infty (\Theta_{\Lambda^*}(it) - 1)t^{d/2-s-1} dt + \frac{1}{s-d/2} \end{aligned}$$

(see, for example, equation (42) in [40]) to reduce to the case of $\Theta(it)$, because $\Lambda_d^* = \Lambda_d$. Note also that Corollary 1.5 and the functional equation for the Epstein zeta function imply that $\zeta_\Lambda(s)$ is minimized at $\Lambda = \Lambda_d$ when $s < 0$ and $\lfloor s \rfloor$ is even, and maximized when $s < 0$ and $\lfloor s \rfloor$ is odd.

Although this corollary was not previously known, it is in principle more tractable than Theorem 1.4, because the lattice hypothesis reduces these assertions to optimization problems in a fixed, albeit large, number of variables.

1.3. Linear programming bounds. Our impetus for proving Theorem 1.4 was Viazovska's solution of the sphere packing problem in eight dimensions [47], as well as our extension to twenty-four dimensions [14]. These papers proved conjectures of Cohn and Elkies [11] about the existence of certain special functions, which imply sphere packing optimality via linear programming bounds. The underlying analytic techniques are by no means limited to sphere packing, and they intrinsically take into account long-range interactions. In particular, by combining the approach of Cohn and Elkies with techniques originated by Yudin [49], Cohn and Kumar [13] extended this framework of linear programming bounds to potential energy minimization in Euclidean space. To prove Theorem 1.4, we prove Conjecture 9.4 in [13] for eight and twenty-four dimensions. (The case of two dimensions remains open.) As a corollary of our construction, we also obtain the values at the origin of the

optimal auxiliary functions in these bounds, which agree with Conjecture 6.1 in [16].

Recall that linear programming bounds work as follows (see [8, 9] for further background). A *Schwartz function* $f: \mathbb{R}^d \rightarrow \mathbb{C}$ is an infinitely differentiable function such that for all $c > 0$, the function $f(x)$ and all its partial derivatives of all orders decay as $O(|x|^{-c})$ as $|x| \rightarrow \infty$. We normalize the Fourier transform by

$$\widehat{f}(y) = \int_{\mathbb{R}^d} f(x) e^{-2\pi i \langle x, y \rangle} dx,$$

where $\langle \cdot, \cdot \rangle$ denotes the standard inner product on \mathbb{R}^d . Then linear programming bounds for energy amount to the following proposition:

PROPOSITION 1.6. *Let $p: (0, \infty) \rightarrow [0, \infty)$ be any function, and suppose $f: \mathbb{R}^d \rightarrow \mathbb{R}$ is a Schwartz function. If $f(x) \leq p(|x|)$ for all $x \in \mathbb{R}^d \setminus \{0\}$ and $\widehat{f}(y) \geq 0$ for all $y \in \mathbb{R}^d$, then every subset of \mathbb{R}^d with density ρ has lower p -energy at least $\rho \widehat{f}(0) - f(0)$.*

In other words, we can certify a lower bound for p -energy by exhibiting an auxiliary function f satisfying specific inequalities. There is no reason to believe a sharp lower bound can necessarily be certified in this way. Indeed, in most cases the certifiable bounds seem to be strictly less than the true ground state energy, and the gap between them can be large when the potential function is steep. For example, for configurations of density 1 in \mathbb{R}^3 under the Gaussian potential function $r \mapsto e^{-\alpha r^2}$, the best linear programming bound known is roughly 3.59% less than the lowest energy known when $\alpha = \pi$, and 15.4% less when $\alpha = 2\pi$. Nevertheless, this technique suffices to prove Theorem 1.4.

Cohn and Kumar [13, Proposition 9.3] proved Proposition 1.6 for the special case of periodic configurations \mathcal{C} . Since the proof is short and motivates much of what we do in this paper, we include it here. The proof uses the Poisson summation formula

$$\sum_{x \in \Lambda} f(x + v) = \frac{1}{\text{vol}(\mathbb{R}^d / \Lambda)} \sum_{y \in \Lambda^*} \widehat{f}(y) e^{2\pi i \langle v, y \rangle},$$

which holds when $f: \mathbb{R}^d \rightarrow \mathbb{C}$ is a Schwartz function, $v \in \mathbb{R}^d$, Λ is a lattice in \mathbb{R}^d , and

$$\Lambda^* = \{y \in \mathbb{R}^d : \langle x, y \rangle \in \mathbb{Z} \text{ for all } x \in \Lambda\}$$

is its *dual lattice*.

Proof of Proposition 1.6 for periodic configurations. Because \mathcal{C} is periodic, we can write it as the disjoint union of $\Lambda + v_j$ for $1 \leq j \leq N$, where Λ is a lattice and $v_1, \dots, v_N \in \mathbb{R}^d$. Then the inequality between f and p and the

formula (1.1) for energy yield the lower bound

$$\begin{aligned} E_p(\mathcal{C}) &= \frac{1}{N} \sum_{j,k=1}^N \sum_{x \in \Lambda \setminus \{v_k - v_j\}} p(|x + v_j - v_k|) \\ &\geq \frac{1}{N} \sum_{j,k=1}^N \sum_{x \in \Lambda \setminus \{v_k - v_j\}} f(x + v_j - v_k) \\ &= \frac{1}{N} \sum_{j,k=1}^N \sum_{x \in \Lambda} f(x + v_j - v_k) - f(0). \end{aligned}$$

(We can apply (1.1) because $p \geq 0$: if the sum diverges, then $E_p(\mathcal{C}) = \infty$ anyway.) Applying Poisson summation to this lower bound and using the nonnegativity of \widehat{f} and the equation $N = \rho \operatorname{vol}(\mathbb{R}^d/\Lambda)$ then shows that

$$\begin{aligned} E_p(\mathcal{C}) &\geq \frac{N}{\operatorname{vol}(\mathbb{R}^d/\Lambda)} \sum_{y \in \Lambda^*} \widehat{f}(y) \left| \frac{1}{N} \sum_{j=1}^N e^{2\pi i \langle v_j, y \rangle} \right|^2 - f(0) \\ &\geq \rho \widehat{f}(0) - f(0), \end{aligned}$$

as desired. \square

This proof works only for periodic configurations, but Proposition 1.6 makes no such assumption. The general case was proved by Cohn and de Courcy-Ireland in [10, Proposition 2.2].

Proposition 1.6 shows how to obtain a lower bound for p -energy from an auxiliary function f satisfying certain inequalities, but it says nothing about how to construct f . Optimizing the choice of f to maximize the resulting bound is an unsolved problem in general. Without loss of generality, we can assume that f is a radial function (i.e., $f(x)$ depends only on $|x|$), because all the constraints are invariant under rotation and we can therefore radially symmetrize f by averaging all its rotations. We are faced with an optimization problem over functions of just one radial variable, but this problem too seems to be intractable in general.

Fortunately, one can characterize when the bound is sharp for a periodic configuration. For simplicity, consider a lattice Λ . Examining the loss in the inequalities in the proof given above shows that f proves a sharp bound for $E_p(\Lambda)$ if and only if both

$$(1.2) \quad \begin{aligned} f(x) &= p(|x|) && \text{for all } x \in \Lambda \setminus \{0\}, \text{ and} \\ \widehat{f}(y) &= 0 && \text{for all } y \in \Lambda^* \setminus \{0\}. \end{aligned}$$

Furthermore, equality must hold to second order, because $f(x) \leq p(|x|)$ and $\widehat{f}(y) \geq 0$ for all x and y . Equivalently, if f is radial, then the radial derivatives

of f and \widehat{f} satisfy

$$(1.3) \quad \begin{aligned} f'(x) &= p'(|x|) && \text{for all } x \in \Lambda \setminus \{0\}, \text{ and} \\ \widehat{f}'(y) &= 0 && \text{for all } y \in \Lambda^* \setminus \{0\}. \end{aligned}$$

We will see that these conditions suffice to determine f .

1.4. *Interpolation.* For the analogous problem of energy minimization in compact spaces studied in [13], conditions (1.2) and (1.3) make it simple to construct the optimal auxiliary functions for most of the universal optima that are known. The point configurations are finite sets, and thus we have only finitely many equality constraints for f to achieve a sharp bound. To construct f , one can simply take the lowest-degree polynomial that satisfies these constraints. It is far from obvious that this construction works, i.e., that f satisfies the needed inequalities elsewhere, but at least describing this choice of f is straightforward. The description amounts to polynomial interpolation (more precisely, Hermite interpolation, since one must interpolate both values and derivatives).

In Euclidean space, describing the optimal auxiliary functions is far more subtle. It again amounts to an interpolation problem, this time for radial Schwartz functions. The interpolation points are known explicitly for \mathbb{R}^8 and \mathbb{R}^{24} : the nonzero vectors in E_8 have lengths $\sqrt{2n}$ for integers $n \geq 1$, and those in the Leech lattice have lengths $\sqrt{2n}$ for $n \geq 2$. What is required is to control the values and radial derivatives of f and \widehat{f} at these infinitely many points. However, simultaneously controlling f and \widehat{f} is not easy, and we quickly run up against uncertainty principles [12]. The feasibility of interpolation depends on the exact points at which we are interpolating, and we do not know how to resolve these questions in general.

The fundamental mystery is how polynomial interpolation generalizes to infinite-dimensional function spaces. One important case that has been thoroughly analyzed is Shannon sampling, which amounts to interpolating the values of a band-limited function (i.e., an entire function of exponential type) at linearly spaced points; see [25] for an account of this theory. Shannon sampling suffices to prove that \mathbb{Z} is universally optimal [13, p. 142], but it cannot handle any higher-dimensional cases.

To construct the optimal auxiliary functions in \mathbb{R}^8 and \mathbb{R}^{24} , we prove a new interpolation theorem for radial Schwartz functions. Let $\mathcal{S}_{\text{rad}}(\mathbb{R}^d)$ denote the set of radial Schwartz functions from \mathbb{R}^d to \mathbb{C} . For $f \in \mathcal{S}_{\text{rad}}(\mathbb{R}^d)$, we abuse notation by applying f directly to radial distances (i.e., if $r \in [0, \infty)$, then $f(r)$ denotes the common value of $f(x)$ when $|x| = r$), and we let f' denote the radial derivative. As above, \widehat{f} denotes the d -dimensional Fourier transform of f , which is again a radial function, and \widehat{f}' denotes the radial derivative of \widehat{f} .

THEOREM 1.7. *Let (d, n_0) be $(8, 1)$ or $(24, 2)$. Then every $f \in \mathcal{S}_{\text{rad}}(\mathbb{R}^d)$ is uniquely determined by the values $f(\sqrt{2n})$, $f'(\sqrt{2n})$, $\hat{f}(\sqrt{2n})$, and $\hat{f}'(\sqrt{2n})$ for integers $n \geq n_0$. Specifically, there exists an interpolation basis $a_n, b_n, \tilde{a}_n, \tilde{b}_n \in \mathcal{S}_{\text{rad}}(\mathbb{R}^d)$ for $n \geq n_0$ such that for every $f \in \mathcal{S}_{\text{rad}}(\mathbb{R}^d)$ and $x \in \mathbb{R}^d$,*

$$(1.4) \quad \begin{aligned} f(x) = & \sum_{n=n_0}^{\infty} f(\sqrt{2n}) a_n(x) + \sum_{n=n_0}^{\infty} f'(\sqrt{2n}) b_n(x) \\ & + \sum_{n=n_0}^{\infty} \hat{f}(\sqrt{2n}) \tilde{a}_n(x) + \sum_{n=n_0}^{\infty} \hat{f}'(\sqrt{2n}) \tilde{b}_n(x), \end{aligned}$$

where these series converge absolutely.

One could likely weaken the decay and smoothness conditions on f , along the lines of Proposition 4 in [37], but determining the best possible conditions seems difficult.

Theorem 1.7 tells us that in \mathbb{R}^8 or \mathbb{R}^{24} , the optimal auxiliary function f for a potential function p is uniquely determined by the necessary conditions (1.2) and (1.3), assuming it is a Schwartz function. Specifically, f satisfies the conditions

$$\begin{aligned} f(\sqrt{2n}) &= p(\sqrt{2n}), & f'(\sqrt{2n}) &= p'(\sqrt{2n}), \\ \hat{f}(\sqrt{2n}) &= 0, & \hat{f}'(\sqrt{2n}) &= 0 \end{aligned}$$

for $n \geq n_0$, and (1.4) then gives a formula for f in terms of the interpolation basis, which we will explicitly construct as part of the proof of Theorem 1.7. The same is also true for the auxiliary functions for sphere packing constructed in [47] and [14]:

COROLLARY 1.8. *In \mathbb{R}^8 and \mathbb{R}^{24} , the optimal auxiliary functions for the linear programming bounds for sphere packing or Gaussian potential energy minimization are unique among radial Schwartz functions.*

Theorem 1.7 was conjectured by Viazovska as part of the strategy for her solution of the sphere packing problem in \mathbb{R}^8 . Note that the interpolation formula is not at all obvious, or even particularly plausible. The lack of plausibility accounts for why it had not previously been conjectured, despite the analogy with energy minimization in compact spaces.

The proof of the interpolation formula develops the techniques introduced by Viazovska in [47] into a broader theory. Radchenko and Viazovska took a significant step in this direction by proving an interpolation formula for single roots in one dimension [37], but extending it to double roots introduces further difficulties.

Theorem 1.7 extends naturally to characterize exactly which sequences can occur as $f(\sqrt{2n})$, $f'(\sqrt{2n})$, $\hat{f}(\sqrt{2n})$, and $\hat{f}'(\sqrt{2n})$ for $n \geq n_0$, with f a radial

Schwartz function. The only restriction on these sequences is on their decay rate. To state the result precisely, let $\mathcal{S}(\mathbb{N})$ be the space of rapidly decreasing sequences of complex numbers. In other words, $(x_n)_{n \geq 1} \in \mathcal{S}(\mathbb{N})$ if and only if $\lim_{n \rightarrow \infty} n^k x_n = 0$ for all k .

THEOREM 1.9. *Let (d, n_0) be $(8, 1)$ or $(24, 2)$. Then the map sending $f \in \mathcal{S}_{\text{rad}}(\mathbb{R}^d)$ to*

$$\left((f(\sqrt{2n}))_{n \geq n_0}, (f'(\sqrt{2n}))_{n \geq n_0}, (\hat{f}(\sqrt{2n}))_{n \geq n_0}, (\hat{f}'(\sqrt{2n}))_{n \geq n_0} \right)$$

is an isomorphism from $\mathcal{S}_{\text{rad}}(\mathbb{R}^d)$ to $\mathcal{S}(\mathbb{N})^4$, whose inverse is given by (1.4); i.e., the inverse isomorphism maps

$$\left((\alpha_n)_{n \geq n_0}, (\beta_n)_{n \geq n_0}, (\tilde{\alpha}_n)_{n \geq n_0}, (\tilde{\beta}_n)_{n \geq n_0} \right)$$

to the function

$$\sum_{n=n_0}^{\infty} \alpha_n a_n + \sum_{n=n_0}^{\infty} \beta_n b_n + \sum_{n=n_0}^{\infty} \tilde{\alpha}_n \tilde{a}_n + \sum_{n=n_0}^{\infty} \tilde{\beta}_n \tilde{b}_n.$$

One consequence of this theorem is that there are no linear relations between the values $f(\sqrt{2n})$, $f'(\sqrt{2n})$, $\hat{f}(\sqrt{2n})$, and $\hat{f}'(\sqrt{2n})$ for $n \geq n_0$. By contrast, Poisson summation over E_8 or the Leech lattice gives such a relation between $f(\sqrt{2n})$ and $\hat{f}(\sqrt{2n})$ for $n \geq 0$.

Another consequence is that the values and derivatives of the interpolation basis functions and their Fourier transforms at the interpolation points are all 0 except for a single 1, which cycles through all these possibilities. In terms of the Kronecker delta,

$$\begin{aligned} a_n(\sqrt{2m}) &= \delta_{m,n}, & a'_n(\sqrt{2m}) &= 0, & \hat{a}_n(\sqrt{2m}) &= 0, & \hat{a}'_n(\sqrt{2m}) &= 0, \\ b_n(\sqrt{2m}) &= 0, & b'_n(\sqrt{2m}) &= \delta_{m,n}, & \hat{b}_n(\sqrt{2m}) &= 0, & \hat{b}'_n(\sqrt{2m}) &= 0, \\ \tilde{a}_n(\sqrt{2m}) &= 0, & \tilde{a}'_n(\sqrt{2m}) &= 0, & \hat{\tilde{a}}_n(\sqrt{2m}) &= \delta_{m,n}, & \hat{\tilde{a}}'_n(\sqrt{2m}) &= 0, \\ \tilde{b}_n(\sqrt{2m}) &= 0, & \tilde{b}'_n(\sqrt{2m}) &= 0, & \hat{\tilde{b}}_n(\sqrt{2m}) &= 0, & \hat{\tilde{b}}'_n(\sqrt{2m}) &= \delta_{m,n} \end{aligned}$$

for integers $m, n \geq n_0$. Such a basis is uniquely determined, by the interpolation theorem itself. Furthermore, it follows that $\tilde{a}_n = \hat{a}_n$ and $\tilde{b}_n = \hat{b}_n$.

The function b_1 is characterized by $b_1(\sqrt{2n}) = 0$, $\hat{b}_1(\sqrt{2n}) = 0$, and $\hat{b}'_1(\sqrt{2n}) = 0$ for $n \geq n_0$, while $b'_1(\sqrt{2n}) = 0$ for $n > n_0$ and $b'_1(\sqrt{2n_0}) = 1$. Up to a constant factor, these are the same conditions satisfied by the sphere packing auxiliary functions constructed in [47] for $d = 8$ and [14] for $d = 24$. Thus, the constructions in those papers are subsumed as a special case of the interpolation basis.

The interpolation theorem amounts to constructing certain radial analogues of Fourier quasicrystals. Define a *radial Fourier quasicrystal* to be a radial

tempered distribution T on \mathbb{R}^d such that both T and \widehat{T} are supported on discrete sets of radii. To reformulate the interpolation theorem in these terms, let δ_r denote a spherical delta function with mass 1 on the sphere of radius r about the origin, or equivalently let

$$\int_{\mathbb{R}^d} f \delta_r = f(r)$$

for $f \in \mathcal{S}_{\text{rad}}(\mathbb{R}^d)$, and define δ'_r by

$$\int_{\mathbb{R}^d} f \delta'_r = -f'(r)$$

for $f \in \mathcal{S}_{\text{rad}}(\mathbb{R}^d)$. (Note that when $d > 1$, this is not the radial derivative of δ_r , as obtained via integration by parts. Using the radial derivative would clutter the notation.) If we set

$$T_x = \sum_{n=n_0}^{\infty} a_n(x) \delta_{\sqrt{2n}} - \sum_{n=n_0}^{\infty} b_n(x) \delta'_{\sqrt{2n}} - \delta_{|x|},$$

then

$$\widehat{T}_x = - \sum_{n=n_0}^{\infty} \tilde{a}_n(x) \delta_{\sqrt{2n}} + \sum_{n=n_0}^{\infty} \tilde{b}_n(x) \delta'_{\sqrt{2n}}$$

by Theorem 1.7. Thus, T_x is a radial Fourier quasicrystal.

Dyson [19] highlighted the importance of classifying Fourier quasicrystals in \mathbb{R}^1 , and radial Fourier quasicrystals are a natural generalization of this problem. In the non-radial case, Fourier quasicrystals satisfying certain positivity and uniformity hypotheses can be completely described using Poisson summation [29], but even a conjectural classification remains elusive in general.

1.5. *Proof techniques.* In light of Theorem 1.7 and its interpolation basis, we can write down the only possible auxiliary function f that could prove a sharp bound for E_8 or the Leech lattice under a potential p (with $d = 8$ or 24 , accordingly), at least among radial Schwartz functions:

$$(1.5) \quad f(x) = \sum_{n=n_0}^{\infty} p(\sqrt{2n}) a_n(x) + \sum_{n=n_0}^{\infty} p'(\sqrt{2n}) b_n(x).$$

The proof of Theorem 1.4 then amounts to checking that $f(x) \leq p(|x|)$ for all $x \in \mathbb{R}^d \setminus \{0\}$ and $\widehat{f}(y) \geq 0$ for all $y \in \mathbb{R}^d$. (Once we prove these inequalities, the necessary conditions for a sharp bound become sufficient as well.) As noted above, it suffices to prove the theorem when p is a Gaussian, i.e., $p(r) = e^{-\alpha r^2}$ for some constant $\alpha > 0$.

Thus, our primary technical contribution is to construct the interpolation basis. To do so, we analyze the generating functions

$$(1.6) \quad F(\tau, x) = \sum_{n \geq n_0} a_n(x) e^{2\pi i n \tau} + 2\pi i \tau \sum_{n \geq n_0} \sqrt{2n} b_n(x) e^{2\pi i n \tau}$$

and

$$(1.7) \quad \widetilde{F}(\tau, x) = \sum_{n \geq n_0} \widetilde{a}_n(x) e^{2\pi i n \tau} + 2\pi i \tau \sum_{n \geq n_0} \sqrt{2n} \widetilde{b}_n(x) e^{2\pi i n \tau},$$

where $x \in \mathbb{R}^d$ and τ is in the upper half-plane $\mathbb{H} = \{z \in \mathbb{C} : \text{Im}(z) > 0\}$. These generating functions determine the basis, and in Section 5.4 we prove integral formulas for the basis functions, which generalize the formulas for b_1 from the sphere packing papers [47, 14].

One motivation for the seemingly extraneous factors of $2\pi i \tau \sqrt{2n}$ in these generating functions is that they match (1.5) with $\tau = i\alpha/\pi$ and $p(r) = e^{-\alpha r^2} = e^{\pi i \tau r^2}$, because

$$p(\sqrt{2n}) = e^{2\pi i n \tau} \quad \text{and} \quad p'(\sqrt{2n}) = 2\pi i \tau \sqrt{2n} e^{2\pi i n \tau}.$$

In other words, the auxiliary function f from (1.5) for this Gaussian potential function is given by $f(x) = F(\tau, x)$.

We can write the interpolation formula for a complex Gaussian $x \mapsto e^{\pi i \tau |x|^2}$ in terms of F and \widetilde{F} . Specifically, the Fourier transform of $x \mapsto e^{\pi i \tau |x|^2}$ as a function on \mathbb{R}^d is $x \mapsto (i/\tau)^{d/2} e^{\pi i (-1/\tau)|x|^2}$, and hence the interpolation formula (1.4) for $x \mapsto e^{\pi i \tau |x|^2}$ amounts to the identity

$$(1.8) \quad F(\tau, x) + (i/\tau)^{d/2} \widetilde{F}(-1/\tau, x) = e^{\pi i \tau |x|^2}.$$

In Section 3.1, we will show using a density argument in $\mathcal{S}_{\text{rad}}(\mathbb{R}^d)$ that it suffices to prove the interpolation theorem for complex Gaussians of the form $x \mapsto e^{\pi i \tau |x|^2}$ with $\tau \in \mathbb{H}$. Thus, constructing the interpolation basis amounts to solving the functional equation (1.8) using functions F and \widetilde{F} with expansions of the form (1.6) and (1.7).

These expansions for F and \widetilde{F} are not quite Fourier expansions in τ , because they contain terms proportional to $\tau e^{2\pi i \tau n}$. In particular, they are not periodic in τ , but they are annihilated by the second-order difference operator:

$$(1.9) \quad F(\tau + 2, x) - 2F(\tau + 1, x) + F(\tau, x) = 0$$

and

$$(1.10) \quad \widetilde{F}(\tau + 2, x) - 2\widetilde{F}(\tau + 1, x) + \widetilde{F}(\tau, x) = 0.$$

Subject to suitable smoothness and growth conditions, proving the interpolation theorem amounts to constructing functions F and \widetilde{F} satisfying the functional equations (1.8), (1.9), and (1.10), as we will show in Theorem 3.1.

To solve these functional equations, we use Laplace transforms of quasimodular forms. This approach was introduced by Viazovska in her solution of the sphere packing problem in eight dimensions [47], and we make heavy use of her techniques. In [47], only modular forms of level at most 2 and the quasimodular form E_2 were needed. However, these functions turn out to be insufficient to construct our interpolation basis, and we must augment them with a logarithm of the Hauptmodul λ for $\Gamma(2)$. Using this enlarged set of functions, we can describe F and \tilde{F} explicitly. The proof of the interpolation theorem then amounts to verifying analyticity, growth bounds, and functional equations for our formulas.

Once we have obtained these formulas, only one step remains in the proof of Theorem 1.4. Let p be a Gaussian potential function, and define the auxiliary function f by (1.5). To complete the proof of Theorem 1.4, we must show that $f(x) \leq p(|x|)$ for all $x \in \mathbb{R}^d \setminus \{0\}$ and $\hat{f}(y) \geq 0$ for all $y \in \mathbb{R}^d$. These inequalities look rather different, but we will see that they are actually equivalent to each other, thanks to a duality transformation introduced in Section 6 of [16]. The underlying inequality follows from the positivity of the kernel in the Laplace transform, as well as a truncated version of the kernel when $d = 24$. Unfortunately we have no conceptual proof of this positivity, but we are able to prove it by combining various analytic methods, including interval arithmetic computations. This inequality then completes the proof of universal optimality.

1.6. *Organization of the paper.* We begin by collecting background information about modular forms, elliptic integrals, and radial Schwartz functions in Section 2. Sections 3 and 4 are the heart of the paper. Section 3 shows how to reduce the interpolation theorem to the existence of generating functions with certain properties, and Section 4 describes the generating functions explicitly as integral transforms of kernels obtained by carefully analyzing an action of $\mathrm{PSL}_2(\mathbb{Z})$. It is not obvious that this construction has all the necessary properties, and Section 5 completes the proof of the interpolation theorem by verifying analytic continuation and growth bounds. Proving universal optimality requires additional inequalities, which are established in Section 6. Finally, we discuss generalizations and open problems in Section 7.

2. Preliminaries and background on modular forms

Much of the machinery of our proof rests on properties of classical modular forms, in particular their growth rates and transformation laws. This section summarizes those features which are used later in the paper, as well as background about elliptic integrals and radial Schwartz functions. For more information about modular forms, see [7, 26, 42, 50].

2.1. *Modular and quasimodular forms.* Let \mathbb{H} denote the complex upper half-plane $\{z \in \mathbb{C} : \text{Im}(z) > 0\}$. The group $\text{SL}_2(\mathbb{R})$ acts on \mathbb{H} by fractional linear transformations

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \cdot z = \frac{az + b}{cz + d}.$$

For any integer k and $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \text{SL}_2(\mathbb{R})$, define the slash operator on functions $f: \mathbb{H} \rightarrow \mathbb{C}$ by the rule³

$$(2.1) \quad (f|_k\gamma)(z) = (cz + d)^{-k} f\left(\frac{az + b}{cz + d}\right).$$

We define the *factor of automorphy* $j(\gamma, z)$ by

$$(2.2) \quad j(\gamma, z) = cz + d;$$

note that it satisfies the identity $j(\gamma_1\gamma_2, z) = j(\gamma_1, \gamma_2 z)j(\gamma_2, z)$, which implies that $f|_k(\gamma_1\gamma_2) = (f|_k\gamma_1)|_k\gamma_2$.

Let Γ be a discrete subgroup of $\text{SL}_2(\mathbb{R})$ such that the quotient $\Gamma \backslash \mathbb{H}$ has finite volume. Recall that a holomorphic *modular form* of weight k for Γ is a holomorphic function $f: \mathbb{H} \rightarrow \mathbb{C}$ such that $f|_k\gamma = f$ for all $\gamma \in \Gamma$, and that furthermore satisfies a polynomial boundedness condition at each cusp (see [7, 26, 42] for details). The space of holomorphic modular forms of weight k for Γ will be denoted $\mathcal{M}_k(\Gamma)$. It contains the subspace $\mathcal{S}_k(\Gamma)$ of weight k *cuspidal forms* for Γ ; these are the modular forms that vanish at all the cusps of $\Gamma \backslash \mathbb{H}$. On the other hand, we may relax the definition to allow modular functions that are holomorphic on \mathbb{H} but merely meromorphic at the cusps (equivalently, they satisfy an exponential growth bound near the cusps). This defines the infinite-dimensional space $\mathcal{M}_k^!(\Gamma)$ of *weakly holomorphic* modular forms.

When Γ is a congruence subgroup of $\text{SL}_2(\mathbb{Z})$, i.e., one that contains

$$\Gamma(N) = \left\{ \gamma \in \text{SL}_2(\mathbb{Z}) : \gamma \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \pmod{N} \right\}$$

for some N , the boundedness condition defining $\mathcal{M}_k(\Gamma)$ is simply that $|(f|_k\gamma)(z)|$ is bounded as $\text{Im}(z) \rightarrow \infty$, for every $\gamma \in \text{SL}_2(\mathbb{Z})$. Similarly, $\mathcal{S}_k(\Gamma)$ is defined by the condition that $(f|_k\gamma)(z) \rightarrow 0$ as $\text{Im}(z) \rightarrow \infty$, while $\mathcal{M}_k^!(\Gamma)$ is defined by the condition that $|(f|_k\gamma)(z)|$ is bounded above by a polynomial in $e^{\text{Im}(z)}$. Since $\text{SL}_2(\mathbb{Z})$ is generated by

$$(2.3) \quad T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad S = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

³When necessary, we will use a superscript on the slash notation to disambiguate which variable it applies to. For example, $f(\tau, z) \Big|_2 \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = z^{-2}f(\tau, -1/z)$.

we will often indicate the action of $\mathrm{SL}_2(\mathbb{Z})$ on a modular form for a congruence subgroup by giving the action of the slash operators corresponding to S and T .

The element $-I \in \mathrm{SL}_2(\mathbb{R})$ acts trivially on \mathbb{H} , and thus the action of $\mathrm{SL}_2(\mathbb{R})$ descends to an action of $\mathrm{PSL}_2(\mathbb{R}) = \mathrm{SL}_2(\mathbb{R})/\{\pm I\}$. We write $\bar{\Gamma}$ to denote the image of a subgroup Γ of $\mathrm{SL}_2(\mathbb{R})$ in $\mathrm{PSL}_2(\mathbb{R})$. The group $\mathrm{PSL}_2(\mathbb{Z}) = \overline{\mathrm{SL}_2(\mathbb{Z})}$ has an elegant presentation in terms of the generators S and T , namely $\mathrm{PSL}_2(\mathbb{Z}) = \langle S, T \mid S^2 = (ST)^3 = I \rangle$.

We next describe the structure of the graded rings

$$\mathcal{M}^1(\Gamma) = \bigoplus_{k \in \mathbb{Z}} \mathcal{M}_k^1(\Gamma)$$

and

$$\mathcal{M}(\Gamma) = \bigoplus_{k \in \mathbb{Z}} \mathcal{M}_k(\Gamma)$$

for the cases of interest in this paper, which are the congruence subgroups $\Gamma = \Gamma(N)$ for $N = 1, 2$. In these cases, the weight k for any nonzero modular form is necessarily even because $-I \in \Gamma$.

2.1.1. *Modular forms for $\Gamma(1) = \mathrm{SL}_2(\mathbb{Z})$.* Here all modular forms can be described in terms of the Eisenstein series

$$\begin{aligned} E_k(z) &= \frac{1}{2\zeta(k)} \sum_{\substack{(m,n) \in \mathbb{Z}^2 \\ (m,n) \neq (0,0)}} (mz + n)^{-k} \\ &= 1 - \frac{2k}{B_k} \sum_{n=1}^{\infty} \sigma_{k-1}(n) e^{2\pi i n z} \end{aligned}$$

for even integers $k \geq 4$, where B_k is the k -th Bernoulli number and $\sigma_\ell(n) = \sum_{d|n} d^\ell$ is the ℓ -th power divisor sum function. The ring $\mathcal{M}(\mathrm{SL}_2(\mathbb{Z}))$ is the free polynomial ring with generators

$$\begin{aligned} E_4(z) &= 1 + 240 \sum_{n=1}^{\infty} \sigma_3(n) q^n \quad \text{and} \\ E_6(z) &= 1 - 504 \sum_{n=1}^{\infty} \sigma_5(n) q^n, \end{aligned}$$

where we use the customary shorthand $q = e^{2\pi i z}$. In particular,

$$(2.4) \quad \dim \mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z})) = \left\lfloor \frac{k}{12} \right\rfloor + \begin{cases} 1 & \text{for } k \equiv 0, 4, 6, 8, 10 \pmod{12}, \text{ and} \\ 0 & \text{for } k \equiv 2 \pmod{12} \end{cases}$$

for even integers $k \geq 0$, and the identities $E_8 = E_4^2$, $E_{10} = E_4E_6$ and $E_{14} = E_4^2E_6$ hold because the modular forms of weight 8, 10, or 14 form a one-dimensional space. Let

$$\Delta(z) = \frac{E_4(z)^3 - E_6(z)^2}{1728} = q \prod_{n=1}^{\infty} (1 - q^n)^{24}$$

denote Ramanujan's cusp form of weight 12. The product formula shows that Δ does not vanish on \mathbb{H} and satisfies the decay estimate

$$\Delta(x + iy) = O(e^{-2\pi y})$$

for $y \geq 1$, uniformly in $x \in \mathbb{R}$. In particular, Δ^{-1} is a weakly holomorphic modular form for $\mathrm{SL}_2(\mathbb{Z})$. Furthermore, since Δ vanishes to first order at the unique cusp of $\mathrm{SL}_2(\mathbb{Z})$, we can use it to cancel the pole of any form $f \in \mathcal{M}^!(\mathrm{SL}_2(\mathbb{Z}))$: if f has weight k and a pole of order r at the cusp, then $\Delta^r f \in \mathcal{M}_{k+12r}(\mathrm{SL}_2(\mathbb{Z}))$. It follows that

$$\mathcal{M}^!(\mathrm{SL}_2(\mathbb{Z})) = \mathbb{C}[E_4, E_6, \Delta^{-1}].$$

For example, the modular j -invariant defined by

$$(2.5) \quad j(z) = \frac{E_4(z)^3}{\Delta(z)} = q^{-1} + 744 + 196884q + 21493760q^2 + \dots$$

is in $\mathcal{M}_0^!(\mathrm{SL}_2(\mathbb{Z}))$, and its derivative, which is in $\mathcal{M}_2^!(\mathrm{SL}_2(\mathbb{Z}))$, can be expressed as

$$(2.6) \quad j'(z) = 2\pi i q \frac{dj}{dq} = -2\pi i \frac{E_{14}(z)}{\Delta(z)},$$

since both side share the same leading asymptotics as $\mathrm{Im}(z) \rightarrow \infty$ and $j'\Delta$ lies in the one-dimensional space $\mathcal{M}_{14}(\mathrm{SL}_2(\mathbb{Z}))$.

An important role in this paper (as well as in [47, 14]) is played by the *quasimodular* form

$$(2.7) \quad E_2(z) = 1 - 24 \sum_{n=1}^{\infty} \sigma_1(n) q^n = \frac{1}{2\pi i} \frac{\Delta'(z)}{\Delta(z)},$$

which just barely fails to be modular:

$$(2.8) \quad E_2(z+1) = E_2(z) \quad \text{and} \quad E_2\left(\frac{-1}{z}\right) = z^2 E_2(z) - \frac{6iz}{\pi}.$$

General quasimodular forms for congruence subgroups are polynomials in E_2 with modular form coefficients; they may be also be obtained by differentiating modular forms. More precisely, a holomorphic function $f: \mathbb{H} \rightarrow \mathbb{C}$ is a quasimodular form for $\Gamma(N)$ of weight k and depth at most p if it is an element of $\bigoplus_{j=0}^p E_2^j \mathcal{M}_{k-2j}(\Gamma(N))$. In other words, depth p corresponds to a degree d polynomial in E_2 or to taking the p -th derivative of a modular form (see [6],

[27], and [50, Prop. 20]).⁴ The behavior at ∞ of a quasimodular form, expressed as a polynomial in E_2 , can be read off directly from that of its modular form coefficients.

2.1.2. *Modular forms for $\Gamma(2)$.* Recall the *Jacobi theta functions*

$$\begin{aligned}\Theta_3(z) &= \theta_{00}(z) = \sum_{n \in \mathbb{Z}} e^{\pi i n^2 z}, \\ \Theta_4(z) &= \theta_{01}(z) = \sum_{n \in \mathbb{Z}} (-1)^n e^{\pi i n^2 z}, \quad \text{and} \\ \Theta_2(z) &= \theta_{10}(z) = \sum_{n \in \mathbb{Z}} e^{\pi i (n + \frac{1}{2})^2 z}\end{aligned}$$

(with their historical numbering), which arise in the classical theory of theta functions. We define

$$(2.9) \quad \begin{aligned}U(z) &= \theta_{00}(z)^4, \\ V(z) &= \theta_{10}(z)^4, \quad \text{and} \\ W(z) &= \theta_{01}(z)^4.\end{aligned}$$

These functions are modular forms of weight 2 for $\Gamma(2)$, they satisfy the *Jacobi identity*

$$(2.10) \quad U = V + W,$$

and $\mathcal{M}(\Gamma(2))$ is the polynomial ring generated by V and W . As was the case for $\Gamma = \Gamma(1)$, multiplication by powers of Δ removes singularities at cusps while increasing the weight. Thus any element of $\mathcal{M}^1(\Gamma(2))$ is again the quotient of an element of $\mathcal{M}(\Gamma(2))$ by some power of Δ , with the behavior at cusps determined by the numerator and the power of Δ . (In fact, $\mathcal{M}^1(\Gamma) = \mathcal{M}(\Gamma)[\Delta^{-1}]$ for any congruence subgroup Γ , because Δ is in $\mathcal{M}(\Gamma)$ and vanishes at all cusps.)

The modular forms U , V , and W transform under $\mathrm{SL}_2(\mathbb{Z})$ as follows:

$$(2.11) \quad \begin{aligned}U|_2T &= W, & V|_2T &= -V, & W|_2T &= U, \\ U|_2S &= -U, & V|_2S &= -W, & W|_2S &= -V.\end{aligned}$$

These formulas specify how modular forms for $\Gamma(2)$ transform under the larger group $\mathrm{SL}_2(\mathbb{Z})$. Conversely, every modular form for $\mathrm{SL}_2(\mathbb{Z})$ is a modular form

⁴For a more intrinsic definition of quasimodular form which applies to non-congruence subgroups of $\mathrm{SL}_2(\mathbb{R})$ as well, see [50, Section 5.3].

for $\Gamma(2)$ and thus can be written in terms of U , V , and W . For example,

$$(2.12) \quad \begin{aligned} E_4 &= \frac{1}{2}(U^2 + V^2 + W^2), \\ E_6 &= \frac{1}{2}(U + V)(U + W)(W - V), \quad \text{and} \\ \Delta &= \frac{1}{256}(UVW)^2. \end{aligned}$$

It will also be convenient to use the holomorphic square root of Δ defined by

$$\sqrt{\Delta} = \frac{1}{16}UVW,$$

which is a modular form of weight 6 for $\Gamma(2)$.

Eichler and Zagier [22, Remark after Theorem 8.4] showed as part of a general result that the algebra $\mathcal{M}(\Gamma(2))$ is a six-dimensional free module over $\mathcal{M}_1 := \mathcal{M}(\Gamma(1))$. Their proof shows that

$$(2.13) \quad \mathcal{M}(\Gamma(2)) = \mathcal{M}_1 \oplus U\mathcal{M}_1 \oplus V\mathcal{M}_1 \oplus U^2\mathcal{M}_1 \oplus V^2\mathcal{M}_1 \oplus UVW\mathcal{M}_1,$$

with the only subtlety being to show that the modular form UVW of weight six does not lie in the direct sum of the first five factors. For comparison, UV lies in $\mathcal{M}_1 \oplus U^2\mathcal{M}_1 \oplus V^2\mathcal{M}_1$, because $UV = U^2 + V^2 - E_4$ by (2.10) and (2.12). As \mathcal{M}_1 is itself the free polynomial ring in $U^2 + V^2 + W^2$ and $(U + V)(U + W)(W - V)$, the decomposition (2.13) can also be deduced from the theory of symmetric polynomials.

2.1.3. The modular function λ and its logarithm. The modular function $\lambda = V/U$ mapping \mathbb{H} to $\mathbb{C} \setminus \{0, 1\}$ is a Hauptmodul for the modular curve $X(2) = \Gamma(2) \backslash \mathbb{H}$ (that is, a generator of its function field over \mathbb{C}). For example, it is related to the Hauptmodul j for $\Gamma(1)$ from (2.5) by

$$j = \frac{256(1 - \lambda + \lambda^2)^3}{\lambda^2(1 - \lambda)^2}.$$

The function λ takes the values 0, 1, and ∞ at the cusps ∞ , 0, and -1 , respectively, and its restriction $\lambda(it)$ to the positive imaginary axis decreases from 1 to 0 as t increases from 0 to ∞ . If we let

$$(2.14) \quad \lambda_S(z) := (\lambda|_0 S)(z) = \lambda(-z^{-1}) = 1 - \lambda(z),$$

then these functions also satisfy the properties

$$(2.15) \quad \lambda(z + 1) = \frac{\lambda(z)}{\lambda(z) - 1} = -\frac{\lambda(z)}{\lambda_S(z)} \quad \text{and} \quad \lambda_S(z + 1) = \frac{1}{\lambda_S(z)}$$

for $z \in \mathbb{H}$.

The nonvanishing of λ and λ_S on \mathbb{H} allows us to define

$$\mathcal{L}(z) = \int_0^z \frac{\lambda'(w)}{\lambda(w)} dw \quad \text{and} \quad \mathcal{L}_S(z) = -\int_z^\infty \frac{\lambda'_S(w)}{\lambda_S(w)} dw,$$

where the contours are chosen to approach the singularities 0 or ∞ on vertical lines. These functions satisfy

$$\mathcal{L}(it) = \log(\lambda(it)) \quad \text{and} \quad \mathcal{L}_S(it) = \log(\lambda_S(it)) = \log(1 - \lambda(it))$$

for $t > 0$, and as such are holomorphic functions for which $e^{\mathcal{L}} = \lambda$ and $e^{\mathcal{L}_S} = \lambda_S$; however, they are not in general the principal branches of the logarithms of λ or λ_S . We note the asymptotics

$$(2.16) \quad \begin{aligned} \mathcal{L}(z) &= \pi iz + 4 \log(2) - 8q^{1/2} + O(q) \quad \text{and} \\ \mathcal{L}_S(z) &= -16q^{1/2} - \frac{64q^{3/2}}{3} + O(q^{5/2}) \end{aligned}$$

as $q \rightarrow 0$, where $q^{n/2} = e^{2\pi inz/2}$.

The functions \mathcal{L} and \mathcal{L}_S have the transformation properties

$$(2.17) \quad \begin{aligned} \mathcal{L}|_0T &= \mathcal{L} - \mathcal{L}_S + i\pi, & \mathcal{L}_S|_0T &= -\mathcal{L}_S, \\ \mathcal{L}|_0S &= \mathcal{L}_S, & \mathcal{L}_S|_0S &= \mathcal{L}. \end{aligned}$$

Indeed, the last pair of assertions follows directly from the definitions and holomorphy. The first two assertions, which read

$$\mathcal{L}(z+1) = \mathcal{L}(z) - \mathcal{L}_S(z) + \pi i \quad \text{and} \quad \mathcal{L}_S(z+1) = -\mathcal{L}_S(z),$$

are proved by showing that the derivatives of both sides are equal (using the derivatives of the identities in (2.15)) and by comparing the asymptotics (2.16) to determine the constant of integration.

2.2. Elliptic integrals. We normalize the *complete elliptic integral of the first kind* by

$$K(m) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - m \sin^2 \theta}}$$

and *of the second kind* by

$$E(m) = \int_0^{\pi/2} \sqrt{1 - m \sin^2 \theta} \, d\theta.$$

Note that many references, such as [35, Chapter 19], define K and E in terms of the elliptic modulus k , so that the complete elliptic integrals are what we call $k \mapsto K(k^2)$ and $k \mapsto E(k^2)$. Our normalization is slightly less principled from the perspective of elliptic function theory, but it has the advantage of simplifying various expressions that occur later in our paper.

These elliptic integrals satisfy a plethora of beautiful identities, a few of which we list below. First, E and K are related by

$$(2.18) \quad K'(m) = \frac{E(m)}{2m(1-m)} - \frac{K(m)}{2m}.$$

(Here, K' denotes the derivative of K . In the elliptic function literature, K' is often used instead to denote the elliptic integral with respect to the complementary modulus $k' = \sqrt{1 - k^2}$.) Legendre proved the identity

$$K(m)E(1-m) + E(m)K(1-m) - K(m)K(1-m) = \frac{\pi}{2}$$

(see [32, pp. 68–69]). The two identities above can be combined to obtain

$$(2.19) \quad K(m)K'(1-m) + K'(m)K(1-m) = \frac{\pi}{4m(1-m)}.$$

In other words, the Wronskian of K and $m \mapsto K(1-m)$ has a simple form.

Elliptic integrals are also related to the modular forms of Section 2.1 via classical identities dating back to Jacobi. For $z \in \mathbb{H}$ on the imaginary axis, the key identity is the inversion formula

$$\Theta_3(z)^2 = 2\pi^{-1}K(\lambda(z))$$

(see [48, §21.61 and §22.301] or [41, Theorem 5.8]). It follows that for such z ,

$$(2.20) \quad \begin{aligned} U(z) &= 4\pi^{-2}K(\lambda(z))^2, \\ V(z) &= 4\pi^{-2}\lambda(z)K(\lambda(z))^2, \quad \text{and} \\ W(z) &= 4\pi^{-2}\lambda_S(z)K(\lambda(z))^2, \end{aligned}$$

because $U = \Theta_3^4$, $\lambda = V/U$, and $U = V + W$. Using (2.14) and Jacobi's transformation law

$$\Theta_3(-1/z)^2 = -iz\Theta_3(z)^2$$

(which follows immediately from Poisson summation), we obtain

$$(2.21) \quad \frac{K(1-\lambda(z))}{K(\lambda(z))} = -iz.$$

Differentiation combined with (2.19) yields the identity

$$\lambda'(z) = 4i\pi^{-1}\lambda(z)(1-\lambda(z))K(\lambda(z))^2.$$

Finally, we can use (2.7), (2.12), (2.18), and (2.20) to write

$$(2.22) \quad E_2(z) = 4\pi^{-2}K(\lambda(z))\left(3E(\lambda(z)) - (2-\lambda(z))K(\lambda(z))\right).$$

In Section 6 we will use equations (2.12), (2.20), (2.21), and (2.22) to write the restriction of elements of $\mathcal{M}^!(\Gamma(2))$ (and related quasimodular expressions) to the imaginary axis in terms of elliptic integrals of λ .

The elliptic integrals E and K are holomorphic in the open unit disk. Their behavior near 1 is governed by

$$(2.23) \quad E(1-z) = A_1(z) + A_2(z)\log(z) \quad \text{and} \quad K(1-z) = A_3(z) + A_4(z)\log(z),$$

where each A_j is a holomorphic function on the open unit disk with real Taylor coefficients about the origin (see [35, Section 19.12] for explicit formulas).

Furthermore, A_1 and A_3 have nonnegative coefficients, while A_2 and A_4 have nonpositive coefficients.

2.3. *Radial Schwartz functions.* For a smooth function f on \mathbb{R}^d , define the *Schwartz seminorms* by

$$\|f\|_{\alpha,\beta} = \sup_{x \in \mathbb{R}^d} |x^\alpha \partial^\beta f(x)|,$$

for $\alpha, \beta \in \mathbb{Z}_{\geq 0}^d$, where we use the multi-index notation

$$x^\alpha = x_1^{\alpha_1} \cdots x_d^{\alpha_d} \quad \text{and} \quad \partial^\beta = \left(\frac{\partial}{\partial x_1}\right)^{\beta_1} \cdots \left(\frac{\partial}{\partial x_d}\right)^{\beta_d}.$$

By definition, f is a Schwartz function if and only if $\|f\|_{\alpha,\beta} < \infty$ for all α and β , and these seminorms define the Schwartz space topology on $\mathcal{S}(\mathbb{R}^d)$. The radial Schwartz space $\mathcal{S}_{\text{rad}}(\mathbb{R}^d)$ is the subspace of radial functions in $\mathcal{S}(\mathbb{R}^d)$, with the induced topology.

LEMMA 2.1. *A Schwartz function f on \mathbb{R}^d is radial if and only if there exists an even Schwartz function f_0 on \mathbb{R} such that $f(x) = f_0(|x|)$ for all $x \in \mathbb{R}^d$. Furthermore, the map $f_0 \mapsto f$ is an isomorphism of topological vector spaces from $\mathcal{S}_{\text{rad}}(\mathbb{R}^1)$ to $\mathcal{S}_{\text{rad}}(\mathbb{R}^d)$.*

Of course $\mathcal{S}_{\text{rad}}(\mathbb{R}^1)$ consists of the even functions in $\mathcal{S}(\mathbb{R}^1)$. For a proof of Lemma 2.1 (in fact, of a slightly stronger result), see [23, Section 3].

For our purposes, the significance of Lemma 2.1 is that we can restrict our attention to radial derivatives when dealing with radial Schwartz functions. Let D denote the radial derivative, defined by $Df(x) = f'_0(|x|)$, and define the *radial seminorms* by

$$\|f\|_{k,\ell}^{\text{rad}} = \sup_{x \in \mathbb{R}^d} |x|^k |D^\ell f(x)|$$

for $k, \ell \in \mathbb{Z}_{\geq 0}$. Then Lemma 2.1 tells us that a smooth, radial function f is a Schwartz function if and only if $\|f\|_{k,\ell}^{\text{rad}} < \infty$ for all k and ℓ , and these seminorms characterize the topology of $\mathcal{S}_{\text{rad}}(\mathbb{R}^d)$.

We will also need the first part of the following lemma, which we prove using the techniques from [37, Section 6].

LEMMA 2.2. *The complex Gaussians $x \mapsto e^{\pi i \tau |x|^2}$ with $\tau \in \mathbb{H}$ span a dense subspace of $\mathcal{S}_{\text{rad}}(\mathbb{R}^d)$. In fact, for any $y > 0$, the same is true if we use only complex Gaussians with $\text{Im}(\tau) = y$.*

Proof. Compactly supported functions are dense in $\mathcal{S}_{\text{rad}}(\mathbb{R}^d)$, as is easily shown by multiplying by a suitable bump function. Thus it will suffice to show that compactly supported, smooth, radial functions can be approximated arbitrarily well by linear combinations of complex Gaussians with $\text{Im}(\tau) = y$.

Removing a factor of $e^{\pi y|x|^2}$ shows that every compactly supported, smooth, radial f on \mathbb{R}^d can be written as

$$f(x) = g(|x|^2)e^{-\pi y|x|^2},$$

where g is a smooth, compactly supported function on \mathbb{R} . Let \hat{g} be its one-dimensional Fourier transform

$$\hat{g}(t) = \int_{\mathbb{R}} g(x)e^{-2\pi itx} dx.$$

Then

$$g(|x|^2) = \int_{\mathbb{R}} \hat{g}(t)e^{2\pi it|x|^2} dt = \lim_{T \rightarrow \infty} \int_{-T}^T \hat{g}(t)e^{2\pi it|x|^2} dt$$

by Fourier inversion, and hence

$$f(x) = \lim_{T \rightarrow \infty} \int_{-T}^T \hat{g}(t)e^{\pi i(2t+iy)|x|^2} dt.$$

The functions

$$(2.24) \quad x \mapsto \int_{-T}^T \hat{g}(t)e^{\pi i(2t+iy)|x|^2} dt$$

are Schwartz functions that converge to f in $\mathcal{S}_{\text{rad}}(\mathbb{R}^d)$ as $T \rightarrow \infty$, because \hat{g} is rapidly decreasing and we can therefore control the radial Schwartz seminorms of the error term

$$x \mapsto \int_{\mathbb{R} \setminus [-T, T]} \hat{g}(t)e^{\pi i(2t+iy)|x|^2} dt.$$

Furthermore, for each T , equally spaced Riemann sums for (2.24) converge to this function in $\mathcal{S}_{\text{rad}}(\mathbb{R}^d)$, by the usual error estimate in terms of the derivative. These Riemann sums are linear combinations of complex Gaussians with $\tau = 2t + iy$ for different values of t in \mathbb{R} , as desired. \square

3. Functional equations and the group algebra $\mathbb{C}[\text{PSL}_2(\mathbb{Z})]$

3.1. *From interpolation to functional equations and back.* As mentioned in the introduction, we consider the generating functions

$$(3.1) \quad F(\tau, x) = \sum_{n \geq n_0} a_n(x) e^{2\pi in\tau} + 2\pi i\tau \sum_{n \geq n_0} \sqrt{2n} b_n(x) e^{2\pi in\tau}$$

and

$$(3.2) \quad \tilde{F}(\tau, x) = \sum_{n \geq n_0} \tilde{a}_n(x) e^{2\pi in\tau} + 2\pi i\tau \sum_{n \geq n_0} \sqrt{2n} \tilde{b}_n(x) e^{2\pi in\tau}$$

for the interpolation basis, where $x \in \mathbb{R}^d$ and τ is in the upper half-plane $\mathbb{H} = \{z \in \mathbb{C} : \text{Im}(z) > 0\}$. In equations (1.8)–(1.10), we derived functional equations for F and \tilde{F} from the existence of an interpolation basis. We now show that the converse holds as well: the existence of a well-behaved solution to the

functional equations (1.8)–(1.10) implies an interpolation theorem, regardless of the dimension.

THEOREM 3.1. *Suppose there exist smooth functions $F, \widetilde{F}: \mathbb{H} \times \mathbb{R}^d \rightarrow \mathbb{C}$ such that*

- (1) $F(\tau, x)$ and $\widetilde{F}(\tau, x)$ are holomorphic in τ ,
- (2) $F(\tau, x)$ and $\widetilde{F}(\tau, x)$ are radial in x ,
- (3) for all nonnegative integers k and ℓ , the radial derivative D_x with respect to x satisfies the uniform bounds

$$|x|^k \left| D_x^\ell F(\tau, x) \right| < \alpha_{k,\ell} \operatorname{Im}(\tau)^{-\beta_{k,\ell}} + \gamma_{k,\ell} |\tau|^{\delta_{k,\ell}}$$

and

$$|x|^k \left| D_x^\ell \widetilde{F}(\tau, x) \right| < \alpha_{k,\ell} \operatorname{Im}(\tau)^{-\beta_{k,\ell}} + \gamma_{k,\ell} |\tau|^{\delta_{k,\ell}}$$

for some nonnegative constants $\alpha_{k,\ell}$, $\beta_{k,\ell}$, $\gamma_{k,\ell}$, and $\delta_{k,\ell}$,

- (4) in the special case $(k, \ell) = (0, 0)$,

$$|F(\tau, x)|, |\widetilde{F}(\tau, x)| \leq \alpha_{0,0} \operatorname{Im}(\tau)^{-\beta_{0,0}}$$

for $-1 \leq \operatorname{Re}(\tau) \leq 1$ and $x \in \mathbb{R}^d$, with $\beta_{0,0} > 0$, and

- (5) F and \widetilde{F} satisfy the functional equations (1.8)–(1.10), i.e.,

$$F(\tau + 2, x) - 2F(\tau + 1, x) + F(\tau, x) = 0,$$

$$\widetilde{F}(\tau + 2, x) - 2\widetilde{F}(\tau + 1, x) + \widetilde{F}(\tau, x) = 0, \text{ and}$$

$$F(\tau, x) + (i/\tau)^{d/2} \widetilde{F}(-1/\tau, x) = e^{\pi i \tau |x|^2}.$$

Then F and \widetilde{F} have expansions of the form (3.1) and (3.2) with $n_0 = 1$, for some radial Schwartz functions $a_n, b_n, \widetilde{a}_n, \widetilde{b}_n$. Moreover, for every radial Schwartz function $f: \mathbb{R}^d \rightarrow \mathbb{R}$, the interpolation formula

$$\begin{aligned} f(x) &= \sum_{n=1}^{\infty} f(\sqrt{2n}) a_n(x) + \sum_{n=1}^{\infty} f'(\sqrt{2n}) b_n(x) \\ &\quad + \sum_{n=1}^{\infty} \widehat{f}(\sqrt{2n}) \widetilde{a}_n(x) + \sum_{n=1}^{\infty} \widehat{f}'(\sqrt{2n}) \widetilde{b}_n(x), \end{aligned}$$

holds, and the right side converges absolutely. Finally, for fixed k and ℓ , the radial seminorms

$$\begin{aligned} \sup_{x \in \mathbb{R}^d} |x|^k \left| a_n^{(\ell)}(x) \right|, & \quad \sup_{x \in \mathbb{R}^d} |x|^k \left| b_n^{(\ell)}(x) \right|, \\ \sup_{x \in \mathbb{R}^d} |x|^k \left| \widetilde{a}_n^{(\ell)}(x) \right|, & \quad \sup_{x \in \mathbb{R}^d} |x|^k \left| \widetilde{b}_n^{(\ell)}(x) \right| \end{aligned}$$

all grow at most polynomially in n .

Furthermore, $a_1 = \widetilde{a}_1 = b_1 = \widetilde{b}_1 = 0$ if and only if $F(\tau, x)$ and $\widetilde{F}(\tau, x)$ are $o(e^{-2\pi \operatorname{Im}(\tau)})$ as $\operatorname{Im}(\tau) \rightarrow \infty$ in the strip $-1 \leq \operatorname{Re}(\tau) \leq 1$ with x fixed.

This last statement concerns starting the interpolation formula at $n_0 = 2$, which Theorem 1.7 asserts is the case for $d = 24$. The separate condition (4) is important for ruling out a contribution from $n = 0$ in the interpolation formula; the restriction to the strip $-1 \leq \operatorname{Re}(\tau) \leq 1$ is because generic solutions to the recurrences in part (5) grow linearly in $\operatorname{Re}(\tau)$ (see (3.5)).

Proof. We begin by obtaining the expansion of F . The difference

$$F(\tau + 1, x) - F(\tau, x)$$

is holomorphic in τ and invariant under $\tau \mapsto \tau + 1$, by the functional equation

$$F(\tau + 2, x) - 2F(\tau + 1, x) + F(\tau, x) = 0.$$

Thus, for each x there is a holomorphic function g_x on the punctured disk $\{z \in \mathbb{C} : 0 < |z| < 1\}$ such that

$$F(\tau + 1, x) - F(\tau, x) = g_x(e^{2\pi i\tau}).$$

Furthermore, it follows from part (4) of the hypotheses that

$$\lim_{z \rightarrow 0} g_x(z) = 0,$$

and thus g_x extends to a holomorphic function that vanishes at 0. By taking the Taylor series of g_x about 0, we obtain coefficients $b_n(x)$ for $n \geq 1$ such that

$$(3.3) \quad F(\tau + 1, x) - F(\tau, x) = 2\pi i \sum_{n \geq 1} \sqrt{2n} b_n(x) e^{2\pi i n \tau}.$$

To obtain $a_n(x)$, we instead look at

$$F(\tau, x) - \tau(F(\tau + 1, x) - F(\tau, x)),$$

which is again holomorphic in τ and invariant under $\tau \mapsto \tau + 1$. The parenthetical expression decays exponentially as $\operatorname{Im}(\tau) \rightarrow \infty$ by (3.3), so the bound in part (4) again yields coefficients $a_n(x)$ for $n \geq 1$ such that

$$(3.4) \quad F(\tau, x) - \tau(F(\tau + 1, x) - F(\tau, x)) = \sum_{n \geq 1} a_n(x) e^{2\pi i n \tau},$$

that is,

$$(3.5) \quad F(\tau, x) = \sum_{n \geq 1} a_n(x) e^{2\pi i n \tau} + 2\pi i \tau \sum_{n \geq 1} \sqrt{2n} b_n(x) e^{2\pi i n \tau}.$$

Because of the symmetry of the hypotheses, the case of \tilde{F} works exactly the same way, with coefficients $\tilde{a}_n(x)$ and $\tilde{b}_n(x)$. The assertion at the end of the theorem statement about when $a_1 = \tilde{a}_1 = b_1 = \tilde{b}_1 = 0$ is then an immediate consequence of formula (3.5) and its counterpart for \tilde{F} .

To check that the coefficients are radial Schwartz functions, we note that for any $y > 0$,

$$(3.6) \quad a_n(x) = \int_{-1+iy}^{iy} (F(\tau, x) - \tau(F(\tau+1, x) - F(\tau, x))) e^{-2\pi i n \tau} d\tau$$

and

$$(3.7) \quad b_n(x) = \frac{1}{2\pi i \sqrt{2n}} \int_{-1+iy}^{iy} (F(\tau+1, x) - F(\tau, x)) e^{-2\pi i n \tau} d\tau$$

by orthogonality using (3.4) and (3.3). We can take radial derivatives in x under the integral sign, because all the derivatives are continuous. If we do so and apply part (3) of the hypotheses, we find that the radial seminorms

$$\sup_{x \in \mathbb{R}^d} |x|^k |a_n^{(\ell)}(x)| \quad \text{and} \quad \sup_{x \in \mathbb{R}^d} |x|^k |b_n^{(\ell)}(x)|$$

are all finite, for any k, ℓ , and n . Thus, a_n and b_n are Schwartz functions (see Lemma 2.1). Furthermore, if we take $y = 1/n$ and integrate over the straight line from $-1 + iy$ to iy , we find that these radial seminorms of a_n and b_n grow at most polynomially in n for each k and ℓ . By symmetry, the same holds for \tilde{a}_n and \tilde{b}_n as well.

These estimates imply that the sum

$$\begin{aligned} & \sum_{n=1}^{\infty} f(\sqrt{2n}) a_n(x) + \sum_{n=1}^{\infty} f'(\sqrt{2n}) b_n(x) \\ & + \sum_{n=1}^{\infty} \hat{f}(\sqrt{2n}) \tilde{a}_n(x) + \sum_{n=1}^{\infty} \hat{f}'(\sqrt{2n}) \tilde{b}_n(x), \end{aligned}$$

converges absolutely whenever f is a radial Schwartz function, and that this formula defines a continuous linear functional on $\mathcal{S}_{\text{rad}}(\mathbb{R}^d)$.

All that remains is to prove the interpolation formula. Fix $x_0 \in \mathbb{R}^d$, and define the functional Λ on $\mathcal{S}_{\text{rad}}(\mathbb{R}^d)$ by

$$\begin{aligned} \Lambda(f) &= \sum_{n=1}^{\infty} f(\sqrt{2n}) a_n(x_0) + \sum_{n=1}^{\infty} f'(\sqrt{2n}) b_n(x_0) \\ &+ \sum_{n=1}^{\infty} \hat{f}(\sqrt{2n}) \tilde{a}_n(x_0) + \sum_{n=1}^{\infty} \hat{f}'(\sqrt{2n}) \tilde{b}_n(x_0) \\ &- f(x_0), \end{aligned}$$

so that the interpolation formula for x_0 is equivalent to $\Lambda = 0$. Because Λ is continuous, it suffices to prove that $\Lambda(f)$ vanishes when f is a complex Gaussian, i.e., $f(x) = e^{\pi i \tau |x|^2}$ with $\tau \in \mathbb{H}$, by Lemma 2.2. This condition amounts to the function equation

$$F(\tau, x_0) + (i/\tau)^{d/2} \tilde{F}(-1/\tau, x_0) = e^{\pi i \tau |x_0|^2},$$

because $\widehat{f}(x) = (i/\tau)^{d/2} e^{\pi i(-1/\tau)|x|^2}$. Thus, the interpolation formula holds for all radial Schwartz functions, as desired. \square

Theorem 3.1 reduces Theorem 1.7 to constructing F and \widetilde{F} , but the only hint it gives for how to do so is the functional equations they must satisfy. The rest of Sections 3 and 4 consists of a detailed study of these functional equations, in terms of the right action of $\mathrm{PSL}_2(\mathbb{Z})$ via the slash operator $|_{d/2}^\tau$ in the τ variable (assuming $d/2$ is an even integer). Using the standard generators S and T from (2.3), the equation

$$F(\tau, x) + (i/\tau)^{d/2} \widetilde{F}(-1/\tau, x) = e^{\pi i \tau |x|^2}$$

expresses F in terms of $\widetilde{F}|_{d/2}^\tau S$ and vice versa (because $S^2 = I$). It therefore suffices to construct F , from which we can obtain \widetilde{F} . The remaining functional equations are best stated in terms of the linear extension of the slash operator action (2.1) of $\mathrm{PSL}_2(\mathbb{Z})$ to the group algebra $R = \mathbb{C}[\mathrm{PSL}_2(\mathbb{Z})]$ of finite formal linear combinations of elements of $\mathrm{PSL}_2(\mathbb{Z})$. The equation

$$F(\tau + 2, x) - 2F(\tau + 1, x) + F(\tau, x) = 0$$

says F is annihilated by $(T - I)^2$, while

$$\widetilde{F}(\tau + 2, x) - 2\widetilde{F}(\tau + 1, x) + \widetilde{F}(\tau, x) = 0$$

specifies the action of $S(T - I)^2$ on F (see (4.5) below). Thus, the functional equations specify the action of the right ideal $\mathcal{I} = (T - I)^2 \cdot R + S(T - I)^2 \cdot R$ on F . This ideal does not amount to all of R , and in fact $\dim_{\mathbb{C}}(R/\mathcal{I}) = 6$, as we will see in Proposition 3.9. (For simplicity we write R/\mathcal{I} rather than $\mathcal{I} \backslash R$, despite the fact that \mathcal{I} is a right ideal.) To make further progress, we must understand the structure of \mathcal{I} and the action of $\mathrm{PSL}_2(\mathbb{Z})$ on the six-dimensional vector space R/\mathcal{I} .

3.2. A six-dimensional representation of $\mathrm{SL}_2(\mathbb{Z})$. Many of our arguments use facts about a particular six-dimensional representation σ of $\mathrm{SL}_2(\mathbb{Z})$, which we collect here for later reference. We will see in (3.17) that this representation describes the action of $\mathrm{PSL}_2(\mathbb{Z})$ on R/\mathcal{I} .

Recall that $\mathrm{PSL}_2(\mathbb{Z})$ has the subgroup $\overline{\Gamma(2)}$ of index 6, which is freely generated by $T^2 = \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}$ and $ST^2S = \begin{pmatrix} -1 & 0 \\ 2 & -1 \end{pmatrix}$. The following lemma gives some standard bounds on the length of a word in these generators by the size of the matrix, in a way which will be useful for later applications such as Proposition 4.2. It follows from work of Eichler [21], but we give a direct proof. The idea of column domination that appears in part (1) dates back at least to Markov's 1954 book on algorithms [31, Chapter VI §10 2.5].

Let $\|\gamma\|_{\text{Frob}} = (\text{Tr}(\gamma\gamma^t))^{1/2}$ denote the Frobenius norm of $\gamma \in \text{SL}_2(\mathbb{R})$, i.e.,

$$\left\| \begin{pmatrix} a & b \\ c & d \end{pmatrix} \right\|_{\text{Frob}}^2 = a^2 + b^2 + c^2 + d^2,$$

and we apply this norm also to elements of $\text{PSL}_2(\mathbb{R})$, because $\|\gamma\|_{\text{Frob}} = \|-\gamma\|_{\text{Frob}}$.

LEMMA 3.2. *Let $\gamma_1 = T^2$ and $\gamma_2 = ST^2S$, so that every element $\gamma \in \overline{\Gamma(2)} \subseteq \text{PSL}_2(\mathbb{Z})$ has a unique expression as a finite reduced word $\gamma_1^{e_1}\gamma_2^{f_1}\gamma_1^{e_2}\cdots$, with each $e_i, f_i \in \mathbb{Z} \setminus \{0\}$ except perhaps $e_1 = 0$.*

- (1) *(Column domination property) The second column of γ has strictly greater Euclidean norm than the first column if and only if γ 's reduced word ends in a nonzero power of $\gamma_1 = T^2$.*
- (2) *The Frobenius norm of γ satisfies*

$$|e_1| + |f_1| + |e_2| + \cdots \leq \|\gamma\|_{\text{Frob}}^2 \leq (2 + 4e_1^2)(2 + 4f_1^2)(2 + 4e_2^2) \cdots.$$

- (3) *The initial subwords*

$$\gamma_1^{\text{sgn}(e_1)}, \gamma_1^{2\text{sgn}(e_1)}, \dots, \gamma_1^{e_1}, \gamma_1^{e_1}\gamma_2^{\text{sgn}(f_1)}, \dots, \gamma_1^{e_1}\gamma_2^{f_1}, \dots, \gamma$$

of the reduced word of γ have strictly increasing Frobenius norms.

Of course the column vectors of an element of $\text{PSL}_2(\mathbb{Z})$ are defined only modulo multiplication by ± 1 , but that suffices for their norms to be well defined. The bounds in part (2) are not sharp, but they will suffice for our purposes.

Proof. Note that conjugating by S maps $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ to $\begin{pmatrix} d & -c \\ -b & a \end{pmatrix}$, which interchanges the column norms as well as the generators $\gamma_1 = T^2$ and $\gamma_2 = ST^2S$. Because of this symmetry, part (1) implies that the first column of γ has strictly greater Euclidean norm than the second column if and only if γ 's reduced word ends in a nonzero power of $\gamma_2 = ST^2S$, and that only the identity element of $\overline{\Gamma(2)}$ has columns of the same Euclidean norm. We will prove these three statements together by induction on the total number of factors $\gamma_1^{e_i}$ or $\gamma_2^{f_i}$ in γ 's reduced word. The base case of powers $\gamma_1^{e_1}$ and $\gamma_2^{f_1}$ is straightforward. For the inductive step, by symmetry we reduce to the case where γ has the form

$$\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 1 & 2e \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} a & b + 2ea \\ c & d + 2ec \end{pmatrix},$$

where $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \text{PSL}_2(\mathbb{Z})$ is not the identity element, e is a nonzero integer, and $a^2 + c^2 > b^2 + d^2$ by the inductive assumption. The Euclidean norm squared of γ 's second column is

$$h(e) := b^2 + d^2 + 4e^2(a^2 + c^2) + 4e(ab + cd),$$

and we must show that $h(e) > a^2 + c^2$ when $e \neq 0$. Because $h(e)$ is quadratic in e and $h(0) < a^2 + c^2$, it suffices to show that $h(\pm 1) > a^2 + c^2$. Indeed,

$$\begin{aligned} h(\pm 1) &\geq b^2 + d^2 + 4(a^2 + c^2) - 4\sqrt{a^2 + c^2}\sqrt{b^2 + d^2} \\ &= (2\sqrt{a^2 + c^2} - \sqrt{b^2 + d^2})^2 > a^2 + c^2, \end{aligned}$$

as desired, where the first inequality follows from the Cauchy-Schwarz inequality. This proves part (1).

The upper bound in part (2) follows from the sub-multiplicativity of the Frobenius norm. The lower bound follows from part (3), because there are $|e_1| + |f_1| + |e_2| + \dots$ initial subwords. Finally, part (3) follows from part (1) and the fact that $h(e)$ increases for $e \geq 1$ and decreases for $e \leq -1$ (it is a quadratic function of e whose minimum occurs between $e = -1$ and $e = 1$). \square

We next introduce some representations of $\mathrm{SL}_2(\mathbb{Z})$. First, define the three-dimensional representation $\rho_3: \mathrm{SL}_2(\mathbb{Z}) \rightarrow \mathrm{GL}_3(\mathbb{Z})$ by the formula

$$(3.8) \quad \rho_3 \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a^2 & 2ab & -b^2 \\ ac & ad + bc & -bd \\ -c^2 & -2cd & d^2 \end{pmatrix};$$

it is the restriction of a three-dimensional representation⁵ of $\mathrm{SL}_2(\mathbb{R})$ to $\mathrm{SL}_2(\mathbb{Z})$. We define $\rho_2: \mathrm{SL}_2(\mathbb{Z}) \rightarrow \mathrm{GL}_2(\mathbb{Z})$ by its action on the generators,

$$\rho_2(T) = \rho_2 \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix} \text{ and } \rho_2(S) = \rho_2 \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix};$$

its image is a dihedral group of order 6 and its kernel is $\Gamma(2)$, so ρ_2 is just a faithful representation of the dihedral group $\mathrm{SL}_2(\mathbb{Z})/\Gamma(2)$. Finally, define the function $\vec{v}: \mathrm{SL}_2(\mathbb{Z}) \rightarrow \mathbb{Z}^2$ by $\vec{v}(S) = (0, 0)$ and $\vec{v}(T) = (1, -1)$ (thought of as row vectors), and then in general by the cocycle formula

$$(3.9) \quad \vec{v}(\gamma\gamma') = \vec{v}(\gamma)\rho_2(\gamma') + \vec{v}(\gamma');$$

to check that this cocycle is well defined, we can define it via (3.9) on the free group generated by S and T , and then check that it annihilates S^2 and $(ST)^3$, so that it factors through $\mathrm{PSL}_2(\mathbb{Z})$. Then

$$\rho(\gamma) = \begin{pmatrix} \rho_3(\gamma) & 0 & 0 \\ 0 & 1 & \vec{v}(\gamma) \\ 0 & 0 & \rho_2(\gamma) \end{pmatrix}$$

defines a six-dimensional representation of $\mathrm{SL}_2(\mathbb{Z})$.

⁵There is a unique irreducible, continuous representation of $\mathrm{SL}_2(\mathbb{R})$ of each finite dimension, up to isomorphism.

Many of our later calculations use a conjugate σ of ρ defined by

$$(3.10) \quad \sigma(\gamma) = g_{\rho\sigma}^{-1} \rho(\gamma) g_{\rho\sigma},$$

where

$$g_{\rho\sigma} = \begin{pmatrix} 1 & 0 & 1 & -1 & 0 & -1 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & -1 & 1 & 0 \\ 3 & -1 & -1 & 3 & -1 & -1 \\ -2 & 0 & 2 & -2 & 0 & 2 \\ 2 & -2 & 0 & 2 & -2 & 0 \end{pmatrix},$$

which is characterized by its values

$$\sigma(S) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad \text{and} \quad \sigma(T) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 2 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & -1 & 2 & 0 & 0 \end{pmatrix}$$

on the generators (2.3). See the paragraph after the proof of Proposition 3.9 for more discussion of the role of σ in this paper and its relationship with ρ .

The next result shows that the (integral) matrix entries of $\rho(\gamma)$ and $\sigma(\gamma)$ do not grow quickly in terms of those of γ .

LEMMA 3.3. *There exist absolute constants $C, N > 0$ such that each matrix entry of $\rho \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ and of $\sigma \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ is bounded by $C(a^2 + b^2 + c^2 + d^2)^N$ in absolute value.*

The boundedness assertion in this lemma depends on the realization of the abstract group $\mathrm{SL}_2(\mathbb{Z})$ in integer matrices. In particular, it implies that the restrictions of ρ or σ to free subgroups of $\mathrm{SL}_2(\mathbb{Z})$ satisfy the same bound, a fact that is false for general representations of these subgroups. For example, the entries of $\sigma(T)^n$ grow only polynomially in n , while exponential growth can occur for other representations of the subgroup $\langle T \rangle$.

Proof. The assertions for these two conjugate representations are equivalent. The representation ρ_3 satisfies this boundedness condition by virtue of its explicit algebraic formula in (3.8), while ρ_2 has a finite image. Thus it suffices to verify that $\vec{v}(\gamma)$ with $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ satisfies the claimed bound. Furthermore, formula (3.9) with $\gamma \in \Gamma(2)$ and γ' one of the six coset representatives for $\Gamma(2)$ shows that it suffices to prove this last bound for $\gamma \in \Gamma(2)$. Because $\Gamma(2)$ is the kernel of ρ_2 , formula (3.9) restricted to $\Gamma(2)$ shows that \vec{v} is a homomorphism from $\Gamma(2)$ to $\mathbb{Z} \oplus \mathbb{Z}$. Writing γ as $\gamma_1^{e_1} \gamma_2^{f_1} \gamma_1^{e_2} \cdots$ as in the statement of Lemma 3.2, we see that the entries of $\vec{v}(\gamma)$ are bounded in absolute value by a constant multiple of $|e_1| + |f_1| + |e_2| + \cdots$, and the result follows from part (2) of Lemma 3.2. \square

3.3. *The group algebra $R = \mathbb{C}[\mathrm{PSL}_2(\mathbb{Z})]$.* In constructing a solution to the identities (1.8)–(1.10), it is convenient to use the slash operator action of

$R = \mathbb{C}[\mathrm{PSL}_2(\mathbb{Z})]$. Then (1.8)–(1.10) state that

$$(3.11) \quad F + i^{d/2} \widetilde{F}|_{d/2}^\tau S = e^{\pi i \tau |x|^2} \quad \text{and} \quad F|_{d/2}^\tau (T - I)^2 = \widetilde{F}|_{d/2}^\tau (T - I)^2 = 0,$$

where I denotes the identity element while S and T are defined by (2.3).

This subsection is devoted to studying some properties of R that are used later in the paper, in particular quotients of the translation action of $\mathrm{PSL}_2(\mathbb{Z})$ on R . Recall that $\mathrm{PSL}_2(\mathbb{Z})$ is the free product of the subgroups $\{I, S\}$ and $\{I, ST, STST\}$. If we write

$$x = S \quad \text{and} \quad y = ST,$$

then every element γ of $\Gamma = \mathrm{PSL}_2(\mathbb{Z}) = \langle x, y \mid x^2 = y^3 = 1 \rangle$ has a unique reduced expression as a product $w_1 w_2 \cdots w_\ell$, where $\ell = \ell(\gamma)$ is the length of the product, each w_j is either x , y , or y^2 , and the only allowable consecutive pairs w_j and w_{j+1} are

$$(w_j, w_{j+1}) = (x, y), (x, y^2), (y, x), \text{ or } (y^2, x).$$

We extend the notion of length to $R = \mathbb{C}[\Gamma]$ by defining $\ell(\sum_{\gamma \in \Gamma} c_\gamma \gamma)$ to be the maximum of all $\ell(\gamma)$ for which $c_\gamma \neq 0$ (otherwise, $\ell(0) = -\infty$).

The order two element $x = S$ acts by left multiplication on R , which can be diagonalized into ± 1 eigenspaces using the decomposition

$$(3.12) \quad r = \frac{I + S}{2} r + \frac{I - S}{2} r$$

for $r \in R$. In particular,

$$(3.13) \quad \{r \in R : (S \pm I)r = 0\} = (S \mp I)R.$$

Similarly we obtain

$$\{r \in R : (y - 1)r = 0\} = (y^2 + y + 1)R.$$

from the idempotent decomposition

$$r = \sum_{j=0}^2 \frac{1 + e^{2\pi i j/3} y + e^{4\pi i j/3} y^2}{3} r$$

into three distinct eigenspaces for left multiplication by y .

The equation $(T - I)v = w$ is a discretization of the derivative from single-variable calculus, and it can be solved using a discretization of the integral as follows.

LEMMA 3.4. *Let $w = \sum_{\gamma \in \Gamma} c_\gamma \gamma$ with $c_\gamma \in \mathbb{C}$. Then there exists a solution $v \in R$ to*

$$(T - I)v = (xy - 1)v = w$$

if and only if $\sum_{n \in \mathbb{Z}} c_{(xy)^n \gamma} = 0$, in which case the unique solution in R is $v = \sum_{\gamma \in \Gamma} d_\gamma \gamma$ with $d_\gamma = \sum_{n > 0} c_{(xy)^n \gamma}$.

Proof. Suppose $v = \sum_{\gamma \in \Gamma} d_\gamma \gamma$. Then $(xy - 1)v = w$ means $c_\gamma = d_{(xy)^{-1}\gamma} - d_\gamma$, and hence $\sum_{n \in \mathbb{Z}} c_{(xy)^n \gamma} = 0$ via telescoping. Conversely, if $\sum_{n \in \mathbb{Z}} c_{(xy)^n \gamma} = 0$, then only finitely many of the numbers $d_\gamma := \sum_{n > 0} c_{(xy)^n \gamma}$ are nonzero, and they satisfy $d_{(xy)^{-1}\gamma} - d_\gamma = c_\gamma$, as desired. To see that the solution is unique, note that $(xy - 1)v = 0$ implies $d_\gamma = d_{(xy)^{-1}\gamma}$ for all γ , which can happen only when $v = 0$ because the coefficients have finite support. \square

COROLLARY 3.5. *Suppose $w = \sum_{\gamma} c_\gamma \gamma$ and there exists $\gamma \in \Gamma$ such that $c_{(xy)^n \gamma} \neq 0$ for exactly one $n \in \mathbb{Z}$. Then $w \notin (T - I)R$.*

LEMMA 3.6. *The set of all $v \in R$ for which there exist $w \in R$ satisfying*

$$(T - I)v = (S + I)w$$

is the right ideal $(y^2 - y + 1)(x + 1)R$. In other words,

$$\{v \in R : (xy - 1)v \in (x + 1)R\} = (y^2 - y + 1)(x + 1)R.$$

Proof. Because $xy - 1 = (x + 1)y - (y + 1)$, we see that $(xy - 1)v \in (x + 1)R$ if and only if $(y + 1)v \in (x + 1)R$. However, $y + 1$ is invertible in the ring R , with multiplicative inverse $(y^2 - y + 1)/2$, because $y^3 = 1$. Thus, $(y + 1)v \in (x + 1)R$ is equivalent to $v \in (y^2 - y + 1)(x + 1)R$, as desired. \square

LEMMA 3.7. *The set of all $v \in R$ for which there exist $w \in R$ satisfying*

$$(T - I)v = (S - I)w$$

is the right ideal $(y^2 + y + 1)R$.

Proof. The identity $(xy - 1)(y^2 + y + 1) = (x - 1)(y^2 + y + 1)$ shows that any element of that ideal provides a solution. Conversely, if $(xy - 1)v = (x - 1)w$, then multiplying by x shows that

$$(1 - x)w = (y - x)v = (y - 1)v - (x - 1)v$$

and hence $(y - 1)v \in (x - 1)R$. We will show that $(x - 1)R \cap (y - 1)R = \{0\}$, from which it follows that $(y - 1)v = 0$ and thus $v \in (y^2 + y + 1)R$ as needs to be shown. If $(y - 1)v \in (x - 1)R$, we may write $yv - v = xu - u$, for some $u = \sum_{\gamma} c_\gamma \gamma$ for which $c_\gamma = 0$ if γ 's reduced word begins with x (such γ can be replaced by $-x\gamma$, which does not start with x , because $(x - 1)(-x) = x - 1$). Multiplying both sides by $y^2 + y + 1$ on the left annihilates $(y - 1)v$ and yields $y^2xu + yxu = y^2u + yu - xu + u$. If u is nonzero, then the right side of this equation has length at most $\ell(u) + 1$, while the left side has terms having length $\ell(u) + 2$ which cannot cancel each other. Thus $u = 0$, proving that $(x - I)R \cap (y - I)R = \{0\}$. \square

3.3.1. *Some ideals of R .* Define the right ideals

$$\begin{aligned}
 \mathcal{I} &= (T - I)^2 \cdot R + S(T - I)^2 \cdot R, \\
 \mathcal{I}_+ &= (S + I) \cdot R + (T - I)^2 \cdot R, \\
 (3.14) \quad \mathcal{I}_- &= (S - I) \cdot R + (T - I)^2 \cdot R, \\
 \tilde{\mathcal{I}}_+ &= (T - 2 + T^{-1} - 2S) \cdot R + (I - STS) \cdot R, \text{ and} \\
 \tilde{\mathcal{I}}_- &= (T - 2 + T^{-1} + 2S) \cdot R + (I + STS) \cdot R
 \end{aligned}$$

of R . (We treat ± 1 and \pm synonymously in subscripts.) As mentioned at the end of Section 3.1, \mathcal{I} consists of the elements of R whose action on the generating function F is determined by the functional equations from Theorem 3.1. The ideals \mathcal{I}_\pm play the same role when we decompose F into eigenfunctions for S (see also part (3) of Proposition 3.9), while $\tilde{\mathcal{I}}_\pm$ are characterized by Proposition 3.11. Note in particular that $\mathcal{I} \subseteq \mathcal{I}_\pm$, because $S(T - I)^2 = (S \pm I)(T - I)^2 \mp (T - I)^2$, and $\mathcal{I}_+ \cap \mathcal{I}_- = \mathcal{I}$, because $Sr \equiv \pm r \pmod{\mathcal{I}}$ for $r \in \mathcal{I}_\pm$, so $r \equiv -r \pmod{\mathcal{I}}$ for $r \in \mathcal{I}_+ \cap \mathcal{I}_-$.

PROPOSITION 3.8. *The sums defining the ideals \mathcal{I} , \mathcal{I}_+ , and \mathcal{I}_- are all direct sums (i.e., these ideals are free modules of rank 2 over R).*

Proof. To deal with \mathcal{I} , suppose that $(T - I)^2 r = S(T - I)^2 r'$ for some $r, r' \in R$. Multiply both sides by S and combine to obtain the identity $(I - \varepsilon S)(T - I)^2(r + \varepsilon r') = 0$ for $\varepsilon = \pm 1$. By (3.13), this shows $(T - I)^2(r + \varepsilon r') \in (S + \varepsilon I)R$. From this we see that the assertion for \mathcal{I} follows from those for \mathcal{I}_\pm .

First consider \mathcal{I}_+ and $u, w \in R$ for which $(T - I)^2 u = (S + I)w$. By Lemma 3.6, $(T - I)u \in (y^2 - y + 1)(x + 1)R$, where $x = S$ and $y = ST$ as above. We will prove that there is no u for which $(T - I)u$ is a nonzero member of this ideal, using Corollary 3.5. Suppose $(T - I)u = (y^2 - y + 1)(x + 1)r$ for some $r \in R$. Without loss of generality, we may assume $r = r_0 + yr_1 + y^2 r_2$, where $r_0 \in \mathbb{C}$ and the reduced words occurring in r_1 or r_2 all start with x or are the identity. (The nontrivial part of this assertion is that we can take $r_0 \in \mathbb{C}$, which holds because we can use the identity $(x + 1)x = x + 1$ to incorporate any other terms from r_0 to \mathbb{C} , r_1 , or r_2 .) Then $(y^2 - y + 1)(x + 1)r$ equals

$$\begin{aligned}
 &y^2 x(r_0 + yr_1 + y^2 r_2) - yx(r_0 + yr_1 + y^2 r_2) + x(r_0 + yr_1 + y^2 r_2) \\
 &\quad + y^2(r_0 + yr_1 + y^2 r_2) - y(r_0 + yr_1 + y^2 r_2) + (r_0 + yr_1 + y^2 r_2).
 \end{aligned}$$

Assume now that r_1 and r_2 are not both zero and that $\ell(r_2) \geq \ell(r_1)$, so that $\ell((T - I)u) \leq \ell(r_2) + 3$. Choose $\gamma \in \text{PSL}_2(\mathbb{Z})$ occurring in r_2 with $\ell(\gamma) = \ell(r_2)$. The group elements $(xy)^n yx y^2 \gamma = (y^2 x)^{-n} yx y^2 \gamma$ have length $2n + 2 + \ell(r_2)$ (if $n \geq 1$) or $-2n + 3 + \ell(r_2)$ (if $n \leq 0$), and so cannot occur in $(T - I)u$ unless $n = 0$, when they occur in exactly one place, namely in $-yx y^2 r_2$ (they do not occur in the three terms in the second line because those have length at most

$\ell(r_2) + 1$). Corollary 3.5 then proves there is no solution in this case. The same argument applies if $\ell(r_1) > \ell(r_2)$: if γ occurs in r_1 with $\ell(\gamma) = \ell(r_1)$, then the group elements $(xy)^n yxy\gamma$ occur only in $-yxyr_1$ and with $n = 0$. Thus $r_1 = r_2 = 0$, and unless $r_0 = 0$ we may renormalize to set $r_0 = 1$ and obtain $(T - I)u = y^2x - yx + x + y^2 - y + 1$. Now yx is the only term in this expression of the form $(xy)^n yx$, and we again obtain a contradiction from Corollary 3.5.

The case of \mathcal{I}_- is slightly simpler: here $(T - I)^2u = (S - I)w$ implies $(T - I)u \in (y^2 + y + 1)R$ by Lemma 3.7. Suppose $(T - I)u = (y^2 + y + 1)r$ with $r \in R$. This time there is no loss in generality in assuming $r = r_0 + xr_1$, where $r_0 \in \mathbb{C}$ and r_1 does not begin with x , because $y^2 + y + 1$ annihilates both $y - 1$ and $y^2 - 1$. Now

$$(y^2 + y + 1)r = r_0y^2 + r_0y + r_0 + y^2xr_1 + yxr_1 + xr_1.$$

The terms occurring in $(xy)^n yxr_1$ occur in this expression only if $n = 0$, and thus Corollary 3.5 applies unless possibly $r_1 = 0$. If $r_1 = 0$, then the term $(xy)^n y$ occurs only for $n = 0$, and so we conclude that $(T - I)u = 0$, as desired. \square

PROPOSITION 3.9. *The ideals \mathcal{I} , \mathcal{I}_+ , and \mathcal{I}_- of R have the following properties:*

- (1) $\dim_{\mathbb{C}} R/\mathcal{I} = 6$ and
- (3.15) $M_1 = I, M_2 = T, M_3 = TS, M_4 = S, M_5 = ST, M_6 = STS$
are a basis of R/\mathcal{I} ,
- (2) $\dim_{\mathbb{C}} R/\mathcal{I}_{\pm} = 3$ and I, T, TS are a basis of R/\mathcal{I}_{\pm} , and
- (3) $\mathcal{I}_{\varepsilon} = \{r \in R : (S - \varepsilon I)r \in \mathcal{I}\}$ for $\varepsilon = \pm 1$.

Proof. Consider the six-dimensional representation σ of $\mathrm{PSL}_2(\mathbb{Z})$ defined in (3.10). By linearity σ further extends to an algebra homomorphism from $R = \mathbb{C}[\mathrm{PSL}_2(\mathbb{Z})]$ to $\mathbb{C}^{6 \times 6}$, whose first row vanishes on \mathcal{I} because the first rows of both $\sigma(S(T - I)^2)$ and $\sigma((T - I)^2)$ vanish.

We begin by proving that M_1, \dots, M_6 span R/\mathcal{I} . If \vec{M} denotes the column vector $(M_1, \dots, M_6) \in R^6$, then the calculations

$$\begin{aligned} \vec{M} \cdot S &= \begin{pmatrix} S \\ TS \\ T \\ I \\ STS \\ ST \end{pmatrix} = \sigma(S)\vec{M} \quad \text{and} \\ (3.16) \quad \vec{M} \cdot T &= \begin{pmatrix} T \\ T^2 \\ TST \\ ST \\ ST^2 \\ STST \end{pmatrix} = \begin{pmatrix} T & & & & & \\ -1+2T+(T-1)^2 & & & & & \\ 2-ST+S(T-1)^2T^{-1}S & & & & & \\ ST & & & & & \\ 2ST-S+S(T-1)^2 & & & & & \\ 2S-TS+(T-1)^2T^{-1}S & & & & & \end{pmatrix} \\ &= \sigma(T)\vec{M} + (T - I)^2 \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ T^{-1}S \end{pmatrix} + S(T - I)^2 \cdot \begin{pmatrix} 0 \\ 0 \\ T^{-1}S \\ 0 \\ 1 \\ 0 \end{pmatrix} \end{aligned}$$

show that

$$(3.17) \quad \vec{M} \cdot \gamma \in \sigma(\gamma)\vec{M} + \mathcal{I}^6$$

for every $\gamma \in \mathrm{PSL}_2(\mathbb{Z})$. It follows that γ , which is the first entry of $\vec{M} \cdot \gamma$, is a linear combination of M_1, \dots, M_6 plus an element of \mathcal{I} .

To show that M_1, \dots, M_6 are linearly independent in R/\mathcal{I} , we begin by checking that $\sigma(M_i)$ has first row entries that are all 0 except for a 1 in the i -th position. Because the first row of $\sigma(r)$ vanishes for all $r \in \mathcal{I}$, no nontrivial linear combination of M_1, \dots, M_6 can lie in \mathcal{I} , which completes the proof of part (1). (Note also that examining the first row of σ gives a convenient algorithm for reducing elements of $\mathrm{PSL}_2(\mathbb{Z})$ modulo \mathcal{I} .)

Next we prove part (2). Because I, T, TS, S, ST , and STS span R/\mathcal{I} , and S acts on the left by ∓ 1 modulo \mathcal{I}_\pm , we see that I, T , and TS span R/\mathcal{I}_\pm . Now let $\pi: R \rightarrow (R/\mathcal{I}_+) \oplus (R/\mathcal{I}_-)$ be the direct sum of the projections modulo these ideals. Because $\mathcal{I}_+ \cap \mathcal{I}_- = \mathcal{I}$, the kernel of π is \mathcal{I} , and thus R/\mathcal{I} maps injectively to $(R/\mathcal{I}_+) \oplus (R/\mathcal{I}_-)$. We have seen that R/\mathcal{I}_\pm are both at most three-dimensional, while R/\mathcal{I} is six-dimensional by part (1). Thus, $\dim_{\mathbb{C}} R/\mathcal{I}_\pm = 3$, and I, T , and TS form a basis.

All that remains is to prove part (3). Since $(S - \varepsilon I)(S + \varepsilon I) = 0$ and $(S - \varepsilon I)(T - I)^2 r = S(T - 1)^2 r + (T - 1)^2(-\varepsilon r)$ lies in \mathcal{I} for all $r \in R$, it is clear that left multiplication by $S - \varepsilon I$ maps \mathcal{I}_ε to \mathcal{I} . To show the reverse inclusion, suppose that

$$(S - \varepsilon I)r = (T - I)^2 r_1 + S(T - I)^2 r_2 \in \mathcal{I}$$

for some $r, r_1, r_2 \in R$, and hence after multiplying both sides by S ,

$$-\varepsilon(S - \varepsilon I)r = (T - I)^2 r_2 + S(T - I)^2 r_1.$$

Combining, we see that $2(S - \varepsilon I)r = (S - \varepsilon I)(T - I)^2(r_2 - \varepsilon r_1)$ and hence $(S - \varepsilon I)(2r - (T - I)^2(r_2 - \varepsilon r_1)) = 0$. By (3.13), $2r - (T - I)^2(r_2 - \varepsilon r_1) \in (S + \varepsilon I)R$, which implies $r \in \mathcal{I}_\varepsilon$. \square

Note that (3.17) gives us a natural interpretation of σ in terms of the right action of $\mathrm{PSL}_2(\mathbb{Z})$ on the six-dimensional vector space R/\mathcal{I} . From this perspective, the conjugacy between σ and ρ in Section 3.2 means R/\mathcal{I} must decompose into the direct sum of two three-dimensional right R -modules, namely the subspaces $\mathcal{I}_\pm/\mathcal{I}$ of R/\mathcal{I} , which are spanned by $I \pm S$, $(I \pm S)T$, and $(I \pm S)TS$. Here, $\mathcal{I}_-/\mathcal{I}$ corresponds to ρ_3 , while $\mathcal{I}_+/\mathcal{I}$ has a two-dimensional submodule corresponding to ρ_2 , namely $(\mathcal{I}_+ \cap \mathcal{I}_{\mathrm{aug}})/\mathcal{I}$, where $\mathcal{I}_{\mathrm{aug}}$ is the augmentation ideal of R . (Recall that the augmentation ideal is the two-sided ideal generated by $\gamma - I$ with $\gamma \in \mathrm{PSL}_2(\mathbb{Z})$. It follows immediately from the definitions of \mathcal{I}_\pm that $\mathcal{I}_- \subseteq \mathcal{I}_{\mathrm{aug}}$, while $\mathcal{I}_+ \not\subseteq \mathcal{I}_{\mathrm{aug}}$.)

Since $\mathcal{I} = (T - I)^2 \cdot R + S(T - I)^2 \cdot R$ is free as a right R -module, for each $r \in R$ there exist unique column vectors $\vec{N}_1(r), \vec{N}_2(r) \in R^6$ such that

$$(3.18) \quad \vec{M} \cdot r = \sigma(r)\vec{M} + (T - I)^2 \cdot \vec{N}_1(r) + S(T - I)^2 \cdot \vec{N}_2(r).$$

It follows that

$$(3.19) \quad \vec{N}_i(r_1 r_2) = \sigma(r_1)\vec{N}_i(r_2) + \vec{N}_i(r_1) \cdot r_2$$

for $i = 1, 2$ and $r_1, r_2 \in R$, with the cocycle relation (3.19) describing the composition law for multiple applications of (3.18). Repeated applications of (3.19) result in the more general formula

$$(3.20) \quad \begin{aligned} \vec{N}_i(r_1 r_2 \cdots r_n) &= \sigma(r_1 \cdots r_{n-1})\vec{N}_i(r_n) \\ &\quad + \sigma(r_1 \cdots r_{n-2})\vec{N}_i(r_{n-1}) \cdot r_n \\ &\quad + \sigma(r_1 \cdots r_{n-3})\vec{N}_i(r_{n-2}) \cdot r_{n-1} r_n \\ &\quad + \cdots + \vec{N}_i(r_1) \cdot r_2 \cdots r_n \end{aligned}$$

for more than two factors.

LEMMA 3.10. *There exist positive constants C and N such that for all $\gamma \in \mathrm{PSL}_2(\mathbb{Z})$, the entries of $\vec{N}_i(\gamma)$ have the form $\sum_{\delta \in \mathrm{PSL}_2(\mathbb{Z})} n_\delta \delta$, with $\sum_\delta |n_\delta| \leq C \|\gamma\|_{\mathrm{Frob}}^N$ and $\|\delta\|_{\mathrm{Frob}} \leq C \|\gamma\|_{\mathrm{Frob}}$ whenever $n_\delta \neq 0$.*

Proof. Formula (3.19) reduces the claim to $\gamma \in \overline{\Gamma(2)}$, as can be seen by taking $r_2 \in \overline{\Gamma(2)}$ and r_1 one of the six coset representatives of $\overline{\Gamma(2)}$. Lemma 3.3 shows the existence of constants $C, N > 0$ such that the matrix entries of $\sigma(\gamma)$ are bounded by $C \|\gamma\|_{\mathrm{Frob}}^N$ in absolute value. Factor $\gamma = \gamma_1^{e_1} \gamma_2^{f_1} \gamma_1^{e_2} \cdots$, with $\gamma_1 = T^2$ and $\gamma_2 = ST^2S$ as in Lemma 3.2, and refine the factorization to $\gamma = r_1 \cdots r_n$ with $r_i \in \{\gamma_1^{\pm 1}, \gamma_2^{\pm 1}\}$ and $n = |e_1| + |f_1| + |e_2| + \cdots \leq \|\gamma\|_{\mathrm{Frob}}^2$ by part (2) of Lemma 3.2. By part (3) of Lemma 3.2, $\|r_1 r_2 \cdots r_i\|_{\mathrm{Frob}}$ is an increasing function of i , while $\|r_i r_{i+1} \cdots r_n\|_{\mathrm{Frob}}$ is decreasing. Then (3.20) expresses $\vec{N}_i(\gamma)$ as a combination of n terms, each of which satisfies the asserted bounds. \square

Like all group rings, R is equipped with the anti-involution ι that sends $\sum_\gamma c_\gamma \gamma$ to $\sum_\gamma c_\gamma \gamma^{-1}$.

PROPOSITION 3.11. *Define linear functionals $\phi_\pm: R/\mathcal{I}_\pm \rightarrow \mathbb{C}$ on the basis vectors from Proposition 3.9 by setting*

$$(3.21) \quad \phi_\pm(I) = 0, \quad \phi_\pm(T) = 1, \quad \text{and} \quad \phi_\pm(TS) = 0.$$

Then

$$\tilde{\mathcal{I}}_\pm = \{r \in R : \phi_\pm(r' \cdot \iota(r)) = 0 \text{ for all } r' \in R\}.$$

The motivation for the maps ϕ_{\pm} is that they describe the residues in part (3) of Theorem 4.3, and therefore they play a key role in the contour shifts in Section 5.

Proof. Let $\varepsilon = \pm 1$, let $r_1 = T - 2 + T^{-1} - 2\varepsilon S$ and $r_2 = I - \varepsilon STS = I - \varepsilon T^{-1}ST^{-1}$ be the generators of $\tilde{\mathcal{I}}_{\varepsilon}$ from its definition (3.14), and let

$$J_{\varepsilon} = \{r \in R : \phi_{\varepsilon}(r' \cdot \iota(r)) = 0 \text{ for all } r' \in R\},$$

which we will show equals $\tilde{\mathcal{I}}_{\varepsilon}$.

To prove that $\tilde{\mathcal{I}}_{\varepsilon} \subseteq J_{\varepsilon}$, note first that J_{ε} is a right ideal. It will therefore suffice to show that ϕ_{ε} annihilates $\iota(r_i)$, $T\iota(r_i)$, and $TS\iota(r_i)$ for $i = 1, 2$, because I , T , and TS span $R/\mathcal{I}_{\varepsilon}$ by part (2) of Proposition 3.9. We check in succession that

$$\begin{aligned} \phi_{\varepsilon}(S) &= -\varepsilon\phi_{\varepsilon}(I) = 0, \\ \phi_{\varepsilon}(ST) &= -\varepsilon\phi_{\varepsilon}(T) = -\varepsilon, \\ \phi_{\varepsilon}(T^2) &= \phi_{\varepsilon}(2T - I) = 2\phi_{\varepsilon}(T) = 2, \\ \phi_{\varepsilon}(T^{-1}) &= \phi_{\varepsilon}(2I - T) = -\phi_{\varepsilon}(T) = -1, \\ \phi_{\varepsilon}(T^{-1}S) &= \phi_{\varepsilon}((2I - T)S) = 0, \\ \phi_{\varepsilon}(TST) &= \phi_{\varepsilon}(ST^{-1}S) = -\varepsilon\phi_{\varepsilon}(T^{-1}S) = 0, \\ \phi_{\varepsilon}(ST^{-1}) &= -\varepsilon\phi_{\varepsilon}(T^{-1}) = \varepsilon, \\ \phi_{\varepsilon}(T^{-1}ST^{-1}) &= \phi_{\varepsilon}(STS) = -\varepsilon\phi_{\varepsilon}(TS) = 0, \\ \phi_{\varepsilon}(TST^{-1}) &= \phi_{\varepsilon}((2I - T^{-1})ST^{-1}) = 2\varepsilon, \quad \text{and} \\ \phi_{\varepsilon}(T^2ST) &= \phi_{\varepsilon}((2T - I)ST) = \varepsilon. \end{aligned}$$

It is then straightforward to verify by direct calculation that ϕ_{ε} evaluates to zero on $\iota(r_i)$, $T\iota(r_i)$, and $TS\iota(r_i)$, because $\iota(r_1) = r_1$ and $\iota(r_2) = I - \varepsilon ST^{-1}S = I - \varepsilon TST$. Thus, $\tilde{\mathcal{I}}_{\varepsilon} \subseteq J_{\varepsilon}$.

To complete the proof, we will show that $\dim(R/\tilde{\mathcal{I}}_{\varepsilon}) \leq \dim(R/J_{\varepsilon})$. We first note that the map $\psi: R \rightarrow \text{Hom}_{\mathbb{C}}(R/\mathcal{I}_{\varepsilon}, \mathbb{C})$ taking r to $r' \mapsto \phi_{\varepsilon}(r' \cdot \iota(r))$ has kernel J_{ε} by definition and is surjective, because the linear functionals $\psi(I)$, $\psi(S)$, and $\psi(T)$ satisfy

$$\begin{aligned} \psi(I)(I) &= 0, & \psi(I)(T) &= 1, & \psi(I)(TS) &= 0, \\ \psi(S)(I) &= 0, & \psi(S)(T) &= 0, & \psi(S)(TS) &= 1, \\ \psi(T)(I) &= -1, & \psi(T)(T) &= 0, & \psi(T)(TS) &= 2\varepsilon \end{aligned}$$

and hence span the three-dimensional space of linear functionals. Therefore R/J_{ε} is a three-dimensional vector space, and it suffices to show that I , S , and T span $R/\tilde{\mathcal{I}}_{\varepsilon}$.

To prove that I , S , and T span $R/\tilde{\mathcal{I}}_\varepsilon$, we begin by reducing ST , ST^{-1} , TS , T^{-1} , and T^2 to linear combinations of I , S , and T modulo $\tilde{\mathcal{I}}_\varepsilon$ via

$$\begin{aligned}
ST &= \varepsilon S - \varepsilon r_2 S \\
&\equiv \varepsilon S \pmod{\tilde{\mathcal{I}}_\varepsilon}, \\
ST^{-1} &= \varepsilon S + r_2 ST^{-1} \\
&\equiv \varepsilon S \pmod{\tilde{\mathcal{I}}_\varepsilon}, \\
TS &= 2\varepsilon + 2S - T^{-1}S + r_1 S \\
&\equiv 2\varepsilon + 2S - T^{-1}S \pmod{\tilde{\mathcal{I}}_\varepsilon} \\
&= 2\varepsilon + 2S - \varepsilon T + \varepsilon r_2 T \\
&\equiv 2\varepsilon + 2S - \varepsilon T \pmod{\tilde{\mathcal{I}}_\varepsilon}, \\
T^{-1} &= \varepsilon TS - \varepsilon r_2 TS \\
&\equiv \varepsilon TS \equiv 2 + 2\varepsilon S - T \pmod{\tilde{\mathcal{I}}_\varepsilon}, \quad \text{and} \\
T^2 &= 2T - 1 + 2\varepsilon ST + r_1 T \\
&\equiv 2T - 1 + 2\varepsilon ST \pmod{\tilde{\mathcal{I}}_\varepsilon} \\
&\equiv 2T - 1 + 2S \pmod{\tilde{\mathcal{I}}_\varepsilon}.
\end{aligned}$$

Using these relations, we can reduce any $\gamma \in \bar{\Gamma}$ (and therefore any $r \in R$) to a linear combination of I , S , and T , by starting from the left of the reduced word representing γ . \square

4. Solutions of functional equations and modular form kernels

4.1. *The action of R on holomorphic functions and integral kernels.* We begin by recalling a commonly used class of functions on the upper half-plane \mathbb{H} , which appears in the literature dating at least as far back as 1974 in work of Knopp [28]: those satisfying a bound of the form

$$(4.1) \quad |F(\tau)| \leq \alpha (\operatorname{Im}(\tau))^{-\beta} + |\tau|^\gamma$$

for some $\alpha, \beta, \gamma \geq 0$. Such a bound has already appeared in part (3) of Theorem 3.1, and is satisfied by any power series in $e^{\pi i \tau}$ whose coefficients grow more slowly than some polynomial (e.g., the classical modular forms E_k and theta functions from Section 2.1). Conversely, the boundedness condition in the definition of modular form is automatic for functions satisfying (4.1).

Recall also that a function F has *moderate growth* on the symmetric space \mathbb{H} if

$$(4.2) \quad |F(g \cdot i)| \leq C \|g\|^N$$

for some $C, N \geq 0$, where $g \cdot i = \frac{ai+b}{ci+d}$ denotes the action of $g = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{R})$ on $i \in \mathbb{H}$ (with $i^2 = -1$) and $\|\cdot\|$ is some fixed matrix norm on $\mathrm{SL}_2(\mathbb{R})$, such as the Frobenius norm. This notion is independent of the choice of matrix norm.

In fact, moderate growth is equivalent to (4.1). First, note that the notion of moderate growth does not depend on the choice of g : if $g \cdot i = g' \cdot i$ with $g, g' \in \mathrm{SL}_2(\mathbb{R})$, then $g^{-1}g' \in \mathrm{SO}_2(\mathbb{R})$ and hence $\|g\|_{\mathrm{Frob}} = \|g'\|_{\mathrm{Frob}}$. Now to see the equivalence between the two bounds, write $\tau = x + iy$ and let $g_\tau = y^{-1/2} \begin{pmatrix} y & x \\ 0 & 1 \end{pmatrix}$. Then $g_\tau \cdot i = \tau$ and

$$\begin{aligned} \|g_\tau\|_{\mathrm{Frob}}^2 &= y^{-1} + y^{-1}(x^2 + y^2) \\ &\leq y^{-1} + (y^{-2} + (x^2 + y^2)^2)/2 \\ &= O(y^{-2} + (x^2 + y^2)^2). \end{aligned}$$

Thus, moderate growth implies (4.1). For the other direction, we must bound y^{-1} and $x^2 + y^2$ by polynomials in $\|g_\tau\|_{\mathrm{Frob}}^2$. To do so, we note that

$$y^{-1} \leq \frac{1 + x^2 + y^2}{y} = \|g_\tau\|_{\mathrm{Frob}}^2 \quad \text{and} \quad y^2 \leq \left(\frac{1 + x^2 + y^2}{y} \right)^2 = \|g_\tau\|_{\mathrm{Frob}}^4,$$

and hence

$$x^2 + y^2 = y \frac{x^2 + y^2}{y} \leq \frac{1}{2} \left(y^2 + \frac{(x^2 + y^2)^2}{y^2} \right) \leq \|g_\tau\|_{\mathrm{Frob}}^4,$$

as desired.

We accordingly use the term *moderate growth on \mathcal{S}* to describe functions satisfying the bound (4.1) for $\tau \in \mathcal{S} \subseteq \mathbb{H}$. Following Knopp's notation, let

$$(4.3) \quad \mathcal{P} = \{F: \mathbb{H} \rightarrow \mathbb{C} : F \text{ is holomorphic and satisfies (4.1) for all } \tau \in \mathbb{H}\}$$

denote the space of holomorphic functions having moderate growth on the full upper half-plane. In terms of the unit disk model of the hyperbolic plane, \mathcal{P} corresponds to holomorphic functions on $\{z \in \mathbb{C} : |z| < 1\}$ that are bounded in absolute value by $C(1 - |z|)^{-N}$ for some constants $C, N \geq 0$.

LEMMA 4.1. *Let F be a holomorphic function on \mathbb{H} , and $\mathcal{S} \subseteq \mathbb{H}$. If*

$$|F(g \cdot i)| \leq C \|g\|_{\mathrm{Frob}}^N$$

for all $g \in \mathrm{SL}_2(\mathbb{R})$ such that $g \cdot i \in \mathcal{S}$, then

$$|(F|_k \gamma)(g \cdot i)| \leq C \|\gamma\|_{\mathrm{Frob}}^{N+|k|} \|g\|_{\mathrm{Frob}}^{N+2|k|}$$

for all $\gamma, g \in \mathrm{SL}_2(\mathbb{R})$ such that $g \cdot i \in \gamma^{-1}\mathcal{S}$.

In particular, \mathcal{P} is preserved by the slash operation (2.1). It is consequently a representation space for $\mathrm{SL}_2(\mathbb{Z})$, and for $\mathrm{PSL}_2(\mathbb{Z})$ and thus $R = \mathbb{C}[\mathrm{PSL}_2(\mathbb{Z})]$ when k is even (so that $\pm\gamma$ act the same for $\gamma \in \mathrm{SL}_2(\mathbb{Z})$; see [7, Section 1.1.6]).

Proof. The factor of automorphy $j(g, z) = cz + d$ for a matrix $g = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{R})$ and point $z \in \mathbb{H}$ satisfies the bounds $\|g\|_{\mathrm{Frob}}^{-1} \leq |j(g, i)| \leq \|g\|_{\mathrm{Frob}}$. The upper bound is trivial, while the lower bound follows from $\|g\|_{\mathrm{Frob}}^2 > a^2 + b^2 \geq (c^2 + d^2)^{-1}$, where the last inequality $(a^2 + b^2)(c^2 + d^2) \geq 1 = (ad - bc)^2$ is itself a consequence of the Cauchy-Schwarz inequality. Note that this last inequality also shows that $\|g\|_{\mathrm{Frob}} \geq \sqrt{2}$. Let g_τ be some element of $\mathrm{SL}_2(\mathbb{R})$ for which $g_\tau \cdot i = \tau$. The identity $j(g_1 g_2, z) = j(g_1, g_2 z) j(g_2, z)$ shows that $j(\gamma, \tau) = j(\gamma g_\tau, i) / j(g_\tau, i)$, and thus

$$(4.4) \quad |j(\gamma, \tau)|, |j(\gamma, \tau)|^{-1} \leq \|g_\tau\|_{\mathrm{Frob}} \|\gamma g_\tau\|_{\mathrm{Frob}} \leq \|\gamma\|_{\mathrm{Frob}} \|g_\tau\|_{\mathrm{Frob}}^2$$

for all $\gamma \in \mathrm{SL}_2(\mathbb{R})$ and $\tau \in \mathbb{H}$. Now the desired bound follows from the definition

$$(F|_k \gamma)(z) = j(\gamma, z)^{-k} F(\gamma \cdot z)$$

of the slash operation. \square

We now algebraically reformulate the system (3.11) in terms of this action on \mathcal{P} . For simplicity we assume d is a multiple of 4, so that $\mathrm{PSL}_2(\mathbb{Z})$ can act with weight $d/2$. Then if we let $\tilde{F} = i^{-d/2} (e^{\pi i \tau |x|^2} - F)|_{d/2}^\tau S$, system (3.11) becomes

$$(4.5) \quad F|_{d/2}^\tau (T - I)^2 = 0 \quad \text{and} \quad F|_{d/2}^\tau S (T - I)^2 = e^{\pi i \tau |x|^2} |_{d/2}^\tau S (T - I)^2.$$

Since $\mathcal{I} = (T - I)^2 \cdot R + S(T - I)^2 \cdot R$, these equations govern the slash operator action of \mathcal{I} on F in the τ variable. Bounds on F (e.g., to show membership in \mathcal{P}) will be shown in Section 5. Let

$$(4.6) \quad \mathcal{D} = \left\{ z \in \mathbb{H} : \mathrm{Re}(z) \in (-1, 1), \left| z - \frac{1}{2} \right| > \frac{1}{2}, \left| z + \frac{1}{2} \right| > \frac{1}{2} \right\}$$

and

$$(4.7) \quad \mathcal{F} = \{ z \in \mathbb{H} : \mathrm{Re}(z) \in (0, 1), |z| > 1, |z - 1| > 1 \}$$

be the fundamental domains for $\Gamma(2)$ and $\mathrm{SL}_2(\mathbb{Z})$, respectively, which are shown in Figure 4.1 and satisfy

$$(4.8) \quad \overline{\mathcal{D}} = \overline{\mathcal{F} \cup T^{-1}\mathcal{F} \cup STS\mathcal{F} \cup S\mathcal{F} \cup ST^{-1}\mathcal{F} \cup T\mathcal{S}\mathcal{F}}.$$

The following proposition shows that functions with symmetry properties generalizing (4.5) are determined by their behavior on the closure $\overline{\mathcal{D}}$ of \mathcal{D} .

PROPOSITION 4.2. *Let k be an even integer, and let $h_1, h_2: \mathbb{H} \rightarrow \mathbb{C}$ be continuous functions. Then the following hold:*

- (1) *(Analytic continuation) Suppose h_1 and h_2 are holomorphic. Let $\mathcal{O} \subseteq \mathbb{H}$ denote an open neighborhood of $\overline{\mathcal{D}}$, and let $f: \mathcal{O} \rightarrow \mathbb{C}$ be a holomorphic function satisfying the transformation laws*

$$(4.9) \quad f|_k (T - I)^2 = h_1 \quad \text{and} \quad f|_k S (T - I)^2 = h_2$$

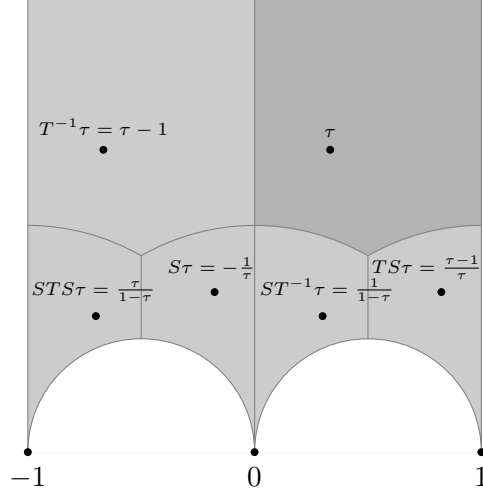


Figure 4.1. The fundamental domain \mathcal{D} for $\Gamma(2)$ defined in (4.6). The six marked points show the images of a point τ in the fundamental domain \mathcal{F} for $\mathrm{SL}_2(\mathbb{Z})$ defined in (4.7).

whenever both sides are defined (that is, on $\mathcal{O} \cap T^{-1}\mathcal{O} \cap T^{-2}\mathcal{O}$ for the first equation, and on $S\mathcal{O} \cap T^{-1}S\mathcal{O} \cap T^{-2}S\mathcal{O}$ for the second equation). Then f extends to a holomorphic function on \mathbb{H} satisfying (4.9).

- (2) (Propagation of the moderate growth bound) Suppose $f: \mathbb{H} \rightarrow \mathbb{C}$ is a continuous function that satisfies the transformation laws (4.9) on \mathbb{H} and grows moderately on \mathcal{D} ; i.e., there exist nonnegative constants C_f and N_f such that

$$(4.10) \quad |f(g \cdot i)| \leq C_f \|g\|_{\mathrm{Frob}}^{N_f}$$

for $g \cdot i \in \mathcal{D}$ (see (4.2)). Suppose also that h_1 and h_2 have moderate growth, and let C_{h_1} , C_{h_2} , N_{h_1} , and N_{h_2} be nonnegative constants such that

$$(4.11) \quad |h_1(g \cdot i)| \leq C_{h_1} \|g\|_{\mathrm{Frob}}^{N_{h_1}} \quad \text{and} \quad |h_2(g \cdot i)| \leq C_{h_2} \|g\|_{\mathrm{Frob}}^{N_{h_2}}$$

for $g \in \mathrm{SL}_2(\mathbb{R})$. Then f has the following moderate growth bound on all of \mathbb{H} : for some constants $C, N \geq 0$ depending only on N_f, N_{h_1}, N_{h_2} , and k ,

$$(4.12) \quad |f(g \cdot i)| \leq C(C_f + C_{h_1} + C_{h_2}) \|g\|_{\mathrm{Frob}}^N$$

for $g \in \mathrm{SL}_2(\mathbb{R})$. In particular, if f, h_1 , and h_2 are all holomorphic, then $f \in \mathcal{P}$.

Proof. For expositional reasons we begin with the proof of part (2). When we refer to a ‘‘constant’’ in this proof, we mean that it can depend only on N_f ,

N_{h_1} , N_{h_2} , and k . By increasing the exponents if necessary, we may assume $N_{h_1} = N_{h_2} = N_f$. Since f is continuous the moderate growth bound (4.10) holds over the closure $\overline{\mathcal{D}}$. Recall the matrices $M_i \in \mathrm{SL}_2(\mathbb{Z})$ from (3.15):

$$(M_1, M_2, M_3, M_4, M_5, M_6) = (I, T, TS, S, ST, STS).$$

It follows from the assumptions and (4.8) that (4.10) holds on $M_1\mathcal{F} = \mathcal{F}$, $M_3\mathcal{F} = TS\mathcal{F}$, $M_4\mathcal{F} = S\mathcal{F}$, and $M_6\mathcal{F} = STS\mathcal{F}$ (i.e., whenever $g \cdot i$ is in these sets). Our first step is to check such an inequality on $M_2\mathcal{F} = T\mathcal{F}$ and $M_5\mathcal{F} = ST\mathcal{F}$.

We can analyze the growth of f on $T\mathcal{F}$ as follows, using f 's moderate growth on $\mathcal{F} \cup T^{-1}\mathcal{F} \subseteq \mathcal{D}$ and the functional equations (4.9). By Lemma 4.1, the moderate growth of f on $T^{-1}\mathcal{F}$ implies that $f|_k T^{-1}$ has moderate growth on \mathcal{F} , with suitably adjusted constants as in the lemma, and the moderate growth of h_1 from (4.11) implies that $h_1|_k T^{-1}$ also has moderate growth. Now we write $f|_k T = f|_k(2I - T^{-1}) + h_1|_k T^{-1}$ by (4.9), to deduce that $f|_k T$ has moderate growth on \mathcal{F} ; hence f has moderate growth on $T\mathcal{F}$ by Lemma 4.1 again. Written out more explicitly, $|f(g \cdot i)| \leq (c_1 C_f + c_2 C_{h_1}) \|g\|_{\mathrm{Frob}}^{N_f + 4|k|}$ on $M_2\mathcal{F} = T\mathcal{F}$, for some constants $c_1, c_2 > 0$. Likewise, the moderate growth on $S\mathcal{F}$ and $ST^{-1}\mathcal{F}$ implies a bound of the form $|f(g \cdot i)| \leq (c'_1 C_f + c'_2 C_{h_2}) \|g\|_{\mathrm{Frob}}^{N_f + 4|k|}$ on $M_5\mathcal{F} = (ST^2)T^{-1}\mathcal{F} = ST\mathcal{F}$, for some constants $c'_1, c'_2 > 0$. Thus, by Lemma 4.1, there exist constants $C_1, N_1 \geq 0$ such that

$$(4.13) \quad |(f|_k M_j)(g \cdot i)| \leq C_1 (C_f + C_{h_1} + C_{h_2}) \|g\|_{\mathrm{Frob}}^{N_1}$$

for $g \cdot i \in \overline{\mathcal{F}}$ and each $j \leq 6$.

For $\tau \in \mathbb{H}$ choose $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z})$ such that $w := \gamma^{-1} \cdot \tau \in \overline{\mathcal{F}}$. Consider (3.18) with $r = \gamma$, so that $\gamma = I \cdot \gamma$ is the first entry of $\sigma(\gamma)\vec{M} + (T - I)^2 \cdot \vec{N}_1(\gamma) + S(T - I)^2 \cdot \vec{N}_2(\gamma)$. We next bound $(f|_k \gamma)(w)$ by expanding it according to this last decomposition. Write the matrix entries of $\sigma(\gamma)$ as $\sigma(\gamma)_{ij}$, and the first vector entries of $\vec{N}_1(\gamma)$ and $\vec{N}_2(\gamma)$ as $\sum_{\delta \in \mathrm{PSL}_2(\mathbb{Z})} n_\delta \delta$ and $\sum_{\delta \in \mathrm{PSL}_2(\mathbb{Z})} n'_\delta \delta$, respectively (bounds on these quantities are given in Lemmas 3.3 and 3.10). Let g_τ and $g_w = \gamma^{-1} g_\tau$ be matrices in $\mathrm{SL}_2(\mathbb{R})$ which map i to τ and w , respectively. Then

$$(4.14) \quad \begin{aligned} (cw + d)^{-k} f(\tau) &= (f|_k \gamma)(g_w \cdot i) \\ &= \sum_{j \leq 6} \sigma(\gamma)_{1j} (f|_k M_j)(g_w \cdot i) \\ &\quad + \sum_{\delta \in \mathrm{PSL}_2(\mathbb{Z})} (n_\delta (h_1|_k \delta)(g_w \cdot i) + n'_\delta (h_2|_k \delta)(g_w \cdot i)). \end{aligned}$$

Invoking (4.10) and (4.11), along with Lemma 4.1 and (4.13), yields the bound

$$\begin{aligned} |(cw + d)^{-k} f(\tau)| &\leq C_2(C_f + C_{h_1} + C_{h_2}) \sum_{j \leq 6} |\sigma(\gamma)_{1j}| \|g_w\|_{\text{Frob}}^{N_2} \\ &\quad + \sum_{\delta} (|n_{\delta}| + |n'_{\delta}|) \|\delta\|_{\text{Frob}}^{N_2} \|g_w\|_{\text{Frob}}^{N_2} \end{aligned}$$

for some constants $C_2, N_2 \geq 0$. The estimates from Lemmas 3.3 and 3.10 show that the sums are at most $C_3 \|\gamma\|_{\text{Frob}}^{N_3} \|g_w\|_{\text{Frob}}^{N_3}$ for some constants $C_3, N_3 \geq 0$. The factor of automorphy $cw + d = j(\gamma, w)$ has a bound of the same form in (4.4), and thus

$$|f(\tau)| \leq C_4(C_f + C_{h_1} + C_{h_2}) \|\gamma\|_{\text{Frob}}^{N_4} \|g_w\|_{\text{Frob}}^{N_4}$$

for some constants $C_4, N_4 \geq 0$.

We now claim that for z in the standard “keyhole” fundamental domain $\{z \in \mathbb{H} : |z| \geq 1, -\frac{1}{2} \leq \text{Re}(z) \leq \frac{1}{2}\}$,

$$(4.15) \quad \|g_z\|_{\text{Frob}} \leq \|\delta g_z\|_{\text{Frob}}$$

for all $\delta \in \text{SL}_2(\mathbb{Z})$, where g_z is some matrix in $\text{SL}_2(\mathbb{R})$ with $g_z \cdot i = z$ (this defines g_z uniquely up to right multiplication by an element of $\text{SO}_2(\mathbb{R})$, so the quantities on both sides of inequality are independent of such a choice). Indeed, writing $z = x + iy$ and $\delta = \begin{pmatrix} p & q \\ r & s \end{pmatrix}$, we may take $g_z = y^{-1/2} \begin{pmatrix} y & x \\ 0 & 1 \end{pmatrix}$, compute the norms squared, and reduce the claim to showing that

$$(x^2 + y^2 - 1)(p^2 + r^2 - 1) + p^2 + q^2 + r^2 + s^2 + 2x(pq + rs) - 2 \geq 0$$

for all $\delta \in \text{SL}_2(\mathbb{Z})$. Using the defining inequalities on z , the expression on the left is at least $p^2 - |pq| + q^2 + r^2 - |rs| + s^2 - 2$, which is nonnegative because the rows of δ are nonzero and the integral quadratic form $m^2 - mn + n^2$ takes positive integer values on integer pairs $(m, n) \neq (0, 0)$.

Half of the fundamental domain \mathcal{F} lies in the keyhole fundamental domain, while the other half lies in its translate by T . Therefore (4.15) and the submultiplicativity of the Frobenius norm imply that there exists a positive constant C'' such that

$$\|g_w\|_{\text{Frob}} \leq C'' \|\delta g_w\|_{\text{Frob}}$$

for all $\delta \in \text{SL}_2(\mathbb{Z})$. Now we can use the inequality

$$\|\gamma\|_{\text{Frob}} \leq \|g_{\tau}\|_{\text{Frob}} \|g_w^{-1}\|_{\text{Frob}} = \|g_{\tau}\|_{\text{Frob}} \|g_w\|_{\text{Frob}} \leq C'' \|g_{\tau}\|_{\text{Frob}}^2$$

(the second step using the fact $\|g_w\|_{\text{Frob}} = \|g_w^{-1}\|_{\text{Frob}}$ for $g_w \in \text{SL}_2(\mathbb{R})$) to deduce that

$$\begin{aligned} |f(\tau)| &\leq C_4(C_f + C_{h_1} + C_{h_2}) \|\gamma\|_{\text{Frob}}^{N_4} \|g_w\|_{\text{Frob}}^{N_4} \\ &\leq C_4(C_f + C_{h_1} + C_{h_2}) (C'')^{N_4} \|g_{\tau}\|_{\text{Frob}}^{3N_4}, \end{aligned}$$

which completes the proof of part (2).

We now turn to the proof of part (1), which shares similar ingredients but instead works with a different basis for R/\mathcal{I} , namely the entries of the column vector

$$\vec{M}' = (M'_1, M'_2, M'_3, M'_4, M'_5, M'_6) = (I, T^{-1}, STS, S, ST^{-1}, TS)$$

coming from (4.8) (i.e., specifying the translates of \mathcal{F} that tile \mathcal{D}). Checking that \vec{M}' consists of a basis amounts to observing that $T^{-1} \equiv 2I - T \pmod{\mathcal{I}}$ and $ST^{-1} \equiv 2S - ST \pmod{\mathcal{I}}$.

As was the case in (3.18), there exist a representation $\sigma': \mathrm{PSL}_2(\mathbb{Z}) \rightarrow \mathrm{GL}_6(\mathbb{Z})$ and maps $\vec{N}'_i: \mathrm{PSL}_2(\mathbb{Z}) \rightarrow R^6$ such that

$$(4.16) \quad \vec{M}' \cdot \gamma = \sigma'(\gamma)\vec{M}' + (T - I)^2 \cdot \vec{N}'_1(\gamma) + S(T - I)^2 \cdot \vec{N}'_2(\gamma)$$

for all $\gamma \in \mathrm{PSL}_2(\mathbb{Z})$, and such that these maps satisfy the analogous cocycle relation to (3.19). In particular, \vec{M}' is an integral change of basis from \vec{M} modulo \mathcal{I}^6 , and thus σ' is the corresponding conjugate of σ .

By shrinking \mathcal{O} if necessary, we assume that its only $\Gamma(2)$ -translates which intersect it are $T^2\mathcal{O}$, $T^{-2}\mathcal{O}$, $ST^2S\mathcal{O}$, and $ST^{-2}S\mathcal{O}$ (coming from the boundaries of \mathcal{D}). There exists an open neighborhood $\mathcal{O}_{\mathcal{F}}$ of $\overline{\mathcal{F}}$ such that $\bigcup_{j \leq 6} M'_j \mathcal{O}_{\mathcal{F}} \subseteq \mathcal{O}$; in particular, $f|_k M'_j$ is defined on $\mathcal{O}_{\mathcal{F}}$ for each $j \leq 6$. By shrinking $\mathcal{O}_{\mathcal{F}}$ if necessary, we may assume that $\gamma \mathcal{O}_{\mathcal{F}}$ intersects $\mathcal{O}_{\mathcal{F}}$ with $\gamma \in \mathrm{PSL}_2(\mathbb{Z})$ only when $\gamma \overline{\mathcal{F}}$ and $\overline{\mathcal{F}}$ share a boundary point. Accordingly, let

$$\begin{aligned} \Omega &= \{\omega \in \mathrm{PSL}_2(\mathbb{Z}) : \omega \mathcal{O}_{\mathcal{F}} \cap \mathcal{O}_{\mathcal{F}} \neq \emptyset\} \\ &= \{S, T, T^{-1}, ST^{-1}, TS, TST^{-1}\}. \end{aligned}$$

Consider a pair $\tau, \tau' \in \mathcal{O}_{\mathcal{F}}$ such that $\tau' = \omega \tau$ for some $\omega \in \Omega$. We claim for each $i \leq 6$ that

$$(4.17) \quad \begin{aligned} (f|_k M'_i \omega)(\tau) &= \sum_{j \leq 6} \sigma'_{ij}(\omega) (f|_k M'_j)(\tau) \\ &\quad + (h_1|_k N'_{1i}(\omega))(\tau) + (h_2|_k N'_{2i}(\omega))(\tau), \end{aligned}$$

where $\sigma'_{ij}(\omega)$ denote the matrix entries of $\sigma'(\omega)$, and $N'_{1i}(\omega)$ and $N'_{2i}(\omega)$ denote the vector entries of $\vec{N}'_1(\omega)$ and $\vec{N}'_2(\omega)$, respectively. This claim would follow immediately from (4.16) if we knew we could apply the functional equations (4.9), and so all we must do is to verify the hypotheses of (4.9), namely that $\gamma \tau \in \mathcal{O} \cap T^{-1}\mathcal{O} \cap T^{-2}\mathcal{O}$ for every term γ that occurs in $N'_{1i}(\omega)$, and $\gamma \tau \in S\mathcal{O} \cap T^{-1}S\mathcal{O} \cap T^{-2}S\mathcal{O}$ for every term γ in $N'_{2i}(\omega)$. To begin, we write (4.16) as

$$(4.18) \quad M'_i \omega - \sum_{j \leq 6} \sigma'_{ij}(\omega) M'_j = (T - I)^2 N'_{1i}(\omega) + S(T - I)^2 N'_{2i}(\omega).$$

Similarly to (3.16), it is straightforward to check for each possible choice of i and ω that either $N'_{1i}(\omega) = N'_{2i}(\omega) = 0$, in which case the hypotheses of (4.9)

hold vacuously and (4.17) follows, or one of $N'_{1i}(\omega)$ and $N'_{2i}(\omega)$ is zero and the other is a group element $\gamma \in \mathrm{PSL}_2(\mathbb{Z})$. In other words, the right side of (4.18) is of the form $(T - I)^2\gamma$ or $S(T - I)^2\gamma$ with $\gamma \in \mathrm{PSL}_2(\mathbb{Z})$ whenever it is nonzero. Since $M'_i\omega\tau = M'_i\tau'$ and all $M'_j\tau$ lie in \mathcal{O} , all the terms on the left side of (4.18) map τ to points in \mathcal{O} ; therefore τ is mapped to \mathcal{O} by all of $T^2\gamma, T\gamma, \gamma$ or $ST^2\gamma, ST\gamma, S\gamma$ (depending on which form the right side has). This assertion is the hypothesis needed for (4.9) to apply at the point $\gamma\tau$, and (4.17) follows by applying the slash operator to f .

Having shown (4.17), we now extend f to arbitrary $w \in \mathbb{H}$ by imitating (4.14) (but with slightly different notation). Namely, we write w as $\gamma\tau$ with $\tau \in \mathcal{O}_{\mathcal{F}}$ and $\gamma \in \mathrm{SL}_2(\mathbb{Z})$, and we define $f(w)$ by

$$j(\gamma, \tau)^{-k} f(w) = \sum_{j \leq 6} \sigma'_{1j}(\gamma) (f|_k M'_j)(\tau) + (h_1|_k N'_{11}(\gamma))(\tau) + (h_2|_k N'_{21}(\gamma))(\tau),$$

where as usual $j(\gamma, \tau)$ is the factor of automorphy from (2.2). That $f(w)$ is well defined follows from (4.17) and the cocycle relation for σ', \vec{N}'_1 , and \vec{N}'_2 analogous to (3.19). Specifically, suppose that $w = \gamma\tau = \gamma'\tau'$, with $\tau, \tau' \in \mathcal{O}_{\mathcal{F}}$ and $\gamma, \gamma' \in \mathrm{PSL}_2(\mathbb{Z})$. Then $\tau' = \omega\tau$ for some $\omega \in \Omega$, and hence $\gamma = \gamma'\omega$. Starting with the definition of $j(\gamma, \tau)^{-k} f(w)$ given above, we expand the right side using $\sigma'(\gamma) = \sigma'(\gamma')\sigma'(\omega)$ and the cocycle relations to obtain

$$\begin{aligned} & \sum_{i \leq 6} \sigma'_{1i}(\gamma') \left(\sum_{j \leq 6} \sigma'_{ij}(\omega) (f|_k M'_j)(\tau) + (h_1|_k N'_{1i}(\omega))(\tau) + (h_2|_k N'_{2i}(\omega))(\tau) \right) \\ & + (h_1|_k N'_{11}(\gamma')\omega)(\tau) + (h_2|_k N'_{21}(\gamma')\omega)(\tau). \end{aligned}$$

Applying (4.17) to the expression in parentheses shows that $j(\gamma, \tau)^{-k} f(w)$ equals

$$\sum_{i \leq 6} \sigma'_{1i}(\gamma') (f|_k M'_i\omega)(\tau) + (h_1|_k N'_{11}(\gamma')\omega)(\tau) + (h_2|_k N'_{21}(\gamma')\omega)(\tau),$$

or equivalently

$$j(\omega, \tau)^{-k} \left(\sum_i \sigma'_{1i}(\gamma') (f|_k M'_i) + (h_1|_k N'_{1i}(\gamma')) + (h_2|_k N'_{2i}(\gamma')) \right) (\omega\tau).$$

Finally, using $\omega\tau = \tau'$ and $j(\gamma, \tau) = j(\gamma', \tau')j(\omega, \tau)$ yields

$$j(\gamma', \tau')^{-k} f(w) = \sum_i \sigma'_{1i}(\gamma') (f|_k M'_i)(\tau') + (h_1|_k N'_{1i}(\gamma'))(\tau') + (h_2|_k N'_{2i}(\gamma'))(\tau'),$$

which is the definition of $f(w)$ as we would obtain by using τ' and γ' . Therefore $f(w)$ is well defined.

We have now defined a holomorphic function on \mathbb{H} agreeing with f on the open neighborhood $\bigcup_{i \leq 6} M'_i \mathcal{O}_{\mathcal{F}}$ of \mathcal{D} (and thus also the original neighborhood

\mathcal{O}). Since the holomorphic identity (4.9) holds for the original function, it must hold for the extension as well. \square

Equation (4.5) recasts the interpolation formula (1.4) from Theorem 1.7 in terms of properties of the function $F: \mathbb{H} \times \mathbb{R}^d \rightarrow \mathbb{R}$. To construct F , we make the Ansatz that $\widetilde{F}|_{d/2}^\tau S$ can (essentially) be written as a Laplace transform, which is equivalent to a contour integral construction introduced by Viazovska in her work on sphere packing [47] and motivated by cycle integrals of modular forms appearing in [18]. Specifically, we will construct an integral kernel \mathcal{K} on $\mathbb{H} \times \mathbb{H}$ such that

$$(4.19) \quad F(\tau, x) = e^{\pi i \tau |x|^2} + 4 \sin(\pi |x|^2 / 2)^2 \int_0^\infty \mathcal{K}(\tau, it) e^{-\pi |x|^2 t} dt,$$

at least for $|x|$ sufficiently large and τ inside the fundamental domain \mathcal{F} for the action of $\mathrm{SL}_2(\mathbb{Z})$ on \mathbb{H} defined in (4.7). Such a formula requires initially restricting τ , because the kernel $\mathcal{K}(\tau, z)$ will have poles; see part (1) of Theorem 4.3. This is the reason we have taken the fundamental domain \mathcal{F} to be different from the usual keyhole fundamental domain for $\mathrm{SL}_2(\mathbb{Z}) \backslash \mathbb{H}$, so that in particular \mathcal{F} does not intersect the imaginary axis $z = it$.

It is natural here to decompose the proposed kernel into eigenfunctions of $|_{d/2}^\tau S$ as $\mathcal{K} = \frac{1}{2}(\mathcal{K}_+ + \mathcal{K}_-)$ using (3.12), where

$$(4.20) \quad \mathcal{K}_\pm(\tau, z) := \mathcal{K}(\tau, z) |_{d/2}^\tau (I \mp S).$$

Note that \mathcal{K}_\pm has eigenvalue ∓ 1 under $|_{d/2}^\tau S$, not ± 1 . However, the notation is consistent with our use of signs elsewhere, such as in part (2) of the next theorem. This labeling reflects the fact that \mathcal{K}_\pm contributes to the decomposition of F into eigenfunctions of the Fourier transform with eigenvalue ± 1 . In terms of the relationship $\widetilde{F} = (e^{\pi i \tau |x|^2} - F)|_{d/2}^\tau S$ between \widetilde{F} and F when d is a multiple of 8, the right side contains $-F|_{d/2}^\tau S$, which introduces an extra minus sign.

The next result, which is proved in Section 4.4, shows the existence of a kernel \mathcal{K} that will be used to construct the solution F of the functional equations (4.5) via (4.19) and later extensions of this formula.

THEOREM 4.3. *For dimensions $d = 8$ and 24 there exist unique meromorphic functions $\mathcal{K} = \mathcal{K}^{(d)}$ and $\mathcal{K}_\pm = \mathcal{K}_\pm^{(d)}$ for $d = 8$ and 24 (related by (4.20)) on $\mathbb{H} \times \mathbb{H}$ satisfying the following properties.*

- (1) *For fixed $z \in \mathbb{H}$ the poles of $\mathcal{K}(\tau, z)$ and $\mathcal{K}_\pm(\tau, z)$ in τ are all simple and contained in the $\mathrm{SL}_2(\mathbb{Z})$ -orbit of z .*
- (2) *The kernel \mathcal{K} satisfies the functional equations*

$$\mathcal{K}(\tau, z) |_{d/2}^\tau (T - I)^2 = 0 \quad \text{and} \quad \mathcal{K}(\tau, z) |_{d/2}^\tau S(T - I)^2 = 0;$$

that is, $\mathcal{K}|_{d/2}^\tau r = 0$ for all $r \in \mathcal{I}$. Also, \mathcal{K}_+ and \mathcal{K}_- satisfy the functional equations

$$\mathcal{K}_\pm(\tau, z) |_{d/2}^\tau (T - I)^2 = 0 \quad \text{and} \quad \mathcal{K}_\pm(\tau, z) |_{d/2}^\tau (S \pm I) = 0;$$

that is, $\mathcal{K}_\pm|_{d/2}^\tau r = 0$ for all $r \in \mathcal{I}_\pm$.

(3) For $z \in \mathbb{H}$ and $r \in R$, the residues of \mathcal{K} and \mathcal{K}_\pm as functions of τ satisfy

$$\text{Res}_{\tau=z} \left(\mathcal{K}|_{d/2}^\tau r \right) = -\frac{1}{2\pi} \phi(r)$$

and

$$\text{Res}_{\tau=z} \left(\mathcal{K}_\pm|_{d/2}^\tau r \right) = -\frac{1}{2\pi} \phi_\pm(r),$$

where $\phi: R/\mathcal{I} \rightarrow \mathbb{C}$ is the linear map defined by

$$\begin{aligned} \phi(I) &= 0, & \phi(T) &= 1, & \phi(TS) &= 0, \\ \phi(S) &= 0, & \phi(ST) &= 0, & \phi(STS) &= 0 \end{aligned}$$

and $\phi_\pm: R/\mathcal{I}_\pm \rightarrow \mathbb{C}$ is the linear map from (3.21) defined by

$$\phi_\pm(I) = 0, \quad \phi_\pm(T) = 1, \quad \phi_\pm(TS) = 0.$$

(4) The functions

$$\Delta(\tau)\Delta(z)(j(\tau) - j(z))\mathcal{K}_\pm^{(8)}(\tau, z)$$

and

$$\Delta(\tau)\Delta(z)^2(j(\tau) - j(z))\mathcal{K}_\pm^{(24)}(\tau, z)$$

are in the class \mathcal{P} both as functions of τ and z . Furthermore, for z fixed the kernels satisfy the bounds

$$(4.21) \quad \mathcal{K}_\pm^{(8)}(\tau, z) = O(|\tau e^{2\pi i\tau}|) \quad \text{and} \quad \mathcal{K}_\pm^{(24)}(\tau, z) = O(|\tau e^{4\pi i\tau}|)$$

as $\text{Im}(\tau) \rightarrow \infty$.

It is not difficult to check that the functional equations for \mathcal{K}_\pm in part (2) are equivalent to those for \mathcal{K} , and the same is true for the residue calculations in part (3). We have stated both cases for completeness.

Our first step in proving Theorem 4.3 is to solve the functional equations satisfied by \mathcal{K}_\pm . Part (2) of the theorem asserts that $\mathcal{K}_\pm(\tau, z) |_{d/2}^\tau r = 0$ for all $r \in \mathcal{I}_\pm$, and we will see in Proposition 4.10 that $\mathcal{K}_\pm(\tau, z) |_{2-d/2}^z r = 0$ for all $r \in \tilde{\mathcal{I}}_\pm$. Furthermore, part (4) reduces the problem to the case of functions in \mathcal{P} , with the factors of $\Delta(\tau)$ and $\Delta(z)$ changing the weights of the actions in τ and z .

4.2. *Functions in \mathcal{P} annihilated by \mathcal{I}_\pm and $\tilde{\mathcal{I}}_\pm$.* Given a right ideal J of $R = \mathbb{C}[\mathrm{PSL}_2(\mathbb{Z})]$ and an even integer k , let

$$\mathrm{Ann}_k(J, \mathcal{P}) = \{f \in \mathcal{P} : f|_k r = 0 \text{ for all } r \in J\}.$$

The following four propositions describe $\mathrm{Ann}_k(J, \mathcal{P})$ for $J = \mathcal{I}_\pm = (S \pm I) \cdot R + (T - I)^2 \cdot R$ and $\tilde{\mathcal{I}}_\pm = (T - 2 + T^{-1} \mp 2S) \cdot R + (I \mp STS) \cdot R$ from (3.14).

PROPOSITION 4.4. *Let k be an even integer. The space $\mathrm{Ann}_k(\mathcal{I}_+, \mathcal{P})$, i.e., the solutions $f \in \mathcal{P}$ to the system*

$$(4.22) \quad f|_k(T - I)^2 = 0 \quad \text{and} \quad f|_k(S + I) = 0,$$

is equal to

$$(4.23) \quad \varphi_2 \mathcal{M}_{k-2}(\mathrm{SL}_2(\mathbb{Z})) + \varphi_0 \mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z})) + \varphi_{-2} \mathcal{M}_{k+2}(\mathrm{SL}_2(\mathbb{Z})),$$

where

$$\varphi_2(\tau) = \tau E_2(\tau)^2 - \frac{6i}{\pi} E_2(\tau), \quad \varphi_0(\tau) = \tau E_2(\tau) - \frac{3i}{\pi}, \quad \text{and} \quad \varphi_{-2}(\tau) = \tau.$$

In particular, the dimension of the space of solutions equals $\max(0, \lceil \frac{k}{4} \rceil + 1)$.

Proof. Suppose that $f \in \mathcal{P}$ is a solution to (4.22). Set

$$g_0 := f|_k(T - I), \quad g_1 := f, \quad \text{and} \quad g_2 := f|_k(T - I)S,$$

from which it follows that

$$(4.24) \quad \begin{aligned} \begin{pmatrix} g_0|_k T \\ g_1|_k T \\ g_2|_k T \end{pmatrix} &= \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 2 & 1 \end{pmatrix} \begin{pmatrix} g_0 \\ g_1 \\ g_2 \end{pmatrix} \quad \text{and} \\ \begin{pmatrix} g_0|_k S \\ g_1|_k S \\ g_2|_k S \end{pmatrix} &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} g_0 \\ g_1 \\ g_2 \end{pmatrix}. \end{aligned}$$

Define h_0, h_1, h_2 by

$$(4.25) \quad \begin{pmatrix} h_0(\tau) \\ h_1(\tau) \\ h_2(\tau) \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ -2\tau & 2 & 0 \\ \tau^2 & -2\tau & 1 \end{pmatrix} \begin{pmatrix} g_0(\tau) \\ g_1(\tau) \\ g_2(\tau) \end{pmatrix}.$$

Denote the above matrix by $M(\tau)$, and the column vectors by $H(\tau)$ and $G(\tau)$, so that $H(\tau) = M(\tau)G(\tau)$, and denote the matrices from (4.24) for the actions of $|_k T$ and $|_k S$ on G by T_G and S_G , respectively. Then

$$(H|_k T)(\tau) = M(\tau + 1)T_G M(\tau)^{-1}H(\tau) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} H(\tau) = H(\tau)$$

and

$$(H|_k S)(\tau) = M(-1/\tau)S_G M(\tau)^{-1}H(\tau) = \begin{pmatrix} \tau^2 & \tau & 1 \\ 0 & 1 & 2/\tau \\ 0 & 0 & 1/\tau^2 \end{pmatrix} H(\tau).$$

In other words,

$$(4.26) \quad \begin{aligned} h_2|_{k-2}T &= h_2 & h_2|_{k-2}S &= h_2 \\ h_1|_kT &= h_1, & (h_1|_kS)(\tau) &= h_1(\tau) + 2\tau^{-1}h_2(\tau), \\ h_0|_{k+2}T &= h_0, & \text{and } (h_0|_{k+2}S)(\tau) &= h_0(\tau) + \tau^{-1}h_1(\tau) + \tau^{-2}h_2(\tau). \end{aligned}$$

Therefore, $h_2 \in \mathcal{M}_{k-2}(\mathrm{SL}_2(\mathbb{Z}))$ because of this invariance and since it has moderate growth (it is an element of \mathcal{P}). It follows from (2.8) and the transformation properties of h_1 that $h_1 - \frac{\pi i}{3}h_2E_2 \in \mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z}))$; in particular, h_1 is a quasimodular form of weight k and depth at most 1 for $\mathrm{SL}_2(\mathbb{Z})$. Similarly, $h_0 - \frac{\pi i}{6}h_1E_2 - \frac{\pi^2}{36}h_2E_2^2 \in \mathcal{M}_{k+2}(\mathrm{SL}_2(\mathbb{Z}))$, and h_0 is therefore a quasimodular form of weight $k+2$ and depth at most 2 for $\mathrm{SL}_2(\mathbb{Z})$.

Thus we have shown the existence of modular forms $f_0 \in \mathcal{M}_{k+2}(\mathrm{SL}_2(\mathbb{Z}))$, $f_1 \in \mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z}))$, and $f_2 \in \mathcal{M}_{k-2}(\mathrm{SL}_2(\mathbb{Z}))$ such that $h_0 = f_0 + f_1E_2 + f_2E_2^2$. Expanding and comparing with the last transformation law for $h_0|_{k+2}S$ in (4.26), we deduce from the periodicity of h_0 , h_1 , and h_2 that $h_1 = -\frac{6i}{\pi}(f_1 + 2f_2E_2)$ and $h_2 = -\frac{36}{\pi^2}f_2$, and thus

$$f = g_1 = \tau h_0 + \frac{1}{2}h_1 = \varphi_{-2}f_0 + \varphi_0f_1 + \varphi_2f_2.$$

Hence f lies in (4.23), and it is straightforward to verify that all elements of (4.23) satisfy the conditions in (4.22). Finally, the dimension assertion follows directly from (2.4). \square

PROPOSITION 4.5. *Let k be an even integer. The space $\mathrm{Ann}_k(\mathcal{I}_-, \mathcal{P})$, i.e., the space of solutions $f \in \mathcal{P}$ to the system*

$$(4.27) \quad f|_k(T-I)^2 = 0 \quad \text{and} \quad f|_k(S-I) = 0,$$

is equal to

$$(4.28) \quad \psi_4 \mathcal{M}_{k-4}(\mathrm{SL}_2(\mathbb{Z})) + \psi_2 \mathcal{M}_{k-2}(\mathrm{SL}_2(\mathbb{Z})) + \psi_0 \mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z})),$$

where

$$\psi_4 = \xi_4 \cdot \mathcal{L} + (\xi_4|_4S) \cdot \mathcal{L}_S, \quad \psi_2 = \xi_2 \cdot \mathcal{L} + (\xi_2|_2S) \cdot \mathcal{L}_S, \quad \text{and} \quad \psi_0 = 1,$$

with

$$\xi_4 = U^2 + W^2 - 2V^2 \quad \text{and} \quad \xi_2 = U + W$$

defined in terms of the theta functions in (2.9). In particular, the dimension of the space of solutions equals $\max(0, \lceil \frac{k-2}{4} \rceil + 1)$.

Proof. As with the proof of Proposition 4.4, it is straightforward to use (2.11) and (2.17) to verify that all elements of (4.28) satisfy (4.27), as well as to deduce the dimension formula from (2.4). Thus we will show that any solution $f \in \mathcal{P}$ to (4.27) lies in (4.28). Set $h_0 := f$, $h_1 := f|_k(T - I)S$, and $h_2 := f|_k(T - I)$, from which it follows that

$$\begin{pmatrix} h_0|_k T \\ h_1|_k T \\ h_2|_k T \end{pmatrix} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} h_0 \\ h_1 \\ h_2 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} h_0|_k S \\ h_1|_k S \\ h_2|_k S \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} h_0 \\ h_1 \\ h_2 \end{pmatrix}.$$

From this we see that $h_2|_k T$ and $h_2|_k(ST^2S)$ equal h_2 ; since $f \in \mathcal{P}$, $h_2(\tau) = f(\tau + 1) - f(\tau)$ grows at most polynomially as $\text{Im}(\tau) \rightarrow \infty$ and hence $h_2 \in \mathcal{M}_k(\Gamma_0(2))$, where $\Gamma_0(2) = \langle T, ST^2S \rangle$ is the subgroup of matrices in $\text{SL}_2(\mathbb{Z})$ whose bottom-left entries are even. Furthermore, $h_2|_k(I + S + ST) = 0$ and h_0 satisfies the system

$$(4.29) \quad h_0|_k(S - I) = 0 \quad \text{and} \quad h_0|_k(T - I) = h_2.$$

A solution to (4.29) is given by the function

$$g_0 := \frac{1}{i\pi} (h_2 \cdot \mathcal{L} + h_1 \cdot \mathcal{L}_S),$$

as can be seen by inserting the transformation laws (2.17), and thus $h_0 - g_0 \in \mathcal{M}_k(\text{SL}_2(\mathbb{Z}))$, since it satisfies the homogeneous version of (4.29) and inherits polynomial growth from \mathcal{P} and (2.16).

Thus

$$f = h_0 = h \cdot \mathcal{L} + (h|_k S) \cdot \mathcal{L}_S + g,$$

where $h = \frac{1}{i\pi} h_2 \in \mathcal{M}_k(\Gamma_0(2))$ satisfies $h|_k(I + S + ST) = 0$, and $g \in \mathcal{M}_k(\text{SL}_2(\mathbb{Z}))$. We now invoke (2.13) and write h uniquely as

$$h = f_1 + Uf_2 + Vf_3 + U^2f_4 + V^2f_5 + UVWf_6,$$

where $f_1 \in \mathcal{M}_k(\text{SL}_2(\mathbb{Z}))$, $f_2, f_3 \in \mathcal{M}_{k-2}(\text{SL}_2(\mathbb{Z}))$, $f_4, f_5 \in \mathcal{M}_{k-4}(\text{SL}_2(\mathbb{Z}))$, and $f_6 \in \mathcal{M}_{k-6}(\text{SL}_2(\mathbb{Z}))$. Using (2.11), we can compute the set of all solutions to the system $h|_k(I + S + ST) = h|_k(T - I) = 0$ in $\mathcal{M}_k(\Gamma(2))$. For instance, the latter condition alone forces $f_6 = f_4 = 0$ and $f_2 = -2f_3$. We find that the space of solutions is $\xi_4 \mathcal{M}_{k-4}(\text{SL}_2(\mathbb{Z})) + \xi_2 \mathcal{M}_{k-2}(\text{SL}_2(\mathbb{Z}))$, which then implies f lies in (4.28). \square

For small values of k the solution spaces in Propositions 4.4 and 4.5 are small enough to rule out certain asymptotic behavior. For example, the following lemma, which is used below to show various uniqueness statements, can be proved by direct computation of asymptotics as $\text{Im}(\tau) \rightarrow \infty$ using q -expansions.

LEMMA 4.6. *No nonzero $f \in \text{Ann}_4(\mathcal{I}_\pm, \mathcal{P})$ satisfies the bound $f(\tau) = o(1)$ as $\text{Im}(\tau) \rightarrow \infty$. Likewise, no nonzero $f \in \text{Ann}_{12}(\mathcal{I}_\pm, \mathcal{P})$ satisfies the bound $f(\tau) = o(e^{-2\pi \text{Im}(\tau)})$ as $\text{Im}(\tau) \rightarrow \infty$.*

PROPOSITION 4.7. *Let k be an even integer. The space $\text{Ann}_k(\tilde{\mathcal{I}}_+, \mathcal{P})$, i.e., the solutions $f \in \mathcal{P}$ to the system*

$$(4.30) \quad f|_k(T - 2 + T^{-1} - 2S) = 0 \quad \text{and} \quad f|_k(I - STS) = 0,$$

is equal to

$$(4.31) \quad \tilde{\varphi}_2 \mathcal{M}_{k-2}(\text{SL}_2(\mathbb{Z})) + \tilde{\varphi}_0 \mathcal{M}_k(\text{SL}_2(\mathbb{Z})) + \tilde{\varphi}_{-2} \mathcal{M}_{k+2}(\text{SL}_2(\mathbb{Z})),$$

where

$$\tilde{\varphi}_2(z) = z^2((E_2|_2S)(z))^2, \quad \tilde{\varphi}_0(z) = z^2(E_2|_2S)(z), \quad \text{and} \quad \tilde{\varphi}_{-2}(z) = z^2.$$

In particular, the dimension of the space of solutions equals $\max(0, \lceil \frac{k}{4} \rceil + 1)$.

Proof. Given a solution $f \in \mathcal{P}$ to (4.30), let

$$g_0 = f|_kS, \quad g_1 = -\frac{1}{2}f|_k(I + S - T), \quad \text{and} \quad g_2 = f.$$

Using the fact that $I - STS = S(I - T)S$, one verifies that g_0, g_1, g_2 satisfy the transformation law (4.24). As was shown in the proof of Proposition 4.4, g_0 is consequently a quasimodular form of weight $k + 2$ and depth at most 2 for $\text{SL}_2(\mathbb{Z})$. Thus, $g_0 \in E_2^2 \mathcal{M}_{k-2}(\text{SL}_2(\mathbb{Z})) + E_2 \mathcal{M}_k(\text{SL}_2(\mathbb{Z})) + \mathcal{M}_{k+2}(\text{SL}_2(\mathbb{Z}))$. It follows that $f = g_0|_kS$ lies in (4.31). The other aspects of the proof are straightforward to verify as above. \square

PROPOSITION 4.8. *Let k be an even integer. The space $\text{Ann}_k(\tilde{\mathcal{I}}_-, \mathcal{P})$, i.e., the solutions $f \in \mathcal{P}$ to the system*

$$(4.32) \quad f|_k(T - 2 + T^{-1} + 2S) = 0 \quad \text{and} \quad f|_k(I + STS) = 0,$$

is equal to

$$(4.33) \quad \tilde{\psi}_4 \mathcal{M}_{k-4}(\text{SL}_2(\mathbb{Z})) + \tilde{\psi}_2 \mathcal{M}_{k-2}(\text{SL}_2(\mathbb{Z})) + \tilde{\psi}_0 \mathcal{M}_k(\text{SL}_2(\mathbb{Z})),$$

where

$$\tilde{\psi}_4 = U^2 - V^2, \quad \tilde{\psi}_2 = W, \quad \text{and} \quad \tilde{\psi}_0 = \mathcal{L}.$$

In particular, the dimension of the space of solutions equals $\max(0, \lceil \frac{k-2}{4} \rceil + 1)$.

Proof. For the same reasons as before, we again restrict our attention to showing that solutions $f \in \mathcal{P}$ to (4.32) lie in (4.33). Let $g = f|_k(S + T - I)$. We check that $g|_kS = g|_kT = g$, and so $g \in \mathcal{M}_k(\text{SL}_2(\mathbb{Z}))$ since it has moderate growth. Because

$$(g \cdot \mathcal{L})|_k(S + T - I) = \pi ig,$$

the function $h := f - \frac{1}{\pi i} g \cdot \mathcal{L}$ has moderate growth and satisfies the homogeneous equations

$$h|_k(S + T - I) = 0 \quad \text{and} \quad h|_k S(T + I) = 0,$$

with the latter equation being a restatement of the second equation in (4.32) since $\mathcal{L}_S|_0(T + I) = 0$. Then h is a modular form of weight k for $\Gamma(2)$, because

$$T^2 - I = (S + T - I)(T + I) - S(T + I)$$

and

$$ST^2S - I = (ST + S)(TS - S).$$

We complete the proof by arguing, as in the proof of Proposition 4.5, and again using (2.13), that these conditions force

$$h \in \tilde{\psi}_4 \mathcal{M}_{k-4}(\mathrm{SL}_2(\mathbb{Z})) + \tilde{\psi}_2 \mathcal{M}_{k-2}(\mathrm{SL}_2(\mathbb{Z})). \quad \square$$

4.3. Uniqueness of \mathcal{K}_\pm and its transformation properties. The characterizations of $\mathrm{Ann}_k(\mathcal{I}_\pm, \mathcal{P})$ in Section 4.2 can now be used to establish the uniqueness assertion in Theorem 4.3. Indeed, suppose $\mathcal{K}(\tau, z)$ and $\mathcal{K}'(\tau, z)$ are two kernels satisfying conditions (1)–(4). Then for fixed $z \in \mathbb{H}$, the function $\tau \mapsto \mathcal{K}_\pm(\tau, z) - \mathcal{K}'_\pm(\tau, z)$ is annihilated by $|\tau|_{d/2}^\tau r$ for all $r \in \mathcal{I}_\pm$ by part (2), and it is holomorphic at all $\tau \in \mathbb{H}$ by parts (1) and (3). Furthermore, it is in \mathcal{P} by part (4) combined with the following lemma (recall that $\mathcal{I} \subseteq \mathcal{I}_\pm$). By Lemma 4.6 the growth condition (4.21) forces $\mathcal{K}_\pm(\tau, z) - \mathcal{K}'_\pm(\tau, z)$ to vanish identically, and hence uniqueness follows.

LEMMA 4.9. *Suppose $f: \mathbb{H} \rightarrow \mathbb{C}$ is holomorphic, k is an even integer, $f|_k r = 0$ for all $r \in \mathcal{I}$, and $\tau \mapsto \Delta(\tau)(j(\tau) - j(z))f(\tau)$ is in \mathcal{P} for some fixed $z \in \mathbb{H}$. Then $f \in \mathcal{P}$.*

Proof. The function f has moderate growth on \mathcal{D} , because

$$\left(\Delta(\tau)(j(\tau) - j(z))\right)^{-1}$$

is bounded above by polynomials in $|\tau|$ and $\mathrm{Im}(\tau)$ as τ approaches any cusp from inside \mathcal{D} (specifically, Δ is a cusp form and j has a pole at infinity). Now Part (2) of Proposition 4.2 with $h_1 = h_2 = 0$ shows that $f \in \mathcal{P}$, as desired. \square

Next we show that the kernels $K_\pm(\tau, z)$ also satisfy modular functional equations in the variable z . In order to do this, first we generalize the residue statements of part (3) of Theorem 4.3 to an action in the variable z , in addition to τ . Suppose first that f is a meromorphic function on \mathbb{H} , with at most simple poles. Then for any $\alpha \in \mathrm{SL}_2(\mathbb{Z})$ and $k \in \mathbb{Z}$,

$$(4.34) \quad \mathrm{Res}_{\tau=\tau_0}(f|_k \alpha)(\tau) = j(\alpha, \tau_0)^{2-k} \mathrm{Res}_{\tau=\alpha\tau_0} f(\tau)$$

in terms of the factor of automorphy from (2.2). Therefore

$$\mathrm{Res}_{\tau=z} \left(\mathcal{K}|_{d/2}^\tau \alpha|_{2-d/2}^z \right)(\tau, z) = \mathrm{Res}_{\tau=\alpha z} \mathcal{K}(\tau, \alpha z),$$

since both sides are equal to $\text{Res}_{\tau=z} j(\alpha, z)^{d/2-2} (\mathcal{K}|_{d/2}^\tau \alpha)(\tau, \alpha z)$. This allows us to compute

$$\begin{aligned} \text{Res}_{\tau=z} (\mathcal{K}|_{d/2}^\tau \alpha|_{2-d/2}^z \beta)(\tau, z) &= \text{Res}_{\tau=z} (\mathcal{K}|_{d/2}^\tau \alpha \beta^{-1}|_{d/2}^\tau \beta|_{2-d/2}^z \beta)(\tau, z) \\ &= \text{Res}_{\tau=\beta z} (\mathcal{K}|_{d/2}^\tau \alpha \beta^{-1})(\tau, \beta z) \end{aligned}$$

for $\alpha, \beta \in \text{SL}_2(\mathbb{Z})$. Of course these identities also hold with \mathcal{K} replaced by \mathcal{K}_\pm . Combining them with (4.34), we see that part (3) of Theorem 4.3 generalizes to

$$(4.35) \quad \text{Res}_{\tau=\gamma z} \mathcal{K}_\pm|_{d/2}^\tau \alpha|_{2-d/2}^z \beta = -\frac{j(\gamma, z)^{d/2-2}}{2\pi} \phi_\pm(\alpha\gamma\beta^{-1})$$

for $\alpha, \beta, \gamma \in \text{PSL}_2(\mathbb{Z})$. Furthermore, for all $r \in R = \mathbb{C}[\text{PSL}_2(\mathbb{Z})]$ and $\alpha \in \text{PSL}_2(\mathbb{Z})$, we have the residue formula

$$(4.36) \quad \text{Res}_{\tau=\alpha z} (\mathcal{K}_\pm|_{2-d/2}^z r)(\tau, z) = -\frac{j(\alpha, z)^{d/2-2}}{2\pi} \phi_\pm(\alpha \cdot \iota(r));$$

indeed, by linearity it suffices to verify this formula in the case that $r = \iota(r)^{-1} \in \text{PSL}_2(\mathbb{Z})$, in which case it follows from (4.35).

PROPOSITION 4.10. *Let \mathcal{K}_\pm be the kernels whose existence and uniqueness are guaranteed by Theorem 4.3. Then*

$$\mathcal{K}_\pm(\tau, z)|_{2-d/2}^z r = 0$$

for all $r \in \tilde{\mathcal{I}}_\pm$.

Proof. Let $r \in \tilde{\mathcal{I}}_\pm$ and consider the function $g_r := \mathcal{K}_\pm|_{2-d/2}^z r$ on $\mathbb{H} \times \mathbb{H}$. Part (1) of Theorem 4.3 asserts that all possible poles of $g_r(\tau, z)$ in τ lie at points $\tau = \alpha z$, where $\alpha \in \text{SL}_2(\mathbb{Z})$. The residues at such points are computed by formula (4.36), and actually vanish since $\phi_\pm(\alpha \cdot \iota(r)) = 0$ by Proposition 3.11. Thus $\tau \mapsto g_r(\tau, z)$ is holomorphic, and it is in \mathcal{P} by Lemma 4.9 and part (4) of Theorem 4.3. Thus it vanishes by Lemma 4.6 and the bounds (4.21). \square

4.4. Proof of Theorem 4.3 and kernel asymptotics. We can now write down the kernels in Theorem 4.3 explicitly. We claim that they are given by

$$\begin{aligned} \mathcal{K}_+^{(d)}(\tau, z) &= \begin{pmatrix} \varphi_{-2}(\tau) \\ \varphi_0(\tau) \\ \varphi_2(\tau) \end{pmatrix}^t \cdot \Upsilon_+^{(d)}(\tau, z) \cdot \begin{pmatrix} \tilde{\varphi}_{-2}(z) \\ \tilde{\varphi}_0(z) \\ \tilde{\varphi}_2(z) \end{pmatrix} \quad \text{and} \\ \mathcal{K}_-^{(d)}(\tau, z) &= \begin{pmatrix} \psi_0(\tau) \\ \psi_2(\tau) \\ \psi_4(\tau) \end{pmatrix}^t \cdot \Upsilon_-^{(d)}(\tau, z) \cdot \begin{pmatrix} \tilde{\psi}_0(z) \\ \tilde{\psi}_2(z) \\ \tilde{\psi}_4(z) \end{pmatrix} \end{aligned}$$

in terms of the bases defined in Propositions 4.4 through 4.8, where the coefficient matrices $\Upsilon_\pm^{(d)}$ are specified below. Let

$$(f_{-2}, f_0, f_2, \dots, f_{14}) = (E_{10}/\Delta, 1, E_{14}/\Delta, E_4, E_6, E_8, E_{10}, \Delta, E_{14}),$$

let Π_{k_1, k_2, k_3} be the diagonal matrix $\text{diag}(f_{k_1}, f_{k_2}, f_{k_3})$, and let us abbreviate $j_\tau = j(\tau)$, $j_z = j(z)$, $j_{\tau, z} = j(\tau) - j(z)$, and $N = 1728$. Then we define

$$\Upsilon_+^{(8)}(\tau, z) = \frac{\Pi_{6,4,2}(\tau) \begin{pmatrix} j_{\tau, z} & 0 & 1 \\ -2j_{\tau, z} & -2 & 0 \\ 1 & 0 & 0 \end{pmatrix} \Pi_{12,10,8}(z)}{36\pi^{-2}i\Delta(z)(j(\tau) - j(z))},$$

$$\Upsilon_+^{(24)}(\tau, z) = \frac{\Pi_{14,12,10}(\tau) \begin{pmatrix} 6 & 0 & Nj_{\tau, z}^{-1} - 6 \\ -12j_\tau + 5N & -2Nj_{\tau, z}^{-1} & 12j_\tau - 7N \\ Nj_{\tau, z}^{-1} + 6 & 0 & -6 \end{pmatrix} \Pi_{4,2,0}(z)}{36N\pi^{-2}i\Delta(z)},$$

$$\Upsilon_-^{(8)}(\tau, z) = \frac{\Pi_{4,2,0}(\tau) \begin{pmatrix} -2N & 0 & 0 \\ 0 & 1 & -1 \\ 0 & N - j_\tau & j_\tau \end{pmatrix} \Pi_{10,8,6}(z)}{2N\pi\Delta(z)(j(\tau) - j(z))},$$

and

$$\Upsilon_-^{(24)}(\tau, z) = \frac{\Pi_{12,10,8}(\tau) \begin{pmatrix} -2N & -2Nj_{\tau, z} & 0 \\ 0 & j_\tau + 2j_{\tau, z} & -1 \\ 0 & N - 2j_{\tau, z} - j_\tau & 1 \end{pmatrix} \Pi_{2,0,-2}(z)}{2N\pi\Delta(z)(j(\tau) - j(z))}.$$

Note in particular that in accordance with Propositions 4.4 through 4.8, $\Upsilon_+^{(d)}$ has rows of weight $d/2 + 2$, $d/2$, and $d/2 - 2$ in τ and columns of weight $4 - d/2$, $2 - d/2$, and $-d/2$ in z , while $\Upsilon_-^{(d)}$ has rows of weight $d/2$, $d/2 - 2$, and $d/2 - 4$ in τ and columns of weight $2 - d/2$, $-d/2$, and $-2 - d/2$ in z .

Poles occur in the entries of $\Upsilon_\pm^{(d)}(\tau, z)$ only from dividing by $j(\tau) - j(z)$. Thus, the poles of these matrix entries in τ are contained in the $\text{SL}_2(\mathbb{Z})$ -orbit of z , and they are all simple poles unless $j'(z) = 0$. Because $j' = -2\pi i E_4^2 E_6 / \Delta$ by (2.6), that can happen only if $E_4(z) = 0$ or $E_6(z) = 0$. The Eisenstein series E_4 and E_6 have single roots on the $\text{SL}_2(\mathbb{Z})$ -orbits of $e^{2\pi i/3}$ and i , respectively, and no other roots by [7, Proposition 5.6.5]; the function $j = 1728E_4^3 / (E_4^3 - E_6^2)$ takes the values 0 and 1728 on these orbits. Using these facts, one can check that the matrices $\Upsilon_\pm^{(d)}(\tau, z)$ never have poles in τ of order greater than one.

We can calculate residues by using the identity

$$\lim_{\tau \rightarrow z} \frac{f(\tau)(\tau - z)}{j(\tau) - j(z)} = \frac{f(z)}{j'(z)} = \frac{if(z)\Delta(z)}{2\pi E_{14}(z)}$$

for a holomorphic function f on a neighborhood of z , where we interpret the right side by continuity if $f(z) = j'(z) = 0$. We find that for both $d = 8$ and 24 ,

$$\begin{aligned} \operatorname{Res}_{\tau=z} \Upsilon_+^{(d)}(\tau, z) &= \frac{\pi}{72} \begin{pmatrix} 0 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \text{and} \\ \operatorname{Res}_{\tau=z} \Upsilon_-^{(d)}(\tau, z) &= \frac{i}{6912\pi^2\Delta(z)} \begin{pmatrix} -3456\Delta(z) & 0 & 0 \\ 0 & E_4(z)^2 & -E_6(z) \\ 0 & -E_6(z) & E_4(z) \end{pmatrix}. \end{aligned}$$

For matrices $\alpha, \beta \in \operatorname{SL}_2(\mathbb{Z})$,

$$(\mathcal{K}_+^{(d)}|_{d/2}\alpha|_{2-d/2}\beta)(\tau, z) = \begin{pmatrix} (\varphi_{-2}|-2\alpha)(\tau) \\ (\varphi_0|0\alpha)(\tau) \\ (\varphi_2|2\alpha)(\tau) \end{pmatrix}^t \cdot \Upsilon_+^{(d)}(\tau, z) \cdot \begin{pmatrix} (\tilde{\varphi}_{-2}|-2\beta)(z) \\ (\tilde{\varphi}_0|0\beta)(z) \\ (\tilde{\varphi}_2|2\beta)(z) \end{pmatrix}$$

and

$$(\mathcal{K}_-^{(d)}|_{d/2}\alpha|_{2-d/2}\beta)(\tau, z) = \begin{pmatrix} (\psi_0|0\alpha)(\tau) \\ (\psi_2|2\alpha)(\tau) \\ (\psi_4|4\alpha)(\tau) \end{pmatrix}^t \cdot \Upsilon_-^{(d)}(\tau, z) \cdot \begin{pmatrix} (\tilde{\psi}_0|0\beta)(z) \\ (\tilde{\psi}_2|2\beta)(z) \\ (\tilde{\psi}_4|4\beta)(z) \end{pmatrix},$$

using the $\operatorname{SL}_2(\mathbb{Z})$ -automorphy properties of the matrix entries of $\Upsilon_{\pm}^{(d)}(\tau, z)$.

Theorem 4.3 can now be straightforwardly verified from these formulas. The uniqueness was already shown in Section 4.3, we have seen that property (1) holds, and property (2) follows from Propositions 4.4 and 4.5 and the weights of the coefficients of φ_k and ψ_k . The residue property (3) follows from computing $\operatorname{Res}_{\tau=z} \mathcal{K}_+^{(d)}|_{d/2}\alpha$ as

$$\frac{\pi}{72} \begin{pmatrix} (\varphi_{-2}|-2\alpha)(z) \\ (\varphi_0|0\alpha)(z) \\ (\varphi_2|2\alpha)(z) \end{pmatrix}^t \cdot \begin{pmatrix} 0 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} \tilde{\varphi}_{-2}(z) \\ \tilde{\varphi}_0(z) \\ \tilde{\varphi}_2(z) \end{pmatrix}$$

and $\operatorname{Res}_{\tau=z} \mathcal{K}_-^{(d)}|_{d/2}\alpha$ as

$$\frac{i}{6912\pi^2\Delta(z)} \begin{pmatrix} (\psi_0|0\alpha)(z) \\ (\psi_2|2\alpha)(z) \\ (\psi_4|4\alpha)(z) \end{pmatrix}^t \cdot \begin{pmatrix} -3456\Delta(z) & 0 & 0 \\ 0 & E_4(z)^2 & -E_6(z) \\ 0 & -E_6(z) & E_4(z) \end{pmatrix} \cdot \begin{pmatrix} \tilde{\psi}_0(z) \\ \tilde{\psi}_2(z) \\ \tilde{\psi}_4(z) \end{pmatrix}$$

for $\alpha \in \{I, T, TS\}$. Finally, the membership in \mathcal{P} asserted in property (4) follows from the formulas by using $j\Delta \in \mathcal{P}$, and (4.21) follows from a q -expansion calculation. This completes the proof of Theorem 4.3.

For the detailed analysis of the generating functions F and \tilde{F} in Section 5, we will need to understand the non-decaying asymptotics of $\mathcal{K}_{\pm}^{(d)}(\tau, it)$ as $t \rightarrow \infty$ with $t \in \mathbb{R}$. To do so, we expand $\mathcal{K}_{\pm}^{(d)}(\tau, z)$ as a series in powers of $e^{\pi iz}$, whose coefficients are functions of τ and polynomials in z of degree at most 2, and we define $\mathcal{G}_{\pm}^{(d)}(\tau, z)$ to be the sum of the $e^{n\pi iz}$ terms for $n \leq 0$. Then $\mathcal{K}_{\pm}^{(d)}(\tau, it) = \mathcal{G}_{\pm}^{(d)}(\tau, it) + O(t^2 e^{-\pi t})$ as $t \rightarrow \infty$.

Explicit calculation shows that these functions can be expanded in z as

$$\mathcal{G}_{\pm}^{(d)}(\tau, z) = \sum_{k=-1}^0 \sum_{j=0}^1 z^j e^{2\pi i k z} \mathcal{G}_{k,j,\pm}^{(d)}(\tau),$$

where the coefficient functions $\mathcal{G}_{k,j,\pm}^{(d)}(\tau)$ are polynomials in τ , $E_2(\tau)$, $U(\tau)$, $V(\tau)$, $W(\tau)$, $\mathcal{L}(\tau)$, and $\mathcal{L}_S(\tau)$, and so in particular they lie in \mathcal{P} . In fact, $\mathcal{G}_{-1,j,\pm}^{(8)} = 0$, as will be important in Section 6. We furthermore define $\mathcal{G}^{(d)} = \frac{1}{2}(\mathcal{G}_+^{(d)} + \mathcal{G}_-^{(d)})$ to correspond with $\mathcal{K}^{(d)}$, and set $\mathcal{G}_{k,j}^{(d)} = \frac{1}{2}(\mathcal{G}_{k,j,+}^{(d)} + \mathcal{G}_{k,j,-}^{(d)})$ so that

$$(4.37) \quad \mathcal{G}^{(d)}(\tau, z) = \sum_{k=-1}^0 \sum_{j=0}^1 z^j e^{2\pi i k z} \mathcal{G}_{k,j}^{(d)}(\tau).$$

We will need the following lemma in Section 5.

LEMMA 4.11. *Let*

$$(4.38) \quad n_{+,\tau} = 0, \quad n_{-,\tau} = 1, \quad n_{+,z} = 2, \quad n_{-,z} = 1, \quad \widehat{n}_{\tau}^{(8)} = 2, \quad \text{and} \quad \widehat{n}_{\tau}^{(24)} = 4.$$

For each $\delta > 0$ and $\gamma \in \mathrm{PSL}_2(\mathbb{Z})$, there exists a constant $C = C_{\gamma,\delta} > 0$ such that for $d \in \{8, 24\}$,

$$(4.39) \quad \left| (\mathcal{K}_{\pm}^{(d)} |_{d/2}^{\tau} |_{2-d/2}^z S)(\tau, z) \right| \leq C \left| \frac{e^{\pi i(n_{\pm,\tau}\tau + n_{\pm,z}z)} \tau^2 z^2}{\Delta(\tau)\Delta(z)(j(\tau) - j(z))} \right|,$$

$$(4.40) \quad \left| ((\mathcal{K}_{\pm}^{(d)} - \mathcal{G}_{\pm}^{(d)}) |_{d/2}^{\tau} \gamma)(\tau, z) \right| \leq C \left| \frac{e^{\pi i n_{\pm,z} z} \tau^2 z^2}{\Delta(\tau)\Delta(z)(j(\tau) - j(z))} \right|,$$

and

$$(4.41) \quad \left| (\mathcal{K}_{\pm}^{(d)} |_{2-d/2}^z S)(\tau, z) \right| \leq C \left| \frac{e^{\pi i(\widehat{n}_{\tau}^{(d)}\tau + z)} \tau^2 z^2}{\Delta(\tau)\Delta(z)(j(\tau) - j(z))} \right|,$$

for $\mathrm{Im}(\tau), \mathrm{Im}(z) \geq \delta$ with $j(\tau) \neq j(z)$.

Proof. The kernels $\mathcal{K}_{\pm}^{(d)}$ are annihilated by \mathcal{I}_{\pm} under $|_{d/2}^{\tau}$, and one can check that the same is true for $\mathcal{G}_{\pm}^{(d)}$. Thus, to cover all $\gamma \in \mathrm{PSL}_2(\mathbb{Z})$ it suffices to check the cases $\gamma = I$, T , or TS , because they form a basis of R/\mathcal{I}_{\pm} by Proposition 3.9.

For each of these three cases, the explicit formulas for the kernels show that the expressions inside the absolute values on the left sides, when multiplied by $\Delta(\tau)\Delta(z)(j(\tau) - j(z))$, are finite sums of the form $\sum_{j=0}^2 \sum_{k=0}^2 \phi_{jk}(\tau, z) \tau^j z^k$, where ϕ_{jk} is a holomorphic function on $\mathbb{H} \times \mathbb{H}$ satisfying $\phi_{jk}(\tau + 2, z) = \phi_{jk}(\tau, z) = \phi_{jk}(\tau, z + 2)$. The claims then follow from the form of the double power series expansion of $\phi_{jk}(\tau, z)$ in $e^{\pi i \tau}$ and $e^{\pi i z}$, which can be shown by direct calculation to vanish to the asserted order in these exponentials. \square

Note that the denominators of $\Delta(\tau)\Delta(z)(j(\tau) - j(z))$ are not an obstacle to computing asymptotics. For example, if τ is fixed and $z = it$ with $t \in (0, \infty)$, then $\Delta(\tau)\Delta(it)(j(\tau) - j(it))$ approaches $-\Delta(\tau)$ as $t \rightarrow \infty$, and it is asymptotic to $-t^{-12}\Delta(\tau)$ as $t \rightarrow 0$ by modularity, as in the proof of Lemma 4.9.

5. Proof of the interpolation formula

5.1. *The continuation of F from \mathcal{D} to \mathbb{H} .* Let d be 8 or 24, and let \mathcal{K} and \mathcal{K}_\pm be the kernels from Theorem 3.14 for this value of d (we also suppress superscripts (d) for \mathcal{G} and similar terms). As before, we identify radially symmetric functions of $x \in \mathbb{R}^d$ with functions of $r = |x|$. Analytic continuation will be important in both τ and r , and so we view r as a complex variable.

Using the kernel \mathcal{K} , we can now construct the generating function F we need for Theorem 3.1. We start with the formal expression (4.19), which we decompose as $F(\tau, r) = F_1(\tau, r) + F_2(\tau, r)$, where

$$(5.1) \quad F_1(\tau, r) = e^{\pi i \tau r^2} \quad \text{and} \quad F_2(\tau, r) = 4 \sin(\pi r^2/2)^2 \int_0^\infty \mathcal{K}(\tau, it) e^{-\pi r^2 t} dt.$$

We have not yet addressed when the integral is defined. Part (1) of Theorem 4.3 shows that the poles of the integrand in τ are constrained to $\mathrm{SL}_2(\mathbb{Z})$ -translates of the imaginary axis. None of these translates intersects \mathcal{D} aside from the imaginary axis itself, which in fact does not contribute any poles since part (3) of Theorem 4.3 shows that $\mathcal{K}(\tau, it)$ is holomorphic at $\tau = it$ and $\tau = i/t$ (as $\phi(I) = \phi(S) = 0$). Thus, poles are not an obstacle when $\tau \in \mathcal{D}$.

To analyze the convergence of the integral in (5.1), we must understand how $\mathcal{K}(\tau, it)$ behaves as $t \rightarrow 0$ or $t \rightarrow \infty$. Inequality (4.39) (with $\gamma = I$) in Lemma 4.11 shows that it decays exponentially in $1/t$ as $t \rightarrow 0$, while it grows at most exponentially as $t \rightarrow \infty$ because $\mathcal{K}(\tau, it) = \mathcal{G}(\tau, it) + O(t^2 e^{-\pi t})$. Therefore the integral in (5.1) is convergent for $\tau \in \mathcal{D}$ and r in some open set $\mathcal{O} \subseteq \mathbb{C}$ containing all sufficiently large real numbers. More precisely, our analysis of $\mathcal{G}(\tau, it)$ in Section 4.4 shows that it suffices to take $|r| > 0$ for $d = 8$ and $|r| > \sqrt{2}$ for $d = 24$. Furthermore, $F_2(\tau, r)$ is holomorphic as a function of either variable on these sets. (This is a general principle about integrals of analytic functions: by Morera's theorem, it suffices to show that contour integrals vanish, and that reduces to the analyticity of the integrand by Fubini's theorem.)

Theorem 3.1 also involves the function $\widetilde{F} = (e^{\pi i r^2 \tau} - F)|_{d/2}^\tau S = -F_2|_{d/2}^\tau S$ defined just above (4.5). Since $S\mathcal{D} = \mathcal{D}$ and $-\mathcal{K}|_{d/2}^\tau S = \frac{1}{2}(\mathcal{K}_+ - \mathcal{K}_-) = \widehat{\mathcal{K}}$, we may use (5.1) to write

$$(5.2) \quad \widetilde{F}(\tau, r) = 4 \sin(\pi r^2/2)^2 \int_0^\infty \widehat{\mathcal{K}}(\tau, it) e^{-\pi r^2 t} dt$$

for $\tau \in \mathcal{D}$ and $r \in \mathcal{O}$.

We next analytically continue $r \mapsto F_2(\tau, r)$ to an open neighborhood of \mathbb{R} in \mathbb{C} by breaking up the integral as follows. For $\tau \in \mathcal{D}$, $r \in \mathcal{O}$, and fixed $p > 0$ we decompose $F_2(\tau, r)$ as

$$(5.3) \quad F_2(\tau, r) = F_{2,\text{low}}(\tau, r) + F_{2,\text{trunc}}(\tau, r) + F_{2,\text{high}}(\tau, r),$$

where

$$(5.4) \quad \begin{aligned} F_{2,\text{low}}(\tau, r) &= 4 \sin(\pi r^2/2)^2 \int_0^p \mathcal{K}(\tau, it) e^{-\pi r^2 t} dt, \\ F_{2,\text{trunc}}(\tau, r) &= 4 \sin(\pi r^2/2)^2 \int_p^\infty (\mathcal{K}(\tau, it) - \mathcal{G}(\tau, it)) e^{-\pi r^2 t} dt, \quad \text{and} \\ F_{2,\text{high}}(\tau, r) &= 4 \sin(\pi r^2/2)^2 \int_p^\infty \mathcal{G}(\tau, it) e^{-\pi r^2 t} dt \\ &= \frac{4 \sin(\pi r^2/2)^2}{\pi} \sum_{k=-1}^0 e^{-p\pi(2k+r^2)} \left(\frac{\mathcal{G}_{k,0}(\tau)}{2k+r^2} \right. \\ &\quad \left. + \frac{i(1+2kp\pi + p\pi r^2)\mathcal{G}_{k,1}(\tau)}{\pi(2k+r^2)^2} \right). \end{aligned}$$

The first two integrals are absolutely convergent because of the exponential decay in z in (4.39) and (4.40) with $\gamma = I$ (see also the paragraph after Lemma 4.11). Thus both integrals define holomorphic functions for r in a neighborhood of \mathbb{R} in \mathbb{C} . Furthermore, they are both averages of Gaussians, with the first weighted by $\mathcal{K}(\tau, it)$ (which decays exponentially in $1/t$ as $t \rightarrow 0$ by (4.39), and hence damps the contributions of $e^{-\pi r^2 t}$ for t small) and the second by $\mathcal{K}(\tau, it) - \mathcal{G}(\tau, it)$ (which decays exponentially as $t \rightarrow \infty$). To analyze the Schwartz seminorms, we can use the identity

$$(5.5) \quad \max_{r \in \mathbb{R}} |r^c e^{-\pi r^2 t}| = \left(\frac{c}{2\pi e t} \right)^{c/2}$$

for $c \geq 0$ and $t > 0$. It follows by differentiating under the integral sign and using (5.5) to bound the integrand that the first two integrals in (5.4) define Schwartz functions, and that for any fixed $k, \ell \geq 0$, the Schwartz seminorms

$$\max_{r \in \mathbb{R}} \left| r^k \frac{d^\ell}{dr^\ell} F_{2,\text{low}}(\tau, r) \right| \quad \text{and} \quad \max_{r \in \mathbb{R}} \left| r^k \frac{d^\ell}{dr^\ell} F_{2,\text{trunc}}(\tau, r) \right|$$

are bounded as τ ranges over any fixed compact subset of \mathcal{D} . (Recall from Lemma 2.1 that it suffices to use radial seminorms.) Note that the uniformity in τ makes use of (4.40), and not just our previous estimate $\mathcal{K}^{(d)}(\tau, it) = \mathcal{G}^{(d)}(\tau, it) + O(t^2 e^{-\pi t})$ as $t \rightarrow \infty$, although that would suffice to analyze the case of fixed τ .

The explicit evaluation of $F_{2,\text{high}}(\tau, r)$ shows that it is in fact entire in r , since the possible singularities at $r^2 = -2k$ are compensated for by the vanishing of $\sin(\pi r^2/2)^2$ at those points. Furthermore, for any fixed $k, \ell \geq 0$

the map $\tau \mapsto \max_{r \in \mathbb{R}} \left| r^k \frac{d^\ell}{dr^\ell} F_{2,\text{high}}(\tau, r) \right|$ is in \mathcal{P} since each $\mathcal{G}_{k,j} \in \mathcal{P}$. Formulas (5.3) and (5.4) accordingly serve as our definition of $F_2(\tau, r)$, and in turn $F(\tau, r) = e^{\pi i \tau r^2} + F_2(\tau, r)$, for arbitrary $\tau \in \mathcal{D}$ and $r \in \mathbb{R}$. Note that although the integrals in (5.4) all depend on a parameter p , their sum is independent of p for large r by construction and hence for all $r \in \mathbb{R}$ by analytic continuation. Aside from a technical point in the proof of Proposition 5.1 that requires two different choices of p , this parameter will be fixed and hence suppressed from the notation (in Section 6 a similar construction uses the value $p = 1.01$).

Having defined $F_2(\tau, r)$ for $\tau \in \mathcal{D}$, we next turn to its analytic continuation to the full upper half-plane \mathbb{H} . The anticipated transformation laws (4.5) for F can be restated via (5.1) as

$$(5.6) \quad \begin{aligned} F_2(\tau + 2, r) - 2F_2(\tau + 1, r) + F_2(\tau, r) &= 4e^{\pi i r^2(\tau+1)} \sin(\pi r^2/2)^2 \quad \text{and} \\ (F_2|_{\mathcal{D}/2}^\tau S)(\tau + 2, r) - 2(F_2|_{\mathcal{D}/2}^\tau S)(\tau + 1, r) + (F_2|_{\mathcal{D}/2}^\tau S)(\tau, r) &= 0. \end{aligned}$$

In fact, we will use (5.6) to define the extension from \mathcal{D} to \mathbb{H} ; however, since the $\Gamma(2)$ -translates of the open fundamental domain \mathcal{D} do not cover \mathbb{H} (as they omit boundaries), we first prove the following extension just beyond the closure $\overline{\mathcal{D}}$ of \mathcal{D} :

PROPOSITION 5.1. *The function $\tau \mapsto F_2(\tau, r)$ extends to a holomorphic function on an open subset of \mathbb{H} containing $\overline{\mathcal{D}}$, which satisfies the recurrences (5.6) whenever the left sides are defined. Moreover, $r \mapsto F_2(\tau, r)$ is a Schwartz function for each τ , and for any fixed integers $k, \ell \geq 0$ the Schwartz seminorm $\max_{r \in \mathbb{R}} \left| r^k \frac{d^\ell}{dr^\ell} F_2(\tau, r) \right|$ is bounded as τ ranges over any fixed compact subset of its domain.*

Proof. We first show the continuation to the right of $\text{Re}(\tau) = 1$. The continuation to the left of $\text{Re}(\tau) = -1$ is nearly identical, and those across the bottom two semicircles of the boundary of \mathcal{D} are drastically simpler (owing to the homogeneity of the second equation in (5.6) and the absence of poles as one crosses those boundaries).

Let \mathcal{U} denote the interior of the closure of

$$T \left\{ \tau \in \mathcal{F} : \text{Re}(\tau) < \frac{1}{2} \right\} \cup TST^{-1} \left\{ \tau \in \mathcal{F} : \text{Re}(\tau) > \frac{1}{2} \right\}.$$

Then its closure $\overline{\mathcal{U}}$ includes the line $\text{Re}(\tau) = 1$ but intersects no other $\text{SL}_2(\mathbb{Z})$ -translate of the imaginary axis (see Figure 5.1). For $\tau \in \mathcal{U}$ and $|r|$ sufficiently large, define

$$F_2^\sharp(\tau, r) := 4 \sin(\pi r^2/2)^2 \int_0^\infty \mathcal{K}(\tau, it) e^{-\pi r^2 t} dt,$$

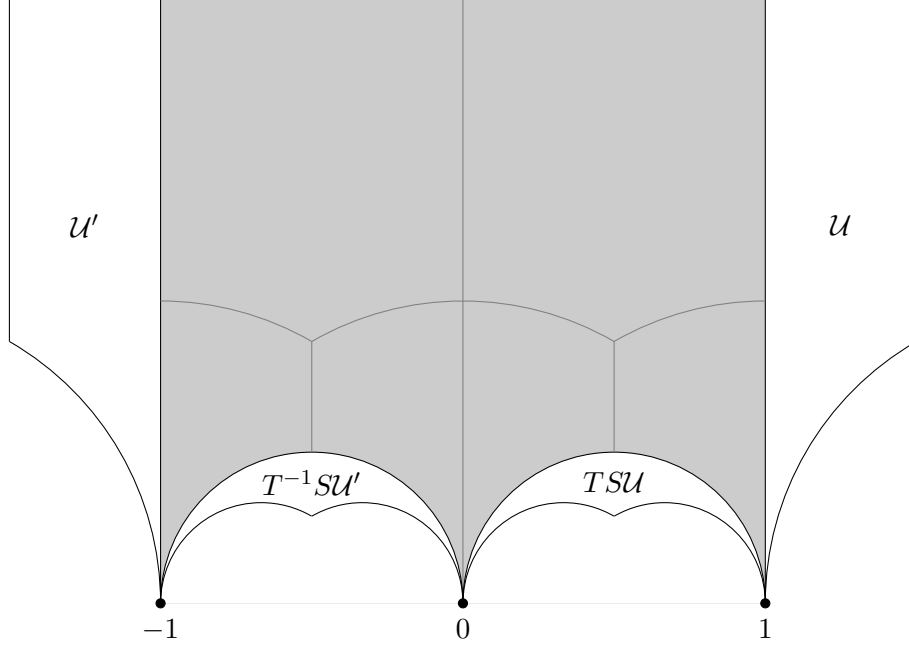


Figure 5.1. The regions \mathcal{U} , $\mathcal{U}' = \{\tau \in \mathbb{C} : -\bar{\tau} \in \mathcal{U}\}$, $TS\mathcal{U} = S\mathcal{U}'$, and $T^{-1}S\mathcal{U}' = S\mathcal{U} = \{\tau \in \mathbb{C} : -\bar{\tau} \in TS\mathcal{U}\}$ in the proof of continuation of $F_2(\tau, r)$. The shaded region is the domain \mathcal{D} from (4.6), and $\overline{\mathcal{D}}$, \mathcal{U} , \mathcal{U}' , $TS\mathcal{U}$, and $T^{-1}S\mathcal{U}'$ together form \mathcal{D}_+ .

i.e., by the same integral formula as in (5.1). It, too, has an analytic continuation to a neighborhood of \mathbb{R} in \mathbb{C} using the integral formulas in (5.4), for exactly the same reason as before.

To relate F_2^\sharp and F_2 , we will examine the poles of $\mathcal{K}(\tau, z)$ using part (3) of Theorem 4.3 and equation (4.36) (with the group algebra element r in this equation given by $r = 1$). For $\tau \in \overline{\mathcal{U}}$ the only possible singularities of the integrand with $z = it$ are at $z = T^{-1}\tau$ or $z = ST^{-1}\tau$, with τ on the left boundary of \mathcal{U} . For $\alpha \in \text{PSL}_2(\mathbb{Z})$, there is a pole at $z = \alpha\tau$ if and only if $\phi(\alpha^{-1}) \neq 0$, because $z = \alpha\tau$ means $\tau = \alpha^{-1}z$, and by (4.36) the residue is

$$\begin{aligned} \text{Res}_{z=\alpha\tau} \mathcal{K}(\tau, z) &= \left(\text{Res}_{w=\alpha^{-1}z} \mathcal{K}(w, z) \right) \Big|_{z=\alpha\tau} \lim_{z \rightarrow \alpha\tau} \frac{z - \alpha\tau}{\tau - \alpha^{-1}z} \\ &= -\frac{j(\alpha^{-1}, \alpha\tau)^{d/2-2}}{2\pi} \phi(\alpha^{-1}) \left(-\frac{1}{j(\alpha, \tau)^2} \right) \\ &= \frac{\phi(\alpha^{-1})}{2\pi j(\alpha, \tau)^{d/2}}. \end{aligned}$$

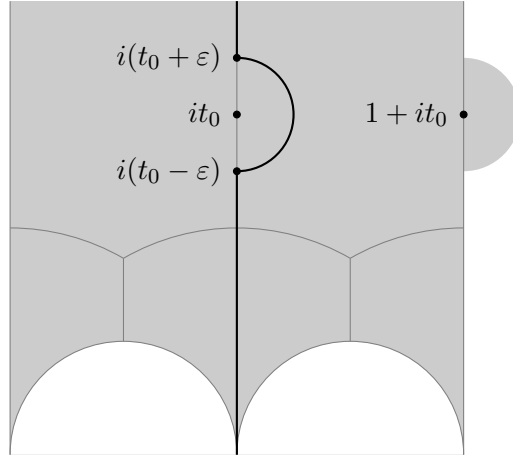


Figure 5.2. A contour achieving analytic continuation for τ near $1 + it_0$.

Thus, there is no pole at $ST^{-1}\tau$, because $\phi(TS) = 0$. On the other hand, there is a pole with residue $1/(2\pi)$ at $z = T^{-1}\tau$, because $\phi(T) = 1$. We must account for this pole if we wish to cross the line $\text{Re}(\tau) = 1$.

To cross this line, we return to the integrals defining $F_2(\tau, r)$ in (5.3) and (5.4), which are contour integrals along pieces of the imaginary axis. Consider a point it_0 on one of these contours; we wish to continue $\tau \mapsto F_2(\tau, r)$ from $\text{Re}(\tau)$ slightly less than 1 to a neighborhood of $1 + it_0$. As shown in Figure 5.2, to do so we can shift the integration in z from the segment from $i(t_0 - \varepsilon)$ to $i(t_0 + \varepsilon)$ to the semicircle $z = it_0 + e^{i\theta}\varepsilon$ with $-\pi/2 \leq \theta \leq \pi/2$, where the radius $\varepsilon = \varepsilon(t_0)$ is taken to be small enough that this semicircle remains inside \mathcal{D} ; it is at this point that we may need two different choices of p (e.g., $p = 1$ and $p = 2$), so that we can ensure that $|p - t_0| > \varepsilon$ and thus ip is either above or below this semicircle. The contours having been moved out of the way of the poles of the integrand, these integrals now give an expression for $F_2(\tau, r)$ that is holomorphic for $T^{-1}\tau$ slightly to the left of the contour, in particular, for τ in a ball of radius $\varepsilon/2$ around $1 + it_0$. We now claim that $F_2(\tau, r)$ is a Schwartz function of r whose Schwartz seminorms are bounded in the region $\{\tau \in \mathbb{C} : |\tau - 1 - it_0| \leq \varepsilon/2\}$. Indeed, the contribution of the integral from the undeformed contour along the imaginary axis retains this property, just as it did for $\tau \in \mathcal{D}$ in the comments following (5.4). Meanwhile, $\mathcal{K}(\tau, z)$ is continuous and hence bounded in terms of t_0 for such τ and for z on the deformed semicircle, which establishes the claimed seminorm bound.

Having shown the analytic continuation of $F_2(\tau, r)$ past $\text{Re}(\tau) = 1$ to an open subset of \mathcal{U} , we next claim that

$$(5.7) \quad F_2(\tau, r) = F_2^\sharp(\tau, r) + 4e^{\pi ir^2(\tau-1)} \sin(\pi r^2/2)^2$$

on this common domain of definition. For sufficiently large r , this identity follows from moving the deformed semicircles back into place and using $\text{Res}_{z=\tau-1} \mathcal{K}(\tau, z) = 1/(2\pi)$, and hence it holds for all $r \in \mathbb{R}$ by analytic continuation.

Arguing similarly, one continues $\tau \mapsto F_2(\tau, r)$ across $\text{Re}(\tau) = -1$ to the reflected region $\mathcal{U}' = \{\tau \in \mathbb{C} : -\bar{\tau} \in \mathcal{U}\}$, as well as across the bottom semicircles $|\tau \pm 1/2| = 1/2$ to $TS\mathcal{U}$ and $T^{-1}S\mathcal{U}' = \{\tau \in \mathbb{C} : -\bar{\tau} \in TS\mathcal{U}\}$. In particular, the integral (5.1) extends holomorphically for large r to these last two domains, because part (3) of Theorem 4.3 shows there is no pole on those bottom semicircles. (Specifically, the residue of $\mathcal{K}(\tau, z)$ at $\tau = \gamma z$ is proportional to $\phi(\gamma)$, and $\phi(STS) = \phi(ST) = \phi(ST^{-1}) = \phi(ST^{-1}S) = 0$; note also that $\phi(TS) = \phi(T^{-1}S) = 0$, so there is no need to take care with inverses.)

So far, we have seen how to analytically continue $\tau \mapsto F_2(\tau, r)$ to all of $\mathcal{D}_+ := \overline{\mathcal{D}} \cup \mathcal{U} \cup \mathcal{U}' \cup TS\mathcal{U} \cup T^{-1}S\mathcal{U}'$, and the boundedness of the Schwartz seminorms holds for the same reason as above. All that remains is to prove the recurrences (5.6). We begin with the first equation in (5.6), namely

$$F_2(\tau, r) \Big|_{d/2}^{\tau} (T - I)^2 = 4e^{\pi i r^2(\tau+1)} \sin(\pi r^2/2)^2$$

whenever $\tau, \tau + 1, \tau + 2 \in \mathcal{D}_+$. The set of such τ is connected (it is the interior of the closure of $\mathcal{U}' \cup T^{-2}\mathcal{U}$), and so by analyticity it suffices to prove this identity when r is sufficiently large and $\tau + 2 \in \mathcal{U}$, in which case $\tau, \tau + 1 \in \mathcal{D}$. Then (5.7) and $\mathcal{K}(\tau, it) \Big|_{d/2}^{\tau} (T - I)^2 = 0$ tell us that

$$\begin{aligned} F_2(\tau, r) \Big|_{d/2}^{\tau} (T - I)^2 &= 4e^{\pi i r^2(\tau+1)} \sin(\pi r^2/2)^2 \\ &\quad + F_2^{\sharp}(\tau, r) \Big|_{d/2}^{\tau} T^2 - 2F_2(\tau, r) \Big|_{d/2}^{\tau} T + F_2(\tau, r) \\ &= 4e^{\pi i r^2(\tau+1)} \sin(\pi r^2/2)^2 \\ &\quad + 4 \sin(\pi r^2/2)^2 \int_0^{\infty} (\mathcal{K}(\tau, it) \Big|_{d/2}^{\tau} (T - I)^2) e^{-\pi r^2 t} dt \\ &= 4e^{\pi i r^2(\tau+1)} \sin(\pi r^2/2)^2. \end{aligned}$$

which is the first identity in (5.6). The second identity states that

$$F_2(\tau, r) \Big|_{d/2}^{\tau} S(T - I)^2 = 0,$$

and it is proved almost exactly the same way. Because \mathcal{D}_+ is invariant under S , the set of τ such that $S\tau, ST\tau, ST^2\tau \in \mathcal{D}_+$ is again connected (it is the same as the set of τ such that $\tau, T\tau, T^2\tau \in \mathcal{D}_+$). We can assume $ST^2\tau \in T^{-1}S\mathcal{U}' = S\mathcal{U}$ and r is sufficiently large. Then $ST\tau, S\tau \in \mathcal{D}$, and each of the three terms in $F_2(\tau, r) \Big|_{d/2}^{\tau} S(T - I)^2$ can be computed using the integral (5.1) when r is large enough. Thus, the second identity follows from $\mathcal{K}(\tau, it) \Big|_{d/2}^{\tau} S(T - I)^2 = 0$. \square

We conclude this subsection with some implications of Proposition 5.1 and both parts of Proposition 4.2.

COROLLARY 5.2. *The function $\tau \mapsto F_2(\tau, r)$ extends to a holomorphic function on \mathbb{H} satisfying the identities*

$$(5.8) \quad F_2|_{d/2}^\tau(T - I)^2 = -e^{\pi i r^2 \tau}|_{d/2}^\tau(T - I)^2 \quad \text{and} \quad F_2|_{d/2}^\tau S(T - I)^2 = 0,$$

and consequently $F = F_1 + F_2$ extends to a holomorphic function on \mathbb{H} satisfying (4.5); in particular, conditions (1) and (5) of Theorem 3.1 hold with $\widetilde{F} = (e^{\pi i \tau |x|^2} - F)|_{d/2}^\tau S$. Furthermore, condition (3) of Theorem 3.1 holds if and only if $\max_{r \in \mathbb{R}} \left| r^k \frac{d^\ell}{dr^\ell} F_2(\tau, r) \right|$ has moderate growth on $\overline{\mathcal{D}}$.

Of course moderate growth on $\overline{\mathcal{D}}$ is equivalent to that on \mathcal{D} , by continuity.

Proof. The extension and the identities in (5.8) follow immediately from part (1) of Proposition 4.2, with $f(\tau) = F_2(\tau, r)$, $h_1 = -e^{\pi i r^2 \tau}|_{d/2}^\tau(T - I)^2$, and $h_2 = 0$. Equation (4.5) is a restatement of condition (5) of Theorem 3.1, since we have defined $\widetilde{F} = (e^{\pi i r^2 \tau} - F)|_{d/2}^\tau S$. As for condition (3) of Theorem 3.1, the corresponding estimate for F_2 , namely that $\max_{r \in \mathbb{R}} \left| r^k \frac{d^\ell}{dr^\ell} F_2(\tau, r) \right|$ has moderate growth on \mathbb{H} , implies those for $F(\tau, r) = e^{\pi i r^2 \tau} + F_2(\tau, r)$ and $\widetilde{F} = -F_2|_{d/2}^\tau S$. (Here we have used that $e^{\pi i r^2 \tau}$ and all its derivatives with respect to r have moderate growth in τ , uniformly in r , which follows from (5.5).) To reduce the moderate growth to $\overline{\mathcal{D}} \subseteq \mathbb{H}$, we can apply part (2) of Proposition 4.2 with $f(\tau) = r^k \frac{d^\ell}{dr^\ell} F_2(\tau, r)$, $h_1 = -r^k \frac{d^\ell}{dr^\ell} e^{\pi i r^2 \tau}|_{d/2}^\tau(T - I)^2$, and $h_2 = 0$. For fixed $r \in \mathbb{R}$ the bound (4.12) then shows moderate growth in τ with constants coming from the Schwartz seminorms of $F_2(\tau, r)$ and h_1 , and the final statement follows by maximizing over $r \in \mathbb{R}$. \square

5.2. Proof of Theorem 1.7. The interpolation formula (1.4) will follow from Theorem 3.1 once we verify all the latter's hypotheses. The radial hypothesis (2) holds by construction, and hypotheses (1) and (5) were just demonstrated in Corollary 5.2, which also reduced hypothesis (3) to checking the moderate growth of $\max_{r \in \mathbb{R}} \left| r^k \frac{d^\ell}{dr^\ell} F_2(\tau, r) \right|$ for $\tau \in \overline{\mathcal{D}}$. Since the seminorm boundedness assertion in Proposition 5.1 gives the boundedness of $\max_{r \in \mathbb{R}} \left| r^k \frac{d^\ell}{dr^\ell} F_2(\tau, r) \right|$ for τ in any fixed compact subset of $\overline{\mathcal{D}}$, it further suffices to verify the moderate growth for τ lying in a neighborhood in $\overline{\mathcal{D}}$ of one of its cusps. Thus to finish the proof of Theorem 1.7 we will show that

$$(5.9) \quad \max_{r \in \mathbb{R}} \left| r^k \frac{d^\ell}{dr^\ell} F_2(\tau, r) \right| \text{ has moderate growth for } \tau \text{ near cusps of } \overline{\mathcal{D}},$$

and that there is an absolute constant $A > 0$ such that

$$(5.10) \quad F^{(8)}(\tau, x), \widetilde{F}^{(8)}(\tau, x) = O(|\tau|^A e^{-\pi \operatorname{Im}(\tau)})$$

and

$$(5.11) \quad F^{(24)}(\tau, x), \widetilde{F}^{(24)}(\tau, x) = O(|\tau|^A e^{-3\pi \operatorname{Im}(\tau)})$$

as $\operatorname{Im}(\tau) \rightarrow \infty$ with $-1 \leq \operatorname{Re}(\tau) \leq 1$. Indeed, (5.10) and (5.11) are stronger than hypothesis (4) and the concluding statement in Theorem 3.1, which allows us to deduce $n_0 = 2$ in $d = 24$ dimensions.

The fundamental domain \mathcal{D} has four cusps, namely -1 , 0 , 1 , and ∞ (see Figure 4.1). Neighborhoods of these cusps are respectively parameterized by the following elements of $\operatorname{SL}_2(\mathbb{Z})$ acting on τ with large imaginary part in the following strips: $T^{-1}S$ applied to $-1 \leq \operatorname{Re}(\tau) \leq 0$; S applied to $-1 \leq \operatorname{Re}(\tau) \leq 1$; TS applied to $0 \leq \operatorname{Re}(\tau) \leq 1$; and I applied to $-1 \leq \operatorname{Re}(\tau) \leq 1$. Since factors of automorphy do not affect moderate growth by (4.4), assertion (5.9) is equivalent to the moderate growth of $\max_{r \in \mathbb{R}} \left| r^k \frac{d^\ell}{dr^\ell} (F_2|_{d/2}^\tau \gamma)(\tau, r) \right|$ for each of these group elements γ and τ with large imaginary part in its corresponding strip. Alternatively, since the corresponding seminorm growth assertion holds for $F_1(\tau, r) = e^{\pi i r^2}$, for each of these γ it is equivalent to replace F_2 by F in this last assertion. For the rest of this subsection we thus take $-1 \leq \operatorname{Re}(\tau) \leq 1$ and $\operatorname{Im}(\tau)$ large.

Our key tool is a contour shift very similar to the proof of [47, Proposition 2]. For $|r|$ and $\operatorname{Im}(\tau)$ both sufficiently large, we write the factor $\sin(\pi r^2/2)^2$ in terms of complex exponentials, incorporate them into the integrand from (5.1), and set $z = it$ to obtain

$$\begin{aligned} F_2(\tau, r) &= i \int_1^{1+i\infty} \mathcal{K}(\tau, z-1) e^{\pi i r^2 z} dz + i \int_{-1}^{-1+i\infty} \mathcal{K}(\tau, z+1) e^{\pi i r^2 z} dz \\ &\quad - 2i \int_0^{i\infty} \mathcal{K}(\tau, z) e^{i\pi r^2 z} dz, \end{aligned}$$

where all the contours are vertical rays. We now claim that a shift to the contours α_{-1} , α_0 , α_1 , and α_∞ shown in Figure 5.3 yields

$$\begin{aligned} (5.12) \quad F(\tau, r) &= e^{\pi i r^2 \tau} + F_2(\tau, r) \\ &= i \int_{\alpha_1} \mathcal{K}(\tau, z-1) e^{\pi i r^2 z} dz + i \int_{\alpha_{-1}} \mathcal{K}(\tau, z+1) e^{\pi i r^2 z} dz \\ &\quad - 2i \int_{\alpha_0} \mathcal{K}(\tau, z) e^{\pi i r^2 z} dz \\ &\quad + i \int_{\alpha_\infty} (\mathcal{K}|_{2-d/2}^z(T+T^{-1}-2))(\tau, z) e^{\pi i r^2 z} dz. \end{aligned}$$

Specifically, we must shift the contours involving $\mathcal{K}(\tau, z-1)$ and $\mathcal{K}(\tau, z+1)$, and the only poles that can intervene in this contour shift are the poles of

$z \mapsto \mathcal{K}(\tau, z \pm 1)$ at $z = \tau$, with residues

$$\operatorname{Res}_{z=\tau} \mathcal{K}(\tau, z \pm 1) = \mp \frac{1}{2\pi}$$

by part (3) of Theorem 4.3. When $\operatorname{Re}(\tau) > 0$, we obtain a contribution from $\mathcal{K}(\tau, z - 1)$ at $z = \tau$, while $\mathcal{K}(\tau, z + 1)$ has no pole at $z = \tau - 1$; when $\operatorname{Re}(\tau) < 0$, we obtain a contribution from $\mathcal{K}(\tau, z + 1)$ at $z = \tau$, while $\mathcal{K}(\tau, z - 1)$ has no pole at $z = \tau + 1$; finally, when $\operatorname{Re}(\tau) = 0$ both contour shifts contribute half as much (alternatively, this case follows by continuity). In each case, the residues cancel the $e^{\pi i r^2 \tau}$ term from $F(\tau, r) = e^{\pi i r^2 \tau} + F_2(\tau, r)$ and we obtain (5.12).

We can rewrite the last integrand in (5.12) using

$$\begin{aligned} \mathcal{K}|_{2-d/2}^z(T + T^{-1} - 2) &= \frac{1}{2} \mathcal{K}_+|_{2-d/2}^z(T + T^{-1} - 2) + \frac{1}{2} \mathcal{K}_-|_{2-d/2}^z(T + T^{-1} - 2) \\ &= \mathcal{K}_+|_{2-d/2}^z S - \mathcal{K}_-|_{2-d/2}^z S \\ &= 2\widehat{\mathcal{K}}|_{2-d/2}^z S \\ &= -2\mathcal{K}|_{d/2}^\tau S|_{2-d/2}^z S, \end{aligned}$$

by Proposition 4.10, the definition of $\widetilde{\mathcal{I}}_\pm$ from (3.14), and (4.20). Thus,

$$\begin{aligned} (5.13) \quad F(\tau, r) &= i \int_{\alpha_1} \mathcal{K}(\tau, z - 1) e^{\pi i r^2 z} dz + i \int_{\alpha_{-1}} \mathcal{K}(\tau, z + 1) e^{\pi i r^2 z} dz \\ &\quad - 2i \int_{\alpha_0} \mathcal{K}(\tau, z) e^{\pi i r^2 z} dz \\ &\quad - 2i \int_{\alpha_\infty} (\mathcal{K}|_{d/2}^\tau S|_{2-d/2}^z S)(\tau, z) e^{\pi i r^2 z} dz. \end{aligned}$$

If we instead start with formula (5.2) for $\widetilde{F} = -F_2|_{d/2}^\tau S$, or with (5.1) for $F_2|_{d/2}^\tau T S$ or $F_2|_{d/2}^\tau T^{-1} S$, then no poles are encountered in these contour shifts, again because of the residue formula from part (3) of Theorem 4.3. Thus after a change of variables (5.13) generalizes to

$$\begin{aligned} (5.14) \quad \Phi(\tau, r) &= i \int_{ST^{-1}\alpha_1} (\mathcal{K}|_{d/2}^\tau \gamma|_{2-d/2}^z S)(\tau, z) e^{\pi i r^2(1-1/z)} \frac{dz}{z^{d/2}} \\ &\quad + i \int_{ST\alpha_{-1}} (\mathcal{K}|_{d/2}^\tau \gamma|_{2-d/2}^z S)(\tau, z) e^{\pi i r^2(-1-1/z)} \frac{dz}{z^{d/2}} \\ &\quad - 2i \int_{S\alpha_0} (\mathcal{K}|_{d/2}^\tau \gamma|_{2-d/2}^z S)(\tau, z) e^{\pi i r^2(-1/z)} \frac{dz}{z^{d/2}} \\ &\quad - 2i \int_{\alpha_\infty} (\mathcal{K}|_{d/2}^\tau S \gamma|_{2-d/2}^z S)(\tau, z) e^{\pi i r^2 z} dz, \end{aligned}$$

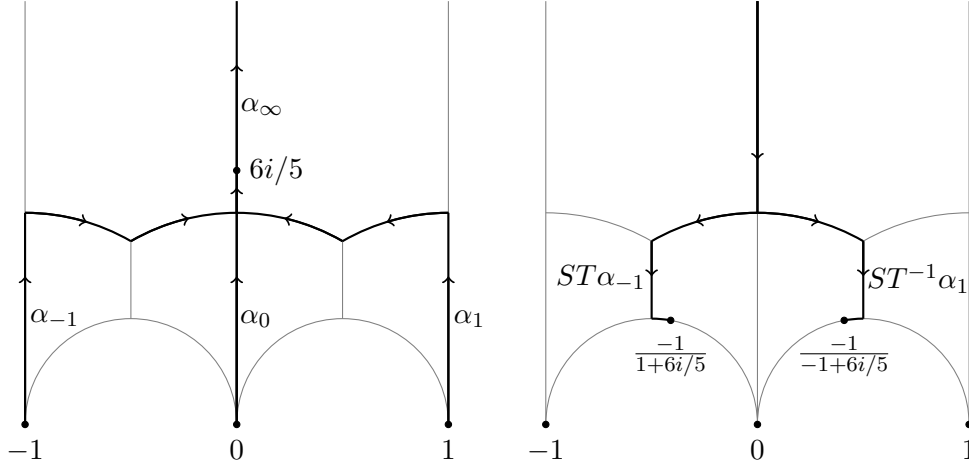


Figure 5.3. The contours α_{-1} , α_0 , α_1 , α_{∞} , $ST\alpha_{-1}$, and $ST^{-1}\alpha_1$ superimposed on the fundamental domain \mathcal{D} shown in Figure 4.1. All four contours on the left share a common terminus at $6i/5$, with α_{-1} , α_0 , and α_1 ending there and α_{∞} starting there, while those on the right go from $i\infty$ to $-1/(\pm 1 + 6i/5)$.

where (Φ, γ) is one of the four pairs

$$(5.15) \quad \begin{array}{ll} (F, I), & (-\tilde{F}, S), \\ (F_2|_{d/2}^{\tau} TS, TS), & (F_2|_{d/2}^{\tau} T^{-1}S, T^{-1}S), \end{array}$$

and we assume $-1 \leq \operatorname{Re}(\tau) \leq 1$ and $\operatorname{Im}(\tau)$ is large. Note that these pairs are exactly the cases we must analyze to treat the four cusps of \mathcal{D} . Since

$$(5.16) \quad \mathcal{K} = \frac{1}{2}(\mathcal{K}_+ + \mathcal{K}_-) \quad \text{and} \quad \widehat{\mathcal{K}} = -\mathcal{K}|_{d/2}^{\tau} S = \frac{1}{2}(\mathcal{K}_+ - \mathcal{K}_-),$$

estimates on the first two kernels in (5.15) are provided in (4.41), and estimates on the last two kernels are provided in (4.39).

Though its derivation initially assumed $|r|$ large, formula (5.14) actually gives an analytic continuation to all $r \in \mathbb{R}$, as can be seen from (4.39) and (4.41), which show that each of its four integrals is absolutely convergent and can be differentiated under the integral sign. In particular, letting

$$e_{k,\ell}(z, r) = r^k \frac{d^\ell}{dr^\ell} e^{\pi i z r^2},$$

we have

$$\begin{aligned}
 (5.17) \quad r^k \frac{d^\ell}{dr^\ell} \Phi(\tau, r) &= i \int_{ST^{-1}\alpha_1} (\mathcal{K}|_{d/2} \gamma|_{2-d/2} \mathcal{S})(\tau, z) e_{k,\ell}(1-1/z, r) \frac{dz}{z^{d/2}} \\
 &\quad + i \int_{ST\alpha_{-1}} (\mathcal{K}|_{d/2} \gamma|_{2-d/2} \mathcal{S})(\tau, z) e_{k,\ell}(-1-1/z, r) \frac{dz}{z^{d/2}} \\
 &\quad - 2i \int_{S\alpha_0} (\mathcal{K}|_{d/2} \gamma|_{2-d/2} \mathcal{S})(\tau, z) e_{k,\ell}(-1/z, r) \frac{dz}{z^{d/2}} \\
 &\quad - 2i \int_{\alpha_\infty} (\mathcal{K}|_{d/2} \mathcal{S} \gamma|_{2-d/2} \mathcal{S})(\tau, z) e_{k,\ell}(z, r) dz.
 \end{aligned}$$

Claims (5.9)–(5.11) are now reduced to bounding the four integrals in (5.17). Each of these four contours in (5.17) lies above $\text{Im}(z) = 1/3$, and consists of a semi-infinite ray along the imaginary axis (possibly) together with a compact curve in \mathbb{H} (see Figure 5.3). Thus for $\text{Im}(\tau)$ sufficiently large the only $\text{SL}_2(\mathbb{Z})$ -translates of τ near any of these contours are $\tau - 1$, τ , and $\tau + 1$, which can only possibly contribute poles for z on the imaginary axis portion of the contour.

We shift the contours (if necessary) to keep z at distance at least $1/4$ from any of these potential poles, in particular by taking the integration over $C_1 \cup C_2 \cup C_3$, where C_1 runs along the compact curve and the imaginary axis between i and $i(\text{Im}(\tau) - 1/4)$, C_2 is a contour between $i(\text{Im}(\tau) - 1/4)$ and $i(\text{Im}(\tau) + 1/4)$ keeping distance at least $1/4$ from any $\text{SL}_2(\mathbb{Z})$ -translate of τ , and C_3 runs along the imaginary axis between $i(\text{Im}(\tau) + 1/4)$ and ∞ (see Figure 5.4).

Next we use (5.16) with the estimates (4.39) and (4.41) from Lemma 4.11 to bound the kernel factors by positive linear combinations of terms of the form

$$\left| \frac{e^{\pi i(B_\tau \tau + B_z z)} \tau^2 z^2}{\Delta(\tau) \Delta(z) (j(\tau) - j(z))} \right|,$$

with the integers B_τ and B_z coming from the exponents on the right sides of those bounds. We claim this last expression is itself bounded by a constant multiple of

$$\left| \frac{e^{\pi i(B_\tau \tau + B_z z)} \tau^2 z^2}{e^{2\pi i \tau} - e^{2\pi i z}} \right|$$

for $\text{Im}(z) \geq 1/3$ and sufficiently large $\text{Im}(\tau)$. Indeed, writing j 's q -expansion (2.5) as

$$j(w) = J(e^{2\pi i w}) = e^{-2\pi i w} + 744 + \tilde{J}(e^{2\pi i w}),$$

where $\tilde{J}(u) = \sum_{n \geq 1} c_j(n) u^n$, we see that $\tilde{J}'(u) = O(1)$ as $|u| \rightarrow 0$ and hence

$$j(\tau) - j(z) = J(e^{2\pi i \tau}) - J(e^{2\pi i z}) = e^{-2\pi i \tau} - e^{-2\pi i z} + \int_{e^{2\pi i z}}^{e^{2\pi i \tau}} \tilde{J}'(u) du,$$

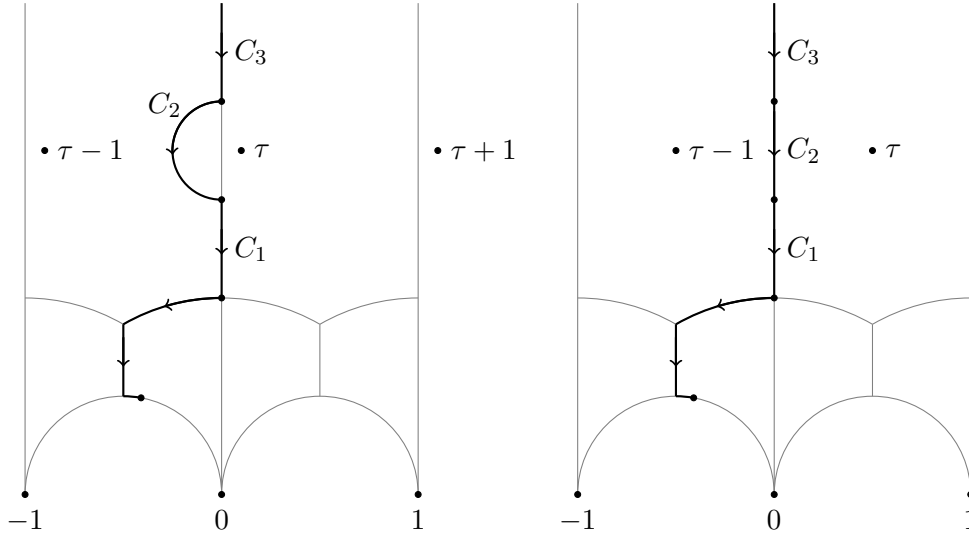


Figure 5.4. The contours C_1 , C_2 , and C_3 (shown here for $ST\alpha_{-1}$) keep distance at least $1/4$ from any \mathbb{Z} -translate of τ .

which is $(e^{2\pi iz} - e^{2\pi i\tau})(e^{-2\pi i(\tau+z)} + O(1))$ for $\text{Im}(\tau), \text{Im}(z) \geq 1/3$. Furthermore, the product formula for Δ implies that $|\Delta(z)| \gg |e^{2\pi iz}|$ for $\text{Im}(z) \geq 1/3$, where \gg indicates inequality up to a positive constant factor, and for sufficiently large $\text{Im}(\tau)$ the $O(1)$ term less is than half the $e^{-2\pi i(\tau+z)}$ added to it; thus $|\Delta(\tau)\Delta(z)(j(\tau) - j(z))| \gg |e^{2\pi i\tau} - e^{2\pi iz}|$, and the claim follows.

To deal with the functions $e_{k,\ell}$ appearing in (5.17), we note that for each k and ℓ , there exists a constant A such that

$$\max_{r \in \mathbb{R}} \left| r^k \frac{d^\ell}{dr^\ell} e^{\pi i z r^2} \right| \ll |z|^A,$$

and the same holds if z is replaced with $-1/z$, $1 - 1/z$, or $-1 - 1/z$ on the left side of the inequality (this follows from (5.5) and $\text{Im}(-1/z) = \text{Im}(z)/|z|^2$). We can assume that $A \geq 0$ because $\text{Im}(z)$ is bounded away from 0. We have thus reduced the verification of (5.9)–(5.11) to estimates for large $\text{Im}(\tau)$ of the three integrals

$$(5.18) \quad I_j(\tau) = \int_{C_j} \left| \frac{e^{\pi i(B_\tau \tau + B_z z)}}{e^{2\pi i\tau} - e^{2\pi iz}} \right| |z|^A dz$$

for $j = 1, 2, 3$, where A is a positive integer depending on k and ℓ . In all cases

$$1 \leq B_z \leq 2 \quad \text{and} \quad B_\tau + B_z \geq 2,$$

by (4.38).

For $z \in C_1$, the denominator $|e^{2\pi i\tau} - e^{2\pi iz}|$ in (5.18) is at least a constant multiple of $|e^{2\pi iz}|$, and

$$|I_1(\tau)| \ll |\tau|^A e^{-\pi B_\tau \operatorname{Im}(\tau)} \left(1 + \int_1^{\operatorname{Im}(\tau)-1/4} e^{(2-B_z)\pi t} dt \right),$$

which is $O(e^{-\pi(B_\tau+B_z-2)\operatorname{Im}(\tau)}|\tau|^{A+1})$. Next, let $z \in C_2$, which keeps distance at least $1/4$ from all integral translates of τ , but has imaginary part within $1/4$ of $\operatorname{Im}(\tau)$; that is,

$$\tau - z \in \left\{ w \in \mathbb{C} : |\operatorname{Im}(w)| \leq \frac{1}{4} \text{ and } |w - n| \geq \frac{1}{4} \text{ for all } n \in \mathbb{Z} \right\}.$$

The image of this last region under the map $w \mapsto e^{2\pi iw}$ is compact but omits 1, and hence is bounded away from 1. It follows that the denominator $|e^{2\pi i\tau} - e^{2\pi iz}| = e^{-2\pi \operatorname{Im}(\tau)} |1 - e^{2\pi i(z-\tau)}|$ is at least some constant multiple of $e^{-2\pi \operatorname{Im}(\tau)}$. Consequently,

$$|I_2(\tau)| \ll e^{-\pi(B_\tau+B_z-2)\operatorname{Im}(\tau)} |\tau|^A.$$

Finally, for $z \in C_3$ the denominator satisfies $|e^{2\pi i\tau} - e^{2\pi iz}| \gg |e^{2\pi i\tau}|$, and the fact that $B_z \geq 1$ allows us to show

$$\begin{aligned} |I_3(\tau)| &\leq e^{-\pi(B_\tau-2)\operatorname{Im}(\tau)} \int_{\operatorname{Im}(\tau)+1/4}^{\infty} e^{-\pi B_z t} t^A dt \\ &\ll e^{-\pi(B_\tau+B_z-2)\operatorname{Im}(\tau)} |\tau|^A. \end{aligned}$$

Combined, $I_1(\tau) + I_2(\tau) + I_3(\tau) = O(e^{-\pi(B_\tau+B_z-2)\operatorname{Im}(\tau)}|\tau|^{A+1})$. Thus (5.9) follows, since $B_\tau + B_z = 2$ in all cases in (4.39) (recall (5.16)). Finally, the estimates (4.41) imply (5.10) (with $B_\tau + B_z = 3$) and (5.11) (with $B_\tau + B_z = 5$), which completes the proof of Theorem 1.9.

5.3. Proof of Theorem 1.9. The following lemma is a direct consequence of applying Lemma 4.6 to $g \pm \tilde{g}$:

LEMMA 5.3. *Let (d, n_0) be $(8, 1)$ or $(24, 2)$. If $g, \tilde{g} \in \mathcal{P}$ satisfy*

$$\begin{aligned} (5.19) \quad &g(\tau + 2) - 2g(\tau + 1) + g(\tau) = 0, \\ &\tilde{g}(\tau + 2) - 2\tilde{g}(\tau + 1) + \tilde{g}(\tau) = 0, \\ &g(\tau) + (i/\tau)^{d/2} \tilde{g}(-1/\tau) = 0, \end{aligned}$$

and $g(\tau), \tilde{g}(\tau) = o(e^{-2\pi(n_0-1)\operatorname{Im}(\tau)})$ as $\operatorname{Im}(\tau) \rightarrow \infty$, then $g = \tilde{g} = 0$.

Recall that the conditions of Theorem 3.1 for $F(\tau, x)$ and $\tilde{F}(\tau, x)$ were shown to hold in the previous subsection. Since $F(\tau, x)$ and $\tilde{F}(\tau, x)$ have the form (3.1) and (3.2), they and their partial derivatives of all orders in x are $o(e^{-2\pi(n_0-1)\operatorname{Im}(\tau)})$ as $\operatorname{Im}(\tau) \rightarrow \infty$, for any fixed x . Furthermore, for any fixed x ,

the functions $F(\tau, x)$ and $\widetilde{F}(\tau, x)$ satisfy the first two equations in (5.19), and an inhomogeneous variant of the third, in which the right side is replaced by $e^{\pi i \tau |x|^2}$. For $m \geq n_0$ and $|x| = \sqrt{2m}$, the pair of functions $g(\tau) = F(\tau, \sqrt{2m}) - e^{2\pi i m \tau}$ and $\widetilde{g}(\tau) = \widetilde{F}(\tau, \sqrt{2m})$ satisfies (5.19). Thus the lemma shows g and \widetilde{g} are identically zero, i.e.,

$$F(\tau, \sqrt{2m}) = e^{2\pi i m \tau} \quad \text{and} \quad \widetilde{F}(\tau, \sqrt{2m}) = 0.$$

In terms of the coefficients of the Fourier series expansion (1.6), we deduce for $m, n \geq n_0$ that $a_n(\sqrt{2m}) = \delta_{n,m}$ and $b_n(\sqrt{2m}) = \widetilde{a}_n(\sqrt{2m}) = \widetilde{b}_n(\sqrt{2m}) = 0$.

Next consider the radial derivatives (i.e., derivatives with respect to $r = |x|$) of equations (1.8)–(1.10), which again have unique solutions for any fixed x by the same logic as above. Suppose $n, m \geq n_0$. At $|x| = \sqrt{2m}$ we similarly deduce that $\frac{\partial F}{\partial r}(\tau, \sqrt{2m}) = 2\pi i \sqrt{2m} \tau e^{2\pi i m \tau}$ and $\frac{\partial \widetilde{F}}{\partial r}(\tau, \sqrt{2m}) = 0$, from which we obtain $b'_n(\sqrt{2m}) = \delta_{n,m}$ and $a'_n(\sqrt{2m}) = \widetilde{a}'_n(\sqrt{2m}) = \widetilde{b}'_n(\sqrt{2m}) = 0$.

Applying the Fourier transform \mathcal{F}_x in x and replacing τ with $-1/\tau$ in equations (1.8)–(1.10) shows that if $(F(\tau, x), \widetilde{F}(\tau, x))$ is a solution to these three equations, then so is $(\mathcal{F}_x \widetilde{F}(\tau, x), \mathcal{F}_x F(\tau, x))$. Applying the lemma to the difference of these two solutions shows that $\widetilde{F}(\tau, x) = \mathcal{F}_x F(\tau, x)$. In terms of the Fourier series (1.6) and (1.7), $\widetilde{a}_n = \widehat{a}_n$ and $\widetilde{b}_n = \widehat{b}_n$. This shows that (1.4) is in fact inverse to the map in the statement of Theorem 1.9. The image of the latter map is contained in $\mathcal{S}(\mathbb{N})^4$ because of the decay of Schwartz functions, and the image of the inverse map is a radial Schwartz function because the radial seminorms of the interpolation basis grow at most polynomially by Theorem 3.1. This completes the proof of Theorem 1.9.

5.4. Integral formulas for the interpolation basis. We can now prove integral formulas for the interpolation basis, which generalize the formulas for the sphere packing auxiliary functions from [47, 14]. These formulas are not needed to prove the interpolation theorem or universal optimality, but they are of interest in their own right, and they help clarify the relationship with the sphere packing constructions.

We begin by noting that for z in any fixed compact subset of \mathbb{H} , whenever $\text{Im}(\tau)$ is sufficiently large the kernels can be expanded as

$$(5.20) \quad \mathcal{K}(\tau, z) = \sum_{n \geq n_0} \alpha_n(z) e^{2\pi i n \tau} + 2\pi i \tau \sum_{n \geq n_0} \sqrt{2n} \beta_n(z) e^{2\pi i n \tau}$$

and

$$(5.21) \quad \widehat{\mathcal{K}}(\tau, z) = \sum_{n \geq n_0} \widetilde{\alpha}_n(z) e^{2\pi i n \tau} + 2\pi i \tau \sum_{n \geq n_0} \sqrt{2n} \widetilde{\beta}_n(z) e^{2\pi i n \tau}$$

for some functions $\alpha_n, \beta_n, \widetilde{\alpha}_n$, and $\widetilde{\beta}_n$ that depend only on the dimension $d \in \{8, 24\}$. To obtain the expansions, we use the q -series in τ for the quasimodular

forms appearing in the explicit constructions of \mathcal{K} and $\widehat{\mathcal{K}}$, as well as the analogous expansions of \mathcal{L} and \mathcal{L}_S , and we write

$$\frac{1}{j(\tau) - j(z)} = \sum_{n \geq 0} \frac{j(z)^n}{j(\tau)^{n+1}}$$

to deal with the factor of $j(\tau) - j(z)$ in the denominator. (Note that $1/j(\tau)$ has an expansion in terms of positive powers of $e^{2\pi i\tau}$.)

PROPOSITION 5.4. *For $d \in \{8, 24\}$, the interpolation basis functions from Theorem 1.7 satisfy*

$$a_n(r) = 4 \sin(\pi r^2/2)^2 \int_0^\infty \alpha_n(it) e^{-\pi r^2 t} dt$$

and

$$b_n(r) = 4 \sin(\pi r^2/2)^2 \int_0^\infty \beta_n(it) e^{-\pi r^2 t} dt$$

whenever $r^2 > 2n$, and

$$\tilde{a}_n(r) = 4 \sin(\pi r^2/2)^2 \int_0^\infty \tilde{\alpha}_n(it) e^{-\pi r^2 t} dt$$

and

$$\tilde{b}_n(r) = 4 \sin(\pi r^2/2)^2 \int_0^\infty \tilde{\beta}_n(it) e^{-\pi r^2 t} dt$$

whenever $r^2 > 0$ for $d = 8$, and whenever $r^2 > 2$ for $d = 24$.

In other words, the interpolation basis functions are integral transforms of the coefficients in the series expansions of \mathcal{K} and $\widehat{\mathcal{K}}$. As usual, one can meromorphically continue the integrals in r by removing the non-decaying terms from the q -expansion of the integrand and handling them separately. Specifically, one can show (using the proof of Proposition 5.4 and the explicit formulas for the kernels \mathcal{K} and $\widehat{\mathcal{K}}$) that the coefficients have expansions of the form

$$(5.22) \quad \begin{aligned} \alpha_n(z) &= -iz e^{-2\pi i n z} + \sum_{m \geq m_0} (\alpha_{0,m,n} + \alpha_{1,m,n} z + \alpha_{2,m,n} z^2) e^{\pi i m z}, \\ \beta_n(z) &= \frac{e^{-2\pi i n z}}{2\pi\sqrt{2n}} + \sum_{m \geq m_0} (\beta_{0,m,n} + \beta_{1,m,n} z + \beta_{2,m,n} z^2) e^{\pi i m z}, \\ \tilde{\alpha}_n(z) &= \sum_{m \geq m_0} (\tilde{\alpha}_{0,m,n} + \tilde{\alpha}_{1,m,n} z + \tilde{\alpha}_{2,m,n} z^2) e^{\pi i m z}, \quad \text{and} \\ \tilde{\beta}_n(z) &= \sum_{m \geq m_0} (\tilde{\beta}_{0,m,n} + \tilde{\beta}_{1,m,n} z + \tilde{\beta}_{2,m,n} z^2) e^{\pi i m z} \end{aligned}$$

for some constants $\alpha_{\ell,m,n}$, $\beta_{\ell,m,n}$, $\tilde{\alpha}_{\ell,m,n}$, and $\tilde{\beta}_{\ell,m,n}$, where $m_0 = 0$ for $d = 8$ and $m_0 = -2$ for $d = 24$. However, we will not need these expansions.

Proof of Proposition 5.4. As in (3.6) and (3.7), we can write the basis functions as integrals involving the generating functions F and \widetilde{F} . We begin with \widetilde{F} , for which the subsequent analysis is a little simpler. For any $y > 0$, the analogues of (3.6) and (3.7) for \tilde{a}_n and \tilde{b}_n are

$$(5.23) \quad \tilde{a}_n(r) = \int_{-1+iy}^{iy} \left(\widetilde{F}(\tau, r) - \tau(\widetilde{F}(\tau+1, r) - \widetilde{F}(\tau, r)) \right) e^{-2\pi i n \tau} d\tau$$

and

$$(5.24) \quad \tilde{b}_n(r) = \frac{1}{2\pi i \sqrt{2n}} \int_{-1+iy}^{iy} \left(\widetilde{F}(\tau+1, r) - \widetilde{F}(\tau, r) \right) e^{-2\pi i n \tau} d\tau.$$

Now we use the identity (5.2), i.e.,

$$(5.25) \quad \widetilde{F}(\tau, r) = 4 \sin(\pi r^2/2)^2 \int_0^\infty \widehat{\mathcal{K}}(\tau, it) e^{-\pi r^2 t} dt,$$

which holds for $\tau \in \mathcal{D}$ and $|r|$ sufficiently large (specifically, $r^2 > 0$ when $d = 8$ and $r^2 > 2$ when $d = 24$). We would like to use the formulas

$$(5.26) \quad \tilde{\alpha}_n(z) = \int_{-1+iy}^{iy} \left(\widehat{\mathcal{K}}(\tau, z) - \tau(\widehat{\mathcal{K}}(\tau+1, z) - \widehat{\mathcal{K}}(\tau, z)) \right) e^{-2\pi i n \tau} d\tau$$

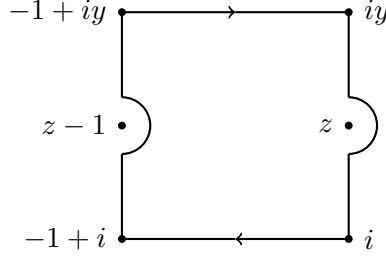
and

$$(5.27) \quad \tilde{\beta}_n(z) = \frac{1}{2\pi i \sqrt{2n}} \int_{-1+iy}^{iy} \left(\widehat{\mathcal{K}}(\tau+1, z) - \widehat{\mathcal{K}}(\tau, z) \right) e^{-2\pi i n \tau} d\tau,$$

which hold for sufficiently large y (depending on z) because of the series expansions (5.20) and (5.21). Before we can use these formulas, we must check whether there is a single choice of y that works for all z on the imaginary axis. Fortunately, any $y \geq 1$ will work. Specifically, it follows from the residue formulas in part (3) of Theorem 4.3 that $\tau \mapsto \widehat{\mathcal{K}}(\tau, z)$ has no poles at z , $-1/z$, $z \pm 1$, or $-1/z \pm 1$. In particular, if z is on the imaginary axis, then this function is holomorphic for $\text{Im}(\tau) \geq 1$ and $-1 \leq \text{Re}(\tau) \leq 1$. Thus, the integrals in (5.26) and (5.27) are independent of y as long as $y \geq 1$, because the integrands are holomorphic and invariant under $\tau \mapsto \tau + 1$.

Now we substitute (5.25) into (5.23) and (5.24) for an arbitrary choice of $y \geq 1$. By the Fubini-Tonelli theorem we can interchange the order of integration. (To prove absolute convergence of the iterated integral, we can use inequalities (4.39) and (4.40) from Lemma 4.11 with $\gamma = I$ to obtain bounds on the integrand as $t \rightarrow 0$ or $t \rightarrow \infty$ that are uniform in τ .) When we do so and apply (5.26) and (5.27), we arrive at the desired formulas for \tilde{a}_n and \tilde{b}_n in terms of $\tilde{\alpha}_n$ and $\tilde{\beta}_n$.

The case of a_n and b_n involves two complications. The function $\tau \mapsto \mathcal{K}(\tau, z)$ has no poles at z , $-1/z$, or $-1/z \pm 1$, but it has poles at $z + 1$ and $z - 1$ with


 Figure 5.5. Contour shift when $\text{Im}(z) > 1$.

residues $-1/(2\pi)$ and $1/(2\pi)$, respectively. Furthermore, we must account for the $e^{\pi i \tau r^2}$ term in (5.1), which says that

$$(5.28) \quad F(\tau, r) = e^{\pi i \tau r^2} + 4 \sin(\pi r^2/2)^2 \int_0^\infty \mathcal{K}(\tau, it) e^{-\pi r^2 t} dt,$$

as long as $\tau \in \mathcal{D}$ and r satisfies $r^2 > 0$ when $d = 8$ and $r^2 > 2$ when $d = 24$. The $e^{\pi i \tau r^2}$ term will turn out to cancel the contributions from the poles.

We begin by analyzing the effects of the poles. As above,

$$\alpha_n(z) = \int_{-1+iy}^{iy} (\mathcal{K}(\tau, z) - \tau(\mathcal{K}(\tau+1, z) - \mathcal{K}(\tau, z))) e^{-2\pi i n \tau} d\tau$$

and

$$\beta_n(z) = \frac{1}{2\pi i \sqrt{2n}} \int_{-1+iy}^{iy} (\mathcal{K}(\tau+1, z) - \mathcal{K}(\tau, z)) e^{-2\pi i n \tau} d\tau$$

when z is on the imaginary axis and y is sufficiently large. If $\text{Im}(z) < 1$, then we can shift the contour in these integrals for α_n and β_n to $y = 1$, as in the case of $\tilde{\alpha}_n$ and $\tilde{\beta}_n$, because the integrand is holomorphic (since $\tau \mapsto \mathcal{K}(\tau, z)$ has no poles at $-1/z$ and $-1/z \pm 1$). We may and shall ignore the case of $z = i$, since it has measure zero in the integrals for a_n and b_n and the integrand is not singular there. If $\text{Im}(z) > 1$, then the integrand has poles at $z - 1$ and z . If we shift the contour to $y = 1$ by passing to the right of these poles, as in Figure 5.5, then this contour shift contributes a residue from integrating the terms involving $\mathcal{K}(\tau + 1, z)$ clockwise around the pole at z . Thus, we obtain the formulas

$$\alpha_n(z) = -iz e^{-2\pi i n z} + \int_{-1+i}^i (\mathcal{K}(\tau, z) - \tau(\mathcal{K}(\tau+1, z) - \mathcal{K}(\tau, z))) e^{-2\pi i n \tau} d\tau$$

and

$$\beta_n(z) = \frac{1}{2\pi i \sqrt{2n}} \left(i e^{-2\pi i n z} + \int_{-1+i}^i (\mathcal{K}(\tau+1, z) - \mathcal{K}(\tau, z)) e^{-2\pi i n \tau} d\tau \right)$$

for $\text{Im}(z) > 1$ (note that the terms coming from the poles are the dominant terms in the asymptotic expansions listed in (5.22)).

Now substituting (5.28) into (3.6) and (3.7) and interchanging the order of integration yields

$$\begin{aligned} a_n(r) &= \int_{-1+i}^i \left(e^{\pi i \tau r^2} - \tau \left(e^{\pi i (\tau+1)r^2} - e^{\pi i \tau r^2} \right) \right) e^{-2\pi i n \tau} d\tau \\ &\quad + 4 \sin(\pi r^2/2)^2 \int_0^1 \alpha_n(it) e^{-\pi r^2 t} dt \\ &\quad + 4 \sin(\pi r^2/2)^2 \int_1^\infty \left(\alpha_n(it) - t e^{2\pi n t} \right) e^{-\pi r^2 t} dt \end{aligned}$$

and

$$\begin{aligned} b_n(r) &= \frac{1}{2\pi i \sqrt{2n}} \int_{-1+i}^i \left(e^{\pi i (\tau+1)r^2} - e^{\pi i \tau r^2} \right) e^{-2\pi i n \tau} d\tau \\ &\quad + 4 \sin(\pi r^2/2)^2 \int_0^1 \beta_n(it) e^{-\pi r^2 t} dt \\ &\quad + 4 \sin(\pi r^2/2)^2 \int_1^\infty \left(\beta_n(it) - \frac{e^{2\pi n t}}{2\pi \sqrt{2n}} \right) e^{-\pi r^2 t} dt. \end{aligned}$$

As above, the estimates (4.39) and (4.40) imply absolute convergence for the original integrals, and then the Fubini-Tonelli theorem shows that the interchanged integrals converge absolutely and the interchange is justified, as long as r satisfies $r^2 > 0$ when $d = 8$ and $r^2 > 2$ when $d = 24$, to justify the application of (5.28). If furthermore $r^2 > 2n$, then $t \mapsto \alpha_n(it) e^{-\pi r^2 t}$ and $t \mapsto \beta_n(it) e^{-\pi r^2 t}$ are integrable over $[1, \infty)$, because the equations

$$\alpha_n(it) e^{-\pi r^2 t} = \left(\alpha_n(it) - t e^{2\pi n t} \right) e^{-\pi r^2 t} + t e^{-\pi(r^2-2n)t}$$

and

$$\beta_n(it) e^{-\pi r^2 t} = \left(\beta_n(it) - \frac{e^{2\pi n t}}{2\pi \sqrt{2n}} \right) e^{-\pi r^2 t} + \frac{e^{-\pi(r^2-2n)t}}{2\pi \sqrt{2n}}$$

express them as the sum of integrable functions. Thus,

$$\int_1^\infty \left(\alpha_n(it) - t e^{2\pi n t} \right) e^{-\pi r^2 t} dt = \int_1^\infty \alpha_n(it) e^{-\pi r^2 t} dt - \int_1^\infty t e^{-\pi(r^2-2n)t} dt$$

and

$$\int_1^\infty \left(\beta_n(it) - \frac{e^{2\pi n t}}{2\pi \sqrt{2n}} \right) e^{-\pi r^2 t} dt = \int_1^\infty \beta_n(it) e^{-\pi r^2 t} dt - \int_1^\infty \frac{e^{-\pi(r^2-2n)t}}{2\pi \sqrt{2n}} dt.$$

All the extraneous terms not involving α_n or β_n cancel, and we obtain the desired formulas for a_n and b_n . \square

6. Positivity of kernels and universal optimality

6.1. *Sharp bounds for energy.* In this section we will prove that E_8 and the Leech lattice are universally optimal (Theorem 1.4). Let d be 8 or 24, with Λ_d being the corresponding lattice and F the generating function from Theorem 3.1. The key inequality is the following proposition:

PROPOSITION 6.1. *Suppose $\operatorname{Re}(\tau) = 0$ and $r > 0$. Then $\widetilde{F}(\tau, r) \geq 0$, with equality if and only if r^2 is an even integer and $r^2 \geq 2n_0$, where $n_0 = 1$ if $d = 8$ and $n_0 = 2$ if $d = 24$.*

The rest of this section is devoted to proving Proposition 6.1, but first we show that it implies universal optimality.

LEMMA 6.2. *For $\alpha > 0$, the function $f: \mathbb{R}^d \rightarrow \mathbb{R}$ defined by $f(x) = F(i\alpha/\pi, x)$ is a Schwartz function and satisfies the inequalities $f(x) \leq e^{-\alpha|x|^2}$ and $\widehat{f}(x) \geq 0$ for all $x \in \mathbb{R}^d$. When $x \neq 0$, equality holds if and only if $|x|$ is the length of a nonzero vector in Λ_d .*

In fact, equality does not hold when $x = 0$ either. That follows from (6.1) below, but we will not need it.

Proof. This function is a Schwartz function since F satisfies condition (3) from Theorem 3.1, so the substantive content of the lemma is the inequalities. The second inequality follows directly from Proposition 6.1, because $\widehat{f}(x) = \widetilde{F}(i\alpha/\pi, x)$ (as shown in Section 5.3). To prove that $f(x) \leq e^{-\alpha|x|^2}$, we use the functional equation $F(\tau, x) + (i/\tau)^{d/2} \widetilde{F}(-1/\tau, x) = e^{\pi i \tau |x|^2}$ with $\tau = i\alpha/\pi$ to obtain

$$e^{-\alpha|x|^2} - f(x) = (\pi/\alpha)^{d/2} \widetilde{F}(i\pi/\alpha, x).$$

Thus, the first inequality amounts to Proposition 6.1 as well, as do the conditions for equality. \square

Although the inequalities $f(x) \leq e^{-\alpha|x|^2}$ and $\widehat{f}(x) \geq 0$ look different, the preceding proof derives them from the same underlying inequality. More generally, Cohn and Miller [16, Section 6] observed a duality principle when the potential function p is a Schwartz function: the auxiliary function f proves a bound for p -energy in Proposition 1.6 if and only if $\widehat{p} - \widehat{f}$ proves a bound for \widehat{p} -energy, and this transformation interchanges the two inequalities. Furthermore, a lattice Λ attains the p -energy bound proved by f if and only if Λ^* attains the \widehat{p} -energy bound proved by $\widehat{p} - \widehat{f}$.

It follows immediately from Lemma 6.2 that Λ_d minimizes energy for all Gaussian potential functions (recall the conditions (1.2) for equality in the linear programming bounds). Furthermore, we can prove uniqueness among periodic configurations as follows. If \mathcal{C} is any periodic configuration in \mathbb{R}^d of

density 1 with the same energy as Λ_d under some Gaussian, then the distances between points in \mathcal{C} must be a subset of those in Λ_d , because of the equality conditions. Without loss of generality we can assume $0 \in \mathcal{C}$. Then, by [11, Lemma 8.2], \mathcal{C} is contained in an even integral lattice (namely, the subgroup of \mathbb{R}^d generated by \mathcal{C}), because all the distances between points in \mathcal{C} are square roots of even integers. Because \mathcal{C} has density 1, it must be the entire lattice. We conclude that it must be isometric to Λ_d , because there is only one such lattice with minimal vector length $\sqrt{2n_0}$ (see [17, Chapters 16 and 18]). Thus, Theorem 1.4 holds for Gaussian potential functions.

Handling other potential functions via linear programming bounds is slightly more technical, because the potential function might decrease too slowly for any Schwartz function to interpolate its values. For example, no Schwartz function can prove a sharp bound for energy under an inverse power law potential in Proposition 1.6. Nevertheless, we will show that Schwartz functions come arbitrarily close to a sharp bound. Suppose we are using a completely monotonic function of squared distance $p: (0, \infty) \rightarrow \mathbb{R}$. By Bernstein's theorem [44, Theorem 9.16], there is some measure μ on $[0, \infty)$ such that

$$p(r) = \int e^{-\alpha r^2} d\mu(\alpha)$$

for all $r \in (0, \infty)$ (which implies that μ must be locally finite). Without loss of generality we can assume $\mu(\{0\}) = 0$, since otherwise all configurations of density 1 have infinite energy. We would like to use

$$f(x) = \int F(i\alpha/\pi, x) d\mu(\alpha)$$

as an auxiliary function for the potential function p , and it might plausibly work under the weaker hypotheses for linear programming bounds proved in [10, Proposition 2.2]. However, it will not be a Schwartz function in general, and we will not analyze the behavior of this integral. Instead, let

$$f_\varepsilon(x) = \int_\varepsilon^{1/\varepsilon} F(i\alpha/\pi, x) d\mu(\alpha),$$

which defines a Schwartz function for each $\varepsilon > 0$ because F satisfies condition (3) of Theorem 3.1. Then

$$\widehat{f}_\varepsilon(y) = \int_\varepsilon^{1/\varepsilon} \widetilde{F}(i\alpha/\pi, y) d\mu(\alpha),$$

and the inequalities $f_\varepsilon(x) \leq p(|x|)$ for all $x \in \mathbb{R}^d \setminus \{0\}$ and $\widehat{f}_\varepsilon(y) \geq 0$ for all $y \in \mathbb{R}^d$ follow from Lemma 6.2. Thus, every configuration in \mathbb{R}^d of density 1 has lower p -energy at least $\widehat{f}_\varepsilon(0) - f_\varepsilon(0)$, by Proposition 1.6. Because of the

sharp bound for each α ,

$$\begin{aligned} \widehat{f}_\varepsilon(0) - f_\varepsilon(0) &= \int_\varepsilon^{1/\varepsilon} E_{r \mapsto e^{-\alpha r^2}}(\Lambda_d) d\mu(\alpha) \\ &= \int_\varepsilon^{1/\varepsilon} \sum_{x \in \Lambda_d \setminus \{0\}} e^{-\alpha|x|^2} d\mu(\alpha) \\ &= \sum_{x \in \Lambda_d \setminus \{0\}} \int_\varepsilon^{1/\varepsilon} e^{-\alpha|x|^2} d\mu(\alpha). \end{aligned}$$

As $\varepsilon \rightarrow 0$, this bound converges to the p -energy of Λ_d by monotone convergence since $\mu(\{0\}) = 0$, and we conclude that Λ_d has minimal p -energy.

Uniqueness among periodic configurations also follows from Bernstein's theorem. Suppose \mathcal{C} is any periodic configuration of density 1 that is not isometric to Λ_d . We have seen that the energy of \mathcal{C} under $r \mapsto e^{-\alpha r^2}$ is strictly greater than that of Λ_d for each $\alpha > 0$, and these energies are continuous functions of α by (1.1). By continuity, for each compact subinterval I of $(0, \infty)$, there exists $\varepsilon > 0$ such that the energy gap between \mathcal{C} and Λ_d is at least ε for all $\alpha \in I$. Thus, Bernstein's theorem and monotone convergence show that $E_p(\mathcal{C}) \geq E_p(\Lambda_d) + \delta$ for some $\delta > 0$. In particular, $E_p(\mathcal{C}) > E_p(\Lambda_d)$ if $E_p(\Lambda_d) < \infty$, as desired. This completes the proof of Theorem 1.4, except for proving Proposition 6.1.

In addition to proving universal optimality, our construction also establishes other properties of the optimal auxiliary functions. For example, the following proposition follows directly from (5.3) and (5.4) for $\tau \in \mathcal{D}$, and for all $\tau \in \mathbb{H}$ by analytic continuation:

PROPOSITION 6.3. *For all $\tau \in \mathbb{H}$ and $d \in \{8, 24\}$,*

$$\begin{aligned} F(\tau, 0) &= 1 + i\mathcal{G}_{0,1}(\tau), \\ F(\tau, \sqrt{2}) &= e^{2\pi i\tau} + i\mathcal{G}_{-1,1}(\tau), \\ \frac{\partial^2}{\partial r^2} \Big|_{r=0} F(\tau, r) &= 2\pi i\tau + 2\pi\mathcal{G}_{0,0}(\tau), \quad \text{and} \\ \frac{\partial}{\partial r} \Big|_{r=\sqrt{2}} F(\tau, r) &= 2\pi i\sqrt{2}e^{2\pi i\tau} + 2\pi\sqrt{2}\mathcal{G}_{-1,0}(\tau). \end{aligned}$$

Equivalently, the proposition specifies these values and derivatives of the interpolation basis functions. It gives another interpretation of the non-decaying asymptotics $\mathcal{G}_{k,j}$ of the kernel \mathcal{K} , and it generalizes the computation of special values of the optimal sphere packing auxiliary functions in [47, Propositions 4 and 8] and [14, Sections 2 and 3].

If one computes $\widetilde{F}(\tau, 0)$ using Proposition 6.3 and the functional equation relating F and \widetilde{F} , one obtains τ times an explicit quasimodular form. Using the theta series for Λ_d and Ramanujan's derivative formulas for modular forms [50, Section 5], a straightforward calculation shows that

$$(6.1) \quad \widetilde{F}(\tau, 0) = -\frac{2\pi i\tau}{d} \sum_{x \in \Lambda_d} |x|^2 e^{\pi i|x|^2\tau}.$$

Equivalently, if f is the auxiliary function from Lemma 6.2 for the potential function $r \mapsto e^{-\alpha r^2}$, then

$$\widehat{f}(0) = \frac{2\alpha}{d} E_{r \mapsto r^2 e^{-\alpha r^2}}(\Lambda_d),$$

in agreement with the prediction in [16, Conjecture 6.1].

6.2. Reduction to positivity of kernels. To complete the proof of universal optimality, all that remains is to prove Proposition 6.1, i.e., the inequality $\widetilde{F}(\tau, r) \geq 0$ and the conditions for equality. For the rest of the section we thus assume $\operatorname{Re}(\tau) = 0$ (in particular, $\tau \in \mathcal{D}$).

The first obstacle to proving that $\widetilde{F}(\tau, r) \geq 0$ is dealing with the integral transform that defines \widetilde{F} in terms of the kernel $\widehat{\mathcal{K}}$. The kernel is written explicitly in terms of well-known special functions, and we will deduce the positivity of the integral at the level of the kernel itself. As in the sphere packing papers [47] and [14], that will involve additional complications for $d = 24$ beyond those that occur in the case of $d = 8$.

Specifically, recall from (5.2) that

$$(6.2) \quad \widetilde{F}(\tau, r) = 4 \sin(\pi r^2/2)^2 \int_0^\infty \widehat{\mathcal{K}}(\tau, it) e^{-\pi r^2 t} dt,$$

which is absolutely convergent for $\tau \in \mathcal{D}$ and $|r|$ sufficiently large, and has an analytic continuation to r in some open neighborhood of \mathbb{R} in \mathbb{C} . We showed in Section 5.1 that this continuation of (6.2) can be achieved by subtracting pieces of the asymptotics of $\mathcal{K}(\tau, it)$ as $t \rightarrow \infty$, as in (5.3) and (5.4). Since Proposition 6.1 does not involve the point $r = 0$, here it suffices to perform a milder truncation by subtracting only the $k = -1$ terms in (4.37), and only for dimension $d = 24$, since for $d = 8$ the integral in (6.2) is absolutely convergent for all $r > 0$.

When $d = 8$, our strategy for proving Proposition 6.1 is to show that $\widehat{\mathcal{K}}^{(8)}(\tau, it) > 0$, which immediately implies both the desired inequality and the equality conditions. The analogous inequality $\widehat{\mathcal{K}}^{(24)}(\tau, it) > 0$ for $d = 24$ holds as well, but additional work is needed to deal with small r . Specifically, we write $\widehat{\mathcal{K}}^{(24)}(\tau, it) = \widehat{\mathcal{E}}(\tau, it) + O(t)$ as $t \rightarrow \infty$, where

$$\widehat{\mathcal{E}}(\tau, z) = \frac{e^{-2\pi iz}}{3456\pi} (z\widehat{\mathcal{E}}_1(\tau) + \widehat{\mathcal{E}}_0(\tau)) \quad \text{and} \quad \widehat{\mathcal{E}}_j(\tau) = \tau\widehat{\mathcal{E}}_{j,1}(\tau) + \widehat{\mathcal{E}}_{j,0}(\tau),$$

with

$$\begin{aligned}\widehat{\mathcal{E}}_{0,0} &= -6912 \log(2)\Delta - 36E_2E_4E_6 + 16E_4^3 + 20E_6^2 + 108E_4\sqrt{\Delta}(V\mathcal{L} + W\mathcal{L}_S), \\ \widehat{\mathcal{E}}_{0,1} &= -\pi i(6E_2^2E_4E_6 - 5E_2E_4^3 - 7E_2E_6^2 + 6E_4^2E_6), \\ \widehat{\mathcal{E}}_{1,0} &= 12\pi i(-E_2E_4E_6 + E_6^2 + 720\Delta), \quad \text{and} \\ \widehat{\mathcal{E}}_{1,1} &= 2\pi^2(E_2^2E_4E_6 - 2E_2E_6^2 - 1728E_2\Delta + E_4^2E_6)\end{aligned}$$

expressed in terms of quasimodular forms, \mathcal{L} , and \mathcal{L}_S .

For $d = 24$ the integral in (6.2) converges absolutely for $|r| > \sqrt{2}$. For the range $0 < |r| \leq \sqrt{2}$ we will use the truncation method from [14], by instead setting $p = 1.01$ and writing

$$\int_0^\infty \widehat{\mathcal{K}}^{(24)}(\tau, it)e^{-\pi r^2 t} dt = \int_0^\infty \widehat{\mathcal{K}}^{\text{trunc}}(\tau, it)e^{-\pi r^2 t} dt + \int_p^\infty \widehat{\mathcal{E}}(\tau, it)e^{-\pi r^2 t} dt,$$

where

$$(6.3) \quad \widehat{\mathcal{K}}^{\text{trunc}}(\tau, it) = \begin{cases} \widehat{\mathcal{K}}^{(24)}(\tau, it) & \text{for } t < p, \text{ and} \\ \widehat{\mathcal{K}}^{(24)}(\tau, it) - \widehat{\mathcal{E}}(\tau, it) & \text{for } t \geq p. \end{cases}$$

The value of p has been chosen to ensure the positivity properties below, in particular so that $\lambda(ip) < 0.49$, where λ is the modular function from Section 2.1.3 (for comparison, $\lambda(i) = 1/2$). The last integral in (6.3) can be evaluated as

$$\begin{aligned}\int_p^\infty \frac{it\widehat{\mathcal{E}}_1(\tau) + \widehat{\mathcal{E}}_0(\tau)}{3456\pi} e^{\pi(2-r^2)t} dt &= \\ &= \frac{e^{-p\pi(r^2-2)}}{(r^2-2)^2} \cdot \frac{\widehat{\mathcal{E}}_0(\tau)\pi(r^2-2) + i\widehat{\mathcal{E}}_1(\tau)(1+p\pi(r^2-2))}{3456\pi^3}.\end{aligned}$$

The singularities from the factor of $(r^2-2)^2$ in the denominator are compensated for by the vanishing of the $\sin(\pi r^2/2)^2$ factor in (6.2). Because $n_0 = 2$ and $\sin(\pi r^2/2)^2$ vanishes at other $r^2 \in 2\mathbb{Z}$, we deduce that Proposition 6.1 is a consequence of the following three statements for $\text{Re}(\tau) = 0$ and $t \in (0, \infty)$:

$$(6.4) \quad \begin{aligned}(1) & \widehat{\mathcal{K}}^{(d)}(\tau, it) > 0 \text{ for } d \in \{8, 24\}, \\ (2) & \widehat{\mathcal{K}}^{\text{trunc}}(\tau, it) > 0 \text{ for } t \geq p, \text{ and} \\ (3) & \widehat{\mathcal{E}}_0(\tau)\pi(r^2-2) + i\widehat{\mathcal{E}}_1(\tau)(1+p\pi(r^2-2)) > 0 \text{ for } r \leq \sqrt{2}.\end{aligned}$$

Statement (3) is itself a consequence of

$$\begin{aligned}(3a) & \widehat{\mathcal{E}}_0(\tau) + ip\widehat{\mathcal{E}}_1(\tau) < 0, \text{ and} \\ (3b) & i\widehat{\mathcal{E}}_1(\tau) > 0.\end{aligned}$$

We have no simple proof of these inequalities, but we will outline below how we have proved them by mathematically rigorous computer calculations.

Proving inequalities of this sort for quasimodular forms also arose in the sphere packing papers [47] and [14], but the computations are much more challenging in our case. In the sphere packing cases, all that was needed was to prove positivity for relatively simple functions of a single variable. Asymptotic calculations reduce the proof to analyzing functions on compact intervals, and that is a straightforward and manageable computation using any of several techniques ([47] used interval arithmetic and [14] used q -expansions).

By contrast, inequalities (1) and (2) in (6.4) involve much more complicated functions of two variables. We must analyze singularities along curves, which are more subtle than the point singularities in one dimension. Furthermore, these curves intersect, and the intersection points are particularly troublesome. In the rest of this section we explain how to overcome these obstacles.

Inequalities (3a) and (3b) involve only a single variable τ , and can be verified using the methods from [14, Appendix A], or the λ function coordinates that we use below for the other inequalities. We thus focus on inequalities (1) and (2), describing the underlying mathematical ideas that were rigorously verified by a computer calculation.

6.3. Passing to the unit square. Recall from Section 2.1.3 that $t \mapsto \lambda(it)$ is a decreasing function mapping $(0, \infty)$ onto $(0, 1)$. Our first step is to express the kernels $\widehat{\mathcal{K}}^{(d)}$ and $\widehat{\mathcal{K}}^{\text{trunc}}$ in terms of functions on the interior of the unit square by inverting the map $(\tau, z) \mapsto (\lambda(\tau), \lambda(z))$. Rewriting the kernels in this way is not logically necessary, but it has the advantage of expressing everything in terms of a small number of functions that can be bounded systematically and efficiently, and we can take advantage of relationships between these functions to obtain more accurate estimates when proving bounds.

Specifically, if we use the identities (2.12), (2.20), (2.21), and (2.22) to write modular forms, z , τ , and E_2 in terms of λ and write $\mathcal{L} = \log(\lambda)$ and $\mathcal{L}_S = \log(1 - \lambda)$ on the imaginary axis, we obtain functions $L^{(d)}$ and L^{trunc} on $(0, 1) \times (0, 1)$ such that

$$\mathcal{K}^{(d)}(\tau, z) = L^{(d)}(\lambda(\tau), \lambda(z)) \quad \text{and} \quad \mathcal{K}^{\text{trunc}}(\tau, z) = L^{\text{trunc}}(\lambda(\tau), \lambda(z))$$

when $\text{Re}(\tau) = \text{Re}(z) = 0$. The resulting functions $L^{(d)}(x, y)$ are rational functions of x , y , and the logarithms and complete elliptic integrals of x , $1 - x$, y , and $1 - y$, while L^{trunc} is slightly more complicated, as described below.

The inequalities (1) and (2) in (6.4) thus transform into the assertions that

$$L^{(d)}(x, y) > 0$$

for $0 < x, y < 1$ and $d = 8$ or 24 , and that

$$L^{\text{trunc}}(x, y) = L^{(24)}(x, y) - \psi^{\text{trunc}}(x, y) > 0$$

for $0 < x < 1$ and $0 < y < 0.49$, where $\psi^{\text{trunc}}(\lambda(\tau), \lambda(z)) = \widehat{\mathcal{E}}(\tau, z)$ and the constant 0.49 is just slightly larger than $\lambda(ip) = \lambda(1.01i) = 0.4891135\dots$. One complication with L^{trunc} is that $\widehat{\mathcal{E}}(\tau, z)$ involves a factor of $e^{-2\pi iz}$, which becomes $e^{2\pi K(1-y)/K(y)}$ by (2.21) when we set $y = \lambda(z)$. We write

$$\psi^{\text{trunc}}(x, y) = e^{2\pi K(1-y)/K(y)} \widetilde{\psi}^{\text{trunc}}(x, y),$$

where $\widetilde{\psi}^{\text{trunc}}(\lambda(\tau), \lambda(z)) = (\widehat{\mathcal{E}}_0(\tau) + z\widehat{\mathcal{E}}_1(\tau))/(3456\pi)$. Observe that

$$L^{\text{trunc}}(x, y) \geq L^{(24)}(x, y)$$

whenever $\widetilde{\psi}^{\text{trunc}}(x, y) \leq 0$, and otherwise $L^{\text{trunc}}(x, y)$ is bounded below by

$$\widetilde{L}^{\text{trunc}}(x, y) := L^{(24)}(x, y) - \left(\frac{256}{y^2} - \frac{256}{y} + 24 + \frac{4 \cdot 10^9}{970299} y^2 \right) \widetilde{\psi}^{\text{trunc}}(x, y)$$

according to (6.5) below. In particular, inequality (1) in (6.4) and the positivity of $\widetilde{L}^{\text{trunc}}(x, y)$ for $0 < x < 1$ and $0 < y < 0.49$ together imply inequality (2).

The lower bound used above can be obtained by truncating the Taylor series of $e^{2\pi K(1-y)/K(y)}$ and bounding the omitted coefficients. It is most convenient to obtain such bounds via complex analysis. For example, the functions $A_j(z)$ in (2.23), along with $E(z)$, $K(z)$, and $\log(1-z)$, all have modulus bounded by 5 on $\{z \in \mathbb{C} : |z| = 0.99\}$, and so their Taylor series coefficients of z^n are bounded above by $5 \cdot 0.99^{-n}$. (This bound of 5, which is easily improved for some of these individual functions, comes from the constant sign of the coefficients of z^n for $n > 1$ and the value at $z = 0.99$.) For the bound needed above, one can check that $z^2 e^{2\pi K(1-z)/K(z)}$ is holomorphic on the open unit disk and

$$(6.5) \quad e^{2\pi K(1-y)/K(y)} \leq \frac{256}{y^2} - \frac{256}{y} + 24 + \frac{4 \cdot 10^9}{970299} y^2$$

for $0 < y < 1/2$, where the error term comes from the bound $|K(z)| \geq 1.3$ for $|z| = 0.99$ (which itself can be shown by evaluation at close points on the circle and derivative bounds).

The next several subsections describe the verification of inequalities (1) and (2) in (6.4). The primary difficulty is dealing with singularities. Since our formulas for the kernels involve denominators of $j(\tau) - j(z)$, which vanish when $\tau = z$ or $\tau = -1/z$, our formulas for $L^{(d)}(x, y)$ and $\widetilde{L}^{\text{trunc}}(x, y)$ naively yield $0/0$ when $x = y$ or $x = 1 - y$. The kernels themselves are not actually singular along these lines, because $\phi(I) = \phi(S) = 0$ in the residue formulas from part (3) of Theorem 4.3, but we must effectively treat the diagonal lines $x = y$ and $x = 1 - y$ as singularities in the formulas. In addition, there are singularities at the edges of the unit square coming from (2.23). In this rest of this section, we describe the methods used to treat these singularities, starting away from any singularities and working our way up to the most singular points: the four corners of the unit square, at which three singularities meet.

In our numerical calculations, it is convenient to remove obviously positive factors from $L^{(d)}(x, y)$ and $\tilde{L}^{\text{trunc}}(x, y)$. To do so, we multiply each of them by

$$(1 - xy)(1 - x(1 - y))(1 - y(1 - x))(1 - (1 - x)(1 - y)),$$

and we furthermore multiply $L^{(8)}(x, y)$ by

$$\frac{\pi^4 K(y)^2 K(1 - x)}{2K(x)^4},$$

$L^{(24)}(x, y)$ by

$$\frac{3\pi^4 y^2 (1 - y)^2 K(y)^{10} K(1 - x)}{K(x)^{12}},$$

and $\tilde{L}^{\text{trunc}}(x, y)$ by

$$\frac{3\pi^{14} y^2 (1 - y)^2 K(y)^{12}}{K(x)^{11}}.$$

For simplicity of notation, in the remainder of Section 6 we use the notation $L^{(d)}(x, y)$ and $\tilde{L}^{\text{trunc}}(x, y)$ to refer to the functions after removing these factors.

6.4. Interval bounds for elliptic integrals. Away from all singularities it is possible to prove positivity via interval arithmetic estimates on $L^{(d)}(x, y)$ and $\tilde{L}^{\text{trunc}}(x, y)$. Interval arithmetic provides rigorous upper and lower bounds on the values of a function over a given interval (see, for example, [34]). It works beautifully for small intervals and well-behaved functions, but the bounds become much less tight for large intervals or near singularities. In practice, instead of simply subdividing intervals to improve the bounds, we obtained better results by using interval arithmetic to evaluate Taylor series expansions, while controlling the error terms by using crude interval arithmetic bounds on partial derivatives, because these error bounds do not need to be tight.

Interval arithmetic for polynomials and logarithms is standard and is part of many software packages. We will next describe how to obtain rigorous interval bounds for the complete elliptic integrals E and K by adapting the arithmetic-geometric mean algorithms for computing them from [3, Chapter 1]. Consider the sequences $(a_n)_{n \geq 0}$ and $(b_n)_{n \geq 0}$ with $a_0 \geq b_0 > 0$ and

$$a_{n+1} = \frac{a_n + b_n}{2} \quad \text{and} \quad b_{n+1} = \sqrt{a_n b_n}.$$

Then $b_n \leq b_{n+1} \leq a_{n+1} \leq a_n$ and both a_n and b_n converge to the same limit $M(a_0, b_0)$ (the *arithmetic-geometric mean* of a_0 and b_0), which is related to the complete elliptic integral K by

$$K(x) = \frac{\pi}{2M(1, \sqrt{1 - x})}$$

for $0 < x < 1$. Since the interval $[b_n, a_n]$ contains $M(a_0, b_0)$, these recurrences give a fast interval-arithmetic algorithm for K .

Computations of E are more subtle and use the formula

$$(6.6) \quad \frac{E(x)}{K(x)} = 1 - \sum_{n \geq 0} 2^{n-1} c_n^2$$

from [3, Algorithm 1.2], where $c_0 = \sqrt{x}$ and

$$c_{n+1} = \frac{a_n - b_n}{2}$$

with a_n and b_n defined as above, starting with $(a_0, b_0) = (1, \sqrt{1-x})$; one can show that $c_{n+1} = c_n^2 / (4a_{n+1})$, which avoids potential precision loss from subtracting a_n and b_n . Since

$$c_n = \frac{a_{n-1} - b_{n-1}}{2} \leq \frac{a_{n-1}}{2} \leq a_n \leq 2a_{n+1},$$

we have

$$c_{n+1} = \frac{c_n^2}{4a_{n+1}} \leq \frac{c_n}{2},$$

and therefore the tail of the series is

$$\sum_{n > m} 2^{n-1} c_n^2 \leq \sum_{n > m} 2^{n-1} (2^{m+1-n} c_{m+1})^2 = 2^{m+1} c_{m+1}^2.$$

From this tail bound, truncating the series in (6.6) yields interval bounds for the ratio $E(x)/K(x)$, and hence $E(x)$ itself in light of the algorithm for $K(x)$ above.

6.5. Near the diagonals and their crossing. After removing factors that are obviously positive as discussed above, the kernels $L^{(d)}(x, y)$ and $\tilde{L}^{\text{trunc}}(x, y)$ have denominator $(x-y)(1-x-y)$, and numerators that vanish at $x = y$ and $x = 1 - y$, as they must in order to be well defined on the interior of the unit square. We use Taylor expansions in one of the variables (along with rigorous interval bounds on partial derivatives, which are themselves expressible in terms of polynomials, logarithms, E , and K) to prove that the kernels are positive near the diagonals. For this purpose it is convenient to work with the coordinate system $(u, v) = (x - y, 1 - x - y)$ and take partial derivatives in u and v .

The most subtle point is the diagonal crossing point $(x, y) = (\frac{1}{2}, \frac{1}{2})$. There both $u = x - y$ and $v = 1 - x - y$ vanish, and so $L^{(d)}(x, y)$ and $\tilde{L}^{\text{trunc}}(x, y)$ can each be written in the form $\frac{f(u, v)}{uv}$, where $f(u, 0) = f(0, v) = 0$ for all u and v . To analyze these functions, we obtain bounds on their Taylor series coefficients by writing

$$\frac{f(u, v)}{uv} = \int_0^1 \int_0^1 f^{(1,1)}(us, vt) ds dt,$$

where $f^{(i,j)}(u, v)$ denotes $(\partial^i/\partial u^i)(\partial^j/\partial v^j)f(u, v)$, and hence

$$\frac{\partial^i}{\partial u^i} \frac{\partial^j}{\partial v^j} \frac{f(u, v)}{uv} = \int_0^1 \int_0^1 s^i t^j f^{(i+1, j+1)}(us, vt) ds dt.$$

It follows that

$$\left| \frac{\partial^i}{\partial u^i} \frac{\partial^j}{\partial v^j} \frac{f(u, v)}{uv} \right| \leq \frac{\max_{0 \leq s, t \leq 1} |f^{(i+1, j+1)}(us, vt)|}{(i+1)(j+1)}.$$

Interval arithmetic bounds on the derivatives then gives rigorous upper bounds on the error terms in the Taylor expansion, which can be used to show positivity close to $(x, y) = (\frac{1}{2}, \frac{1}{2})$.

6.6. Near the edges. For the rest of this section, we reduce to the situation of $0 < x, y \leq \frac{1}{2}$ by changing coordinates from x to $1 - x$ and from y to $1 - y$ as needed. The singularities at the edges come from logarithms as well as the logarithmic behavior of the elliptic integrals $E(z)$ and $K(z)$ near $z = 1$ from (2.23). After substituting those formulas for E and K , we arrive at a sum of powers of logarithms times holomorphic functions. We compute Taylor series for these holomorphic functions in the direction orthogonal to the edge in question, and use interval arithmetic in the tangential direction, while taking into account the Taylor coefficient bounds for special functions mentioned in the paragraph containing (6.5). On narrow strips near the edges we obtain a lower bound for $L^{(d)}(x, y)$ and $\tilde{L}^{\text{trunc}}(x, y)$ as a linear or quadratic polynomial in the logarithm that is responsible for the singularity, whose positivity is straightforward to verify (e.g., using Sturm's theorem or interval arithmetic).

6.7. The corners. The corners are intersections of three distinct singular curves. As in Section 6.6, we change coordinates if necessary so that the corner is at $(x, y) = (0, 0)$. After substituting the formulas in (2.23), we obtain expressions for $L^{(d)}(x, y)$ and $\tilde{L}^{\text{trunc}}(x, y)$ of the form

$$(6.7) \quad \mathcal{H}(x, y) = \frac{1}{x - y} \sum_{i, j \geq 0} h_{i, j}(x, y) \log(x)^i \log(y)^j,$$

where the sum contains only finitely many terms and each coefficient function $h_{i, j}(x, y)$ is holomorphic in $\{x \in \mathbb{C} : |x| < 1\} \times \{y \in \mathbb{C} : |y| < 1\}$. In particular, these coefficient functions can be written in terms of $\log(1 - u)$, $E(u)$, $K(u)$, and the functions $A_j(u)$ from (2.23) for $u = x$ and $u = y$.

Since the kernel $\mathcal{H}(x, y)$ is well defined on the diagonal, the sum in (6.7) must vanish there, but the individual coefficients $h_{i, j}(x, y)$ might not. To

remedy this, we choose $\beta \in \mathbb{Z}$ and write

$$(6.8) \quad \begin{aligned} \mathcal{H}(x, y) &= \sum_{i, j \geq 0} \frac{\tilde{h}_{i, j}(x, y)}{x - y} \log(x)^i \log(y)^j \\ &+ \left(\frac{y}{x}\right)^\beta \sum_{i, j} h_{i, j}(x, x) \frac{\log(x)^i \log(y)^j}{x - y}, \end{aligned}$$

with

$$\tilde{h}_{i, j}(x, y) = h_{i, j}(x, y) - \left(\frac{y}{x}\right)^\beta h_{i, j}(x, x),$$

so that $\tilde{h}_{i, j}(x, x) = 0$ and therefore $\tilde{h}_{i, j}(x, y)/(x - y)$ is holomorphic at $x = y$. This procedure is required in only one corner for $L^{(8)}(x, y)$ and $L^{(24)}(x, y)$ (with $\beta = 0$), and one corner of $\tilde{L}^{\text{trunc}}(x, y)$ (with $\beta = 2$, in order to obtain better estimates).

Each function $\tilde{h}_{i, j}(x, y)$ has a Taylor series expansion $\sum_{n, m \geq 0} b_{n, m} x^n y^m$ that vanishes on the diagonal. In other words,

$$\sum_{n, m \geq 0} b_{n, m} y^n y^m = 0,$$

and therefore

$$\frac{\tilde{h}_{i, j}(x, y)}{x - y} = \sum_{n, m \geq 0} b_{n, m} \frac{x^n y^m - y^n y^m}{x - y} = \sum_{n, m \geq 0} b_{n, m} (x^{n-1} + x^{n-2}y + \dots + y^{n-1}) y^m$$

gives a series expansion of this ratio. The individual coefficients $b_{n, m}$ can be computed from the Taylor series of $\log(1 - z)$, $E(z)$, $K(z)$, and $A_j(z)$, while at the same time the $5 \cdot 0.99^{-n}$ bound on the Taylor coefficients of these special functions gives an upper bound on all $b_{n, m}$. Computing a finite number of coefficients explicitly and using this upper bound on the rest, we obtain a rigorous lower bound on the first sum in (6.8).

When $h_{i, j}(x, x)$ is nonzero, direct computations show that it has a fairly simple form, from which its positivity for small values of x is manifest. For example, $\tilde{L}^{\text{trunc}}(x, y)$ has $h_{i, j}(x, x)$ nonzero only for one corner and two choices of indices (i, j) , where it equals

$$(2 - x)(x - 1)^4(x + 1)(1 - 2x)(x^2 - x + 1)^2 K(x)^2$$

up to a positive constant factor (as well as the obviously positive factors that were removed from $L^{(d)}$ and \tilde{L}^{trunc} earlier, as mentioned above). Similar, and in fact simpler, formulas hold in all other cases, and direct computation shows that the second sum in (6.8), namely

$$\sum_{i, j} h_{i, j}(x, x) \frac{\log(x)^i \log(y)^j}{x - y},$$

can be rewritten as $(\log(y) - \log(x))/(y - x)$ times an explicit, manifestly positive holomorphic function $d(x, y)$. From this we obtain a rigorous lower bound for $\mathcal{H}(x, y)$ for $0 < x, y \leq \frac{1}{2}$, of the form

$$(6.9) \quad \sum_{i,j} p_{i,j}(x, y) \log(x)^i \log(y)^j + d(x, y) \frac{\log(y) - \log(x)}{y - x}$$

with $p_{i,j}(x, y) \in \mathbb{R}[x, y]$ coming from the Taylor series argument above. The coefficient functions $p_{i,j}(x, y)$ and $d(x, y)$ can all be approximated well on small regions using interval arithmetic, as can the quotient $(\log(y) - \log(x))/(y - x)$. To obtain the positivity as both x and y approach zero, we found it efficient in situations where $d(x, y)$ vanishes identically and $p_{i,j}(0, 0) = 0$ to deduce lower bounds on (6.9) and similar expressions via lower bounds on gradients, for which interval arithmetic had better behavior. These arguments complete the proof of Proposition 6.1, and thus Theorem 1.4.

7. Generalizations and open questions

Theorem 1.7 is ideally suited to proving universal optimality for E_8 and the Leech lattice, but the underlying analytic phenomena are not limited to 8 and 24 dimensions. Instead, it seems that the remarkable aspect of these dimensions is the existence of the lattices, while interpolation theorems may hold much more broadly.

OPEN PROBLEM 7.1. *Let d and k be positive integers. If $f \in \mathcal{S}_{\text{rad}}(\mathbb{R}^d)$ satisfies $f^{(j)}(\sqrt{kn}) = \widehat{f}^{(j)}(\sqrt{kn}) = 0$ for all integers $n \geq 0$ and $0 \leq j < k$, then must f vanish identically?*

The answer is yes when $k = d = 1$ by [37, Corollary 1], and it follows for $k = 1$ and all dimensions using the techniques of [37] without much difficulty. It also holds when $(d, k) = (8, 2)$ or $(d, k) = (24, 2)$ by Theorem 1.7, and likely holds more broadly for $k = 2$. As far as we know, interpolation theorems of this form would not lead to any optimality theorems in packing or energy minimization beyond E_8 and the Leech lattice.

The special nature of the interpolation points $\sqrt{2n}$ plays an essential role in our proofs. For example, the functional equations

$$F(\tau + 2, x) - 2F(\tau + 1, x) + F(\tau, x) = 0$$

and

$$\widetilde{F}(\tau + 2, x) - 2\widetilde{F}(\tau + 1, x) + \widetilde{F}(\tau, x) = 0$$

encode algebraic properties of $\sqrt{2n}$, without which we would be unable to construct the interpolation basis. This framework (i.e., Theorem 3.1) generalizes naturally to the interpolation points \sqrt{kn} from Open Problem 7.1, with

the corresponding functional equations using a k -th difference operator in τ . However, our methods cannot apply to $k > 2$ without serious modification.

There is no reason why interpolation theorems should be restricted to radii that are square roots of integers. We expect that far more is true, at the cost of giving up the algebraic structure behind our proofs. In particular, optimizing the linear programming bound for Gaussian energy seems to lead to interpolation formulas, except in low dimensions. Recall that the optimal functions for linear programming bounds seem to work as specified by the following conjecture, which is a variant of [11, Section 7] and [13, Section 9]:

CONJECTURE 7.2. *Fix a dimension $d \geq 3$, density $\rho = 1$, and $\alpha > 0$. Then the optimal linear programming bound $\widehat{f}(0) - f(0)$ from Proposition 1.6 for the potential $p(r) = e^{-\alpha r^2}$ is achieved by some radial Schwartz function f , the radii $|x|$ for which $f(x) = e^{-\alpha|x|^2}$ are the same as the radii $|y|$ for which $\widehat{f}(y) = 0$, they form a discrete, infinite set, and these radii do not depend on α .*

Note that at least one implication holds among the assertions of this conjecture: the radii at which $f(x) = e^{-\alpha|x|^2}$ must be the same as those for which $\widehat{f}(y) = 0$ if all these radii are independent of α , thanks to the duality symmetry from [16, Section 6].

OPEN PROBLEM 7.3. *Let r_1, r_2, \dots be the radii from Conjecture 7.2 for some d . For which d is every $f \in \mathcal{S}_{\text{rad}}(\mathbb{R}^d)$ uniquely determined by the values $f(r_n)$, $f'(r_n)$, $\widehat{f}(r_n)$, and $\widehat{f}'(r_n)$ for $n \geq 1$ through an interpolation formula?*

Numerically constructing the interpolation basis seems to work about as well for general $d \geq 3$ as it does for $d = 8$ or $d = 24$, which suggests that interpolation holds for many or even all such d . In particular, simple variants of the algorithms from [11] and [12] yield interpolation formulas of this sort for all functions of the form $x \mapsto p(|x|^2)e^{-\pi|x|^2}$, where p is a polynomial of degree at most some bound N . As N grows, these interpolation formulas seem to converge to well-behaved limits when $d \geq 3$.

From an interpolation perspective, the numerical evidence suggests that these dimensions behave much like $d = 8$ and $d = 24$. On the other hand, we know of no simple description of the interpolation points r_1, r_2, \dots when $d \notin \{8, 24\}$, and we are not aware of any point configurations in \mathbb{R}^d that meet the optimal linear programming bounds in these cases. In other words, $d = 8$ and $d = 24$ differ both algebraically and geometrically from the other dimensions.

When $d \leq 2$, universally optimal configurations exist (conjecturally for $d = 2$), but the radii r_1, r_2, \dots are more sparsely spaced, seemingly too much so to allow for an interpolation theorem. For $d = 1$, we can in fact rule out an interpolation theorem corresponding to the point configuration \mathbb{Z} :

LEMMA 7.4. *Radial Schwartz functions $f: \mathbb{R} \rightarrow \mathbb{R}$ are not uniquely determined by the values $f(n)$, $f'(n)$, $\widehat{f}(n)$, and $\widehat{f}'(n)$ for integers $n \geq 1$.*

This lemma follows immediately from [37, Theorem 2], but for completeness we will give a simpler, direct proof.

Proof. Let t be the tent function

$$t(x) = \begin{cases} 1 - |x| & \text{if } |x| \leq 1, \text{ and} \\ 0 & \text{otherwise.} \end{cases}$$

Then

$$\widehat{t}(y) = \left(\frac{\sin \pi y}{\pi y} \right)^2,$$

which vanishes to second order at all nonzero integers. Now let b be any even, smooth, nonnegative function with support contained in $[-\frac{1}{2}, \frac{1}{2}]$, and consider the convolution $f = b * t$. This function is smooth and compactly supported, and it is therefore a Schwartz function, whose Fourier transform $\widehat{f} = \widehat{b} \widehat{t}$ again vanishes to second order at all nonzero integers. Furthermore, f vanishes to infinite order at all nonzero integers other than ± 1 , because its support is contained in $[-3/2, 3/2]$. If the interpolation property in the lemma statement held, then f would be uniquely determined by $f(1)$ and $f'(1)$. In other words, there would be just a two-dimensional space of functions of this form. Furthermore, those two dimensions would have to correspond to the support of f and scalar multiplication. Thus, f would be completely determined by the support and total integral of b . However, that is manifestly false: the value

$$f(0) = \int_{-1}^1 b(x)(1 - |x|) dx$$

is not determined by the support and integral of b . \square

The two-dimensional case is more difficult to analyze. If we scale the hexagonal lattice so that it has density 1, then the distances between the lattice points are given by

$$(4/3)^{1/4} \sqrt{j^2 + jk + k^2},$$

where j and k range over the integers. Bernays [1] proved that as $N \rightarrow \infty$, the number of such distances between 0 and N (counted without multiplicity) is asymptotic to

$$\frac{CN^2}{\sqrt{\log N}}$$

for some positive constant C . Thus, the distances in the hexagonal lattice are slightly sparser than those in E_8 or the Leech lattice, for which the corresponding counts of distinct distances are $N^2/2 + O(1)$. This sparsity suggests that the

interpolation property might fail in \mathbb{R}^2 , and numerical computations indicate that it does:

CONJECTURE 7.5. *Let r_1, r_2, \dots be the positive real numbers of the form $(4/3)^{1/4} \sqrt{j^2 + jk + k^2}$, where j and k are integers. Then radial Schwartz functions $f: \mathbb{R}^2 \rightarrow \mathbb{R}$ are not uniquely determined by the values $f(r_n)$, $f'(r_n)$, $\widehat{f}(r_n)$, and $\widehat{f}'(r_n)$ for integers $n \geq 1$.*

More generally, in each dimension we expect that interpolation fails whenever the sequence r_1, r_2, \dots contains only $o(N^2)$ elements between 0 and N as $N \rightarrow \infty$, and perhaps even $(c + o(1))N^2$ elements for some constant $c < \frac{1}{2}$. However, we have not explored this possibility thoroughly. Note that the interpolation property cannot depend solely on the asymptotic growth rate of the radii, because it is sensitive to deleting a single interpolation point. We have no characterization of when the interpolation property holds, and it is unclear just how sensitive it is. For example, does moving (but not removing) finitely many interpolation points preserve the interpolation property?

Cohn and Kumar [13] conjectured that the linear programming bounds are sharp in two dimensions and prove the universal optimality of the hexagonal lattice. There is strong numerical evidence in favor of this conjecture, and in fact the numerics converge far more quickly than in eight or twenty-four dimensions. However, it seems surprisingly difficult to prove that they converge to a sharp bound. Assuming Conjecture 7.5 holds, one cannot prove universal optimality in \mathbb{R}^2 via a straightforward adaptation of the interpolation strategy used in \mathbb{R}^8 and \mathbb{R}^{24} . Instead, a more sophisticated approach may be needed.

Despite Lemma 7.4, universal optimality in \mathbb{R}^1 can be proved using an interpolation theorem for a different function space, namely Shannon sampling for band-limited functions (see [13, p. 142]). Is it possible that universal optimality in \mathbb{R}^2 also corresponds to an interpolation theorem for some space of radial functions? That would establish a satisfying pattern, but we are unable to propose what the relevant function space might be.

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