

RECEIVED: March 6, 2019

REVISED: April 8, 2019

ACCEPTED: April 17, 2019

PUBLISHED: April 23, 2019

Modular graph functions and odd cuspidal functions. Fourier and Poincaré series¹

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ABSTRACT: Modular graph functions are $SL(2, \mathbb{Z})$ -invariant functions associated with Feynman graphs of a two-dimensional conformal field theory on a torus of modulus τ . For one-loop graphs they reduce to real analytic Eisenstein series. We obtain the Fourier series, including the constant and non-constant Fourier modes, of all two-loop modular graph functions, as well as their Poincaré series with respect to $\Gamma_\infty \backslash \mathrm{PSL}(2, \mathbb{Z})$. The Fourier and Poincaré series provide the tools to compute the Petersson inner product of two-loop modular graph functions using Rankin-Selberg-Zagier methods. Modular graph functions which are odd under $\tau \rightarrow -\bar{\tau}$ are cuspidal functions, with exponential decay near the cusp, and exist starting at two loops. Holomorphic subgraph reduction and the sieve algorithm, developed in earlier work, are used to give a lower bound on the dimension of the space \mathfrak{A}_w of odd two-loop modular graph functions of weight w . For $w \leq 11$ the bound is saturated and we exhibit a basis for \mathfrak{A}_w .

KEYWORDS: Scattering Amplitudes, Superstrings and Heterotic Strings

ARXIV EPRINT: [1902.04180](https://arxiv.org/abs/1902.04180)

¹This research is supported in part by the National Science Foundation under grant PHY-16-19926.

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1 Introduction

A modular graph function is a function associated to a certain Feynman graph for a two-dimensional conformal field theory on a torus with complex structure τ . It is invariant under transformations of τ by the modular group $\text{SL}(2, \mathbb{Z})$. Modular graph functions may be decomposed into even and odd pieces depending on their parity under $\tau \rightarrow -\bar{\tau}$, and their *loop order* is given by the number of loops of the corresponding Feynman graph. The

weight w of a modular graph function is half of the degree of homogeneity in the momenta of the graph, and provides a grading on the ring of such functions. One-loop modular graph functions are always even and, for weight w , reduce to real analytic Eisenstein series E_w .

The origin of modular graph functions at higher loop order may be traced back to string theory. The analytic structure of the genus-one superstring amplitude for four strings was analyzed in [1], and the low-energy expansion was organized in terms of modular functions in [2, 3]. A systematic study of modular graph functions was initiated in [4, 5] where they were shown to obey a system of differential and algebraic identities and in [6] where they were shown to be intimately related to single-valued elliptic polylogarithms. Further identities were derived in [7–10]. A key ingredient in the construction of these identities is the Laurent polynomial in $\text{Im}(\tau)$ of the modular graph function. It governs the leading behavior at the cusp $\tau \rightarrow i\infty$ and was obtained in closed form for an infinite class of even two-loop modular graph functions in [11], and for all graphs with four or fewer vertices in [12].

Modular graph *forms*, which associate an $\text{SL}(2, \mathbb{Z})$ non-holomorphic modular form to a certain type of (decorated) graph, were introduced in [13–15], where a systematic method was developed to construct all the identities between them. An alternative construction in terms of Eichler type integrals was developed in [16]. The underlying nature of these identities remains to be fully uncovered, but it is already clear that they generalize to modular graph forms some of the algebraic identities which exist between multiple zeta values (see for example [17–22]). Direct connections between modular graph functions and single-valued elliptic polylogarithms were obtained in [6, 23–25]. The role of multiple zeta values in string amplitudes has been investigated extensively in [26–30]. Generalizations of modular graph functions for Heterotic string amplitudes were studied in [31–33]. Higher genus modular graph functions were introduced and analyzed in [34, 35], building on earlier studies of special cases in [36–38], and further developed in [39–41].

In the present paper, we shall obtain the Fourier series, including constant and non-constant Fourier modes, of arbitrary two-loop modular graph functions, thereby generalizing the results of [11]. The coefficients of the Fourier modes involve odd zeta values as well as a novel generalization of divisor sums. We also construct the Poincaré series of all two-loop modular graph functions in terms of a sum over $\Gamma_\infty \backslash \text{PSL}(2, \mathbb{Z})$, with Γ_∞ the Borel subgroup of $\text{PSL}(2, \mathbb{Z})$, compute the corresponding seed functions, prove absolute convergence of the series, and outline the generalization to arbitrary weight and loop order.

The Fourier and Poincaré series expansions provide all the tools needed to evaluate integrals of two-loop modular graph functions over the fundamental domain of $\text{PSL}(2, \mathbb{Z})$, as well as the Petersson inner product between modular graph functions, using the Rankin-Selberg-Zagier methods. Some of these integrals are needed to evaluate the contributions to the genus-one string amplitudes which are analytic in the external momenta [2, 4].

Finally, we investigate the space \mathfrak{A}_w of odd two-loop modular graph functions of weight w , and show that \mathfrak{A}_w consists entirely of cuspidal functions, namely modular functions which have exponential decay near the cusp. Using the techniques of holomorphic subgraph reduction and the sieve algorithm developed in [13–15] we produce a lower bound on the dimension of \mathfrak{A}_w by exhibiting families of linearly independent odd modular graph functions at each weight. For $w \leq 4$ the space \mathfrak{A}_w is empty, while for $5 \leq w \leq 11$ the lower bound is saturated and we exhibit an explicit basis for \mathfrak{A}_w .

Organization. In section 2, we review the definition and basic properties of general modular graph functions and forms, define their parity under $\tau \rightarrow -\bar{\tau}$, discuss the one-loop and two-loop cases, and prove some basic decomposition formulas for two-loop modular graph functions. In section 3, we obtain the Poincaré series for general modular graph functions, compute the seed functions for the two-loop case and prove absolute convergence of the series. In section 4 we carry out the calculation of the Fourier series expansion for arbitrary two-loop modular graph functions. In section 5 we simplify the result for the constant Fourier mode, and extract the expansion for the non-constant Fourier modes. In section 6, we review the holomorphic subgraph reduction procedure and sieve algorithm, construct infinite families of linearly independent two-loop odd modular graph functions, and produce a lower bound for the dimension of the space \mathfrak{A}_w of odd modular graph functions of weight w . Finally, in section 7 we discuss the action of the Laplace operator on two-loop odd modular graph functions and study Petersson inner products between them. Technical details of the calculations and some explicit formulas for complicated expansion coefficients are relegated to the appendices.

Acknowledgments

We are happy to thank Bill Duke, Michael Green, Boris Pioline, and Oliver Schlotterer for their interest in this project and for several stimulating discussions. The research of ED is supported in part by the National Science Foundation under research grant PHY-16-19926, and was supported by a Fellowship from the Simons Foundation in 2017–2018. The research of JK is supported in part by funding from the Bhaumik Institute.

2 Modular graph functions and forms

In this section, we shall review the definitions and basic properties of modular graph functions and forms, define even and odd modular graph functions, exhibit the action of differential operators, and illustrate the cases of one and two loops.

2.1 Definitions and basic properties

A decorated connected graph (Γ, A, B) with V vertices and R edges is defined as follows. The connectivity matrix Γ of the graph has components Γ_{vr} where the index $v = 1, \dots, V$ labels the vertices of the graph and the index $r = 1, \dots, R$ labels its edges. No edge is allowed to begin and end on the same vertex. When edge r contains vertex v we have $\Gamma_{vr} = \pm 1$, while otherwise we have $\Gamma_{vr} = 0$. The decoration (A, B) of the graph is defined as follows,

$$\begin{aligned} A &= [a_1, \dots, a_R] & a &= a_1 + \dots + a_R \\ B &= [b_1, \dots, b_R] & b &= b_1 + \dots + b_R \end{aligned} \tag{2.1}$$

where $a_r, b_r \in \mathbb{C}$ with $a_r - b_r \in \mathbb{Z}$ for all $r = 1, \dots, R$. The pair (a_r, b_r) is associated with edge r , while a, b are associated with the full decorated graph.

To a decorated graph (Γ, A, B) we associate a complex-valued function on the Poincaré upper half plane \mathcal{H} , defined by the following Kronecker-Eisenstein sum,

$$\mathcal{C}_\Gamma \begin{bmatrix} A \\ B \end{bmatrix} (\tau) = \left(\frac{\tau_2}{\pi}\right)^{\frac{1}{2}a + \frac{1}{2}b} \sum_{p_1, \dots, p_R \in \Lambda'} \prod_{r=1}^R \frac{1}{(p_r)^{a_r} (\bar{p}_r)^{b_r}} \prod_{v=1}^V \delta \left(\sum_{s=1}^R \Gamma_{vs} p_s \right) \quad (2.2)$$

whenever this sum is absolutely convergent. The momentum lattice is given by $\Lambda = \mathbb{Z} + \tau\mathbb{Z}$ for $\tau \in \mathcal{H}$ with $\Lambda' = \Lambda \setminus \{0\}$. The momenta p_r depend holomorphically on \mathcal{H} . We refer to a_r and b_r as the exponents of respectively holomorphic and anti-holomorphic momenta. The Kronecker δ -symbol equals 1 when its argument vanishes and 0 otherwise. The number of loops L is the number of independent momenta, given by $L = R - V + 1$. The domain of absolute convergence of the sums in (2.2) is given by a system of inequalities on the combinations $\text{Re}(a_r + b_r)$, beyond which the functions \mathcal{C} of (2.2) may be defined by analytic continuation in the variables $a_r + b_r$.

The function \mathcal{C}_Γ in (2.2) vanishes whenever the integer $a - b$ is odd, or whenever the graph Γ becomes disconnected upon severing a single edge. A function \mathcal{C}_Γ associated with a connected graph Γ which is the union of two graphs $\Gamma = \Gamma_1 \cup \Gamma_2$ whose intersection $\Gamma_1 \cap \Gamma_2$ consists of a single vertex factorizes into the product $\mathcal{C}_{\Gamma_1} \mathcal{C}_{\Gamma_2}$ with the corresponding partitions of the exponents. Henceforth, we shall assume that $a - b$ is even, and that the graph Γ remains connected upon the removal of any single edge or vertex.

Under $\text{SL}(2, \mathbb{Z})$, the functions defined in (2.2) transform as follows,

$$\mathcal{C}_\Gamma \begin{bmatrix} A \\ B \end{bmatrix} \begin{pmatrix} \alpha\tau + \beta \\ \gamma\tau + \delta \end{pmatrix} = \left(\frac{\gamma\tau + \delta}{\gamma\bar{\tau} + \delta}\right)^{\frac{1}{2}a - \frac{1}{2}b} \mathcal{C}_\Gamma \begin{bmatrix} A \\ B \end{bmatrix} (\tau) \quad (2.3)$$

where $\alpha, \beta, \gamma, \delta \in \mathbb{Z}$ and $\alpha\delta - \beta\gamma = 1$. The *modular weight* of \mathcal{C}_Γ is given by the pair $(\frac{a-b}{2}, \frac{b-a}{2})$ which has integer entries since $a - b$ is even. For $a \neq b$, the function \mathcal{C}_Γ transforms as a non-holomorphic *modular graph form*. For $a = b$ the function \mathcal{C}_Γ is $\text{SL}(2, \mathbb{Z})$ -invariant and referred to as a *modular graph function* of *weight*¹ $w = a = b$.

A modular graph form is invariant under permutations of its vertices and its pairs of exponents (a_r, b_r) . It obeys a momentum conservation identity at each vertex $v = 1, \dots, V$,

$$\sum_{r=1}^R \Gamma_{vr} \mathcal{C}_\Gamma \begin{bmatrix} A - S_r \\ B \end{bmatrix} = \sum_{r=1}^R \Gamma_{vr} \mathcal{C}_\Gamma \begin{bmatrix} A \\ B - S_r \end{bmatrix} = 0 \quad (2.4)$$

The R -dimensional array S_r is defined to have zeroes in all slots except for the r -th,

$$S_r = [0_{r-1}, 1, 0_{R-r}] \quad (2.5)$$

where 0_ℓ stands for an array of ℓ zeros. The momentum conservation identities provide linear algebraic relations between modular graph forms of the same modular weight.

¹This *weight* is not to be confused with the *modular weight*, which vanishes for $a = b$.

2.2 Graphical representation

Though it will not be used much in the present work, we now briefly review the graphical representation of modular graph functions and forms. The generating function of modular graph functions with N vertices is given as follows,

$$\mathcal{B}_N(s_{ij}|\tau) = \prod_{k=1}^N \int_{\Sigma} \frac{d^2 z_k}{\tau_2} \exp \left(\sum_{1 \leq i < j \leq N} s_{ij} G(z_i - z_j|\tau) \right) \quad (2.6)$$

where Σ is a torus with complex structure modulus τ and $G(z_i - z_j|\tau)$ is the scalar Green function on Σ , given as a Fourier sum by

$$G(z|\tau) = \sum_{p \in \Lambda} \frac{\tau_2}{\pi |p|^2} e^{2\pi i(n\alpha - m\beta)} \quad (2.7)$$

for $z = \alpha + \beta\tau$. Modular graph functions may be represented by Feynman graphs on Σ as follows. We begin by representing a Green function graphically by an edge in a Feynman diagram,

$$\begin{array}{c} \circ \text{---} \circ \\ z_i \quad z_j \end{array} = G(z_i - z_j|\tau) \quad (2.8)$$

The integration over the position of a vertex z on which r Green functions end is denoted by an unmarked filled black dot, in contrast with an unintegrated vertex z_i which is represented by a marked unfilled white dot. The basic ingredients in the graphical notation are depicted in the graph below,

$$\begin{array}{c} \bullet \\ \diagup \quad \diagdown \\ \circ \quad \circ \quad \dots \quad \circ \quad \circ \\ z_1 \quad z_2 \quad z_{r-1} \quad z_r \end{array} = \int_{\Sigma} \frac{d^2 z}{\tau_2} \prod_{i=1}^r G(z - z_i|\tau) \quad (2.9)$$

For our purposes, we will be interested only in those cases in which all positions on the torus have been integrated over, and hence all nodes in the diagrams are filled and unmarked.

More generally, modular graph forms may be obtained by considering derivatives of the scalar Green functions, which given rise to differing exponents (a_r, b_r) for the holomorphic and anti-holomorphic momenta p_r, \bar{p}_r . These exponents are represented graphically by decorated edges as follows,

$$\circ \text{---} \boxed{a_r, b_r} \text{---} \circ \approx (p_r)^{-a_r} (\bar{p}_r)^{-b_r} \quad (2.10)$$

As a simple example, for $\Gamma_{1r} = 1$ and $\Gamma_{2r} = -1$, $r = 1, 2, 3$, one has

$$\mathcal{C}_{\Gamma} \begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{bmatrix} = \begin{array}{c} \boxed{a_1, b_1} \\ \curvearrowright \quad \curvearrowleft \\ \bullet \text{---} \boxed{a_2, b_2} \text{---} \bullet \\ \curvearrowleft \quad \curvearrowright \\ \boxed{a_3, b_3} \end{array} \quad (2.11)$$

2.3 Modular graph functions of even and odd parity

Parity is an anti-holomorphic automorphism of the upper half plane $\tau \rightarrow -\bar{\tau}$ under which an arbitrary modular graph form transforms by swapping the arrays A and B ,

$$\mathcal{C}_\Gamma \begin{bmatrix} A \\ B \end{bmatrix} (-\bar{\tau}) = \mathcal{C}_\Gamma \begin{bmatrix} B \\ A \end{bmatrix} (\tau) \quad (2.12)$$

thereby swapping the modular weights $(\frac{a-b}{2}, \frac{b-a}{2})$ and $(\frac{b-a}{2}, \frac{a-b}{2})$. For $a = b$ it is consistent to decompose an arbitrary modular graph function into *even and odd modular graph functions* $\mathcal{C}_\Gamma = \mathcal{S}_\Gamma + \mathcal{A}_\Gamma$ which satisfy,

$$\mathcal{S}_\Gamma \begin{bmatrix} A \\ B \end{bmatrix} (-\bar{\tau}) = \mathcal{S}_\Gamma \begin{bmatrix} A \\ B \end{bmatrix} (\tau) \quad \mathcal{A}_\Gamma \begin{bmatrix} A \\ B \end{bmatrix} (-\bar{\tau}) = -\mathcal{A}_\Gamma \begin{bmatrix} A \\ B \end{bmatrix} (\tau) \quad (2.13)$$

We note that whenever $A = B$ we have $\mathcal{A} = 0$. When the exponents a_r, b_r are all integers, the parity operation on \mathcal{C}_Γ is equivalent to complex conjugation of \mathcal{C}_Γ .

2.4 Action of differential operators

The choice made for the exponent of the τ_2 prefactor in the definition of (2.2) ensures the canonical normalization in which the modular weight vanishes for $a = b$. For $a \neq b$, however, there is no such canonical normalization available, and the action of differential operators is made more convenient by changing normalization to modular forms \mathcal{C}_Γ^+ and \mathcal{C}_Γ^- of respective modular weights $(0, b - a)$ and $(a - b, 0)$ defined as follows,

$$\mathcal{C}_\Gamma^\pm \begin{bmatrix} A \\ B \end{bmatrix} (\tau) = (\tau_2)^{\pm \frac{a-b}{2}} \mathcal{C}_\Gamma \begin{bmatrix} A \\ B \end{bmatrix} (\tau) \quad (2.14)$$

The action of the first order operator $\nabla = 2i\tau_2^2 \partial_\tau$ on modular graph forms \mathcal{C}_Γ^+ is simple since no connection is required, and the same is true for the action of $\bar{\nabla} = -2i\tau_2^2 \partial_{\bar{\tau}}$ on modular graph forms \mathcal{C}_Γ^- . The action of the operators ∇ and $\bar{\nabla}$ may be expressed as follows,

$$\nabla \mathcal{C}_\Gamma^+ \begin{bmatrix} A \\ B \end{bmatrix} = \sum_{r=1}^R a_r \mathcal{C}_\Gamma^+ \begin{bmatrix} A + S_r \\ B - S_r \end{bmatrix} \quad \bar{\nabla} \mathcal{C}_\Gamma^- \begin{bmatrix} A \\ B \end{bmatrix} = \sum_{r=1}^R b_r \mathcal{C}_\Gamma^- \begin{bmatrix} A - S_r \\ B + S_r \end{bmatrix} \quad (2.15)$$

where the row matrix S_r was defined in (2.5). The operator ∇ maps modular graph forms of modular weight $(0, b - a)$ to those of modular weight $(0, b - a - 2)$, and similarly for $\bar{\nabla}$.

The Laplace-Beltrami operator on modular graph functions is the Laplace operator on \mathcal{H} given by $\Delta = 4\tau_2^2 \partial_{\bar{\tau}} \partial_\tau$ and maps the space of modular graph functions into itself,

$$(\Delta + a) \mathcal{C}_\Gamma \begin{bmatrix} A \\ B \end{bmatrix} = \sum_{r,s=1}^R a_r b_s \mathcal{C}_\Gamma \begin{bmatrix} A + S_r - S_s \\ B - S_r + S_s \end{bmatrix} \quad (2.16)$$

The action of the Laplace-Beltrami differentials on modular graph forms may be defined analogously, but will not be needed in this paper. Since the operator Δ commutes with parity $\tau \rightarrow -\bar{\tau}$, it maps even into even, and odd into odd modular graph functions. The explicit formula for these actions may be obtained by simply substituting \mathcal{C} on both sides of the equality in (2.16) by either \mathcal{S}_Γ or \mathcal{A}_Γ .

2.5 One-loop modular graph forms and Eisenstein series

The combinatorial complexity of modular graphs forms increases rapidly with the number of loops. At one loop, the number of vertices equals the number of edges, so that all vertices are bivalent. The case $V = R = 1$ is excluded since the edge begins and ends on the same vertex. For $V = R \geq 2$ all one-loop modular graphs forms are given for $a_r - b_r \in \mathbb{Z}$ by,

$$\mathcal{C} \begin{bmatrix} a_1 & a_2 \\ b_1 & b_2 \end{bmatrix} = (-)^{a_2+b_2} \mathcal{C} \begin{bmatrix} a & 0 \\ b & 0 \end{bmatrix} \quad (2.17)$$

where a, b are given by (2.1). The non-holomorphic Eisenstein series E_s is defined by,

$$E_s(\tau) = \sum_{p \in \Lambda'} \frac{\tau_2^s}{\pi^s |p|^{2s}} = \sum_{\substack{m, n \in \mathbb{Z} \\ (m, n) \neq (0, 0)}} \frac{\tau_2^s}{\pi^s |m\tau + n|^{2s}} \quad (2.18)$$

The Fourier series of E_s for $s \in \mathbb{C}$ is given by,

$$E_s(\tau) = \frac{2\zeta(2s)}{\pi^s} \tau_2^s + \frac{2\Gamma(s - \frac{1}{2})\zeta(2s - 1)}{\Gamma(s)\pi^{s-\frac{1}{2}}\tau_2^{s-1}} + \frac{4\sqrt{\tau_2}}{\Gamma(s)} \sum_{N=1}^{\infty} N^{s-\frac{1}{2}} \sigma_{1-2s}(N) K_{s-\frac{1}{2}}(2\pi N\tau_2) \left(e^{2\pi i N\tau_1} + e^{-2\pi i N\tau_1} \right) \quad (2.19)$$

where K is the modified Bessel function and $\sigma_z(N) = \sum_{0 < d|N} d^z$ is the divisor sum. The Poincaré series representation of E_s is given by

$$E_s(\tau) = \frac{2\zeta(2s)}{\Gamma(s)} \sum_{\gamma \in \Gamma_{\infty} \backslash \text{SL}(2, \mathbb{Z})} (\text{Im}\gamma(\tau))^s \quad (2.20)$$

The one-loop modular graph forms of (2.17) may all be expressed in terms of E_s . There are no odd modular graph functions to one-loop order, and the Eisenstein series are the only even modular graph functions to one-loop order. Successive application of the derivatives ∇ and $\bar{\nabla}$ to E_s produces all one-loop modular graph forms,

$$\nabla^k E_s = \frac{\Gamma(s+k)}{\Gamma(s)} \mathcal{C}^+ \begin{bmatrix} s+k & 0 \\ s-k & 0 \end{bmatrix} \quad \bar{\nabla}^k E_s = \frac{\Gamma(s+k)}{\Gamma(s)} \mathcal{C}^- \begin{bmatrix} s-k & 0 \\ s+k & 0 \end{bmatrix} \quad (2.21)$$

For integer $s = k \geq 2$ the derivative is proportional to a holomorphic Eisenstein series G_{2k} ,

$$\nabla^k E_k(\tau) = \frac{\Gamma(2k)}{\Gamma(k)} (\tau_2)^{2k} G_{2k}(\tau) \quad G_{2k}(\tau) = \sum_{p \in \Lambda'} \frac{1}{\pi^k p^{2k}} \quad (2.22)$$

For integer s the Fourier series of E_s simplifies and may be recast as follows,

$$E_k(\tau) = -\frac{B_{2k}}{(2k)!} (-4\pi\tau_2)^k + \frac{4(2k-3)! \zeta(2k-1)}{(k-2)! (k-1)! (4\pi\tau_2)^{k-1}} + \frac{2}{(k-1)!} \sum_{N=1}^{\infty} N^{k-1} \sigma_{1-2k}(N) P_k(4N\pi\tau_2) (q^N + \bar{q}^N) \quad (2.23)$$

where $q = e^{2\pi i \tau}$, B_{2k} are the Bernoulli numbers, and $P_k(x)$ is a polynomial in $1/x$ given by,

$$P_k(x) = \sum_{m=0}^{k-1} \frac{(k+m-1)!}{m! (k-m-1)! x^m} \quad (2.24)$$

2.6 Two-loop modular graph forms

Two-loop modular graph forms are given by the following Kronecker-Eisenstein sum,

$$\mathcal{C} \begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{bmatrix} = \sum_{p_1, p_2, p_3 \in \Lambda'} \frac{\tau_2^w \delta_{p_1+p_2+p_3, 0}}{\pi^w p_1^{a_1} p_2^{a_2} p_3^{a_3} \bar{p}_1^{b_1} \bar{p}_2^{b_2} \bar{p}_3^{b_3}} \quad (2.25)$$

where the weight w is given by,

$$2w = a + b = a_1 + a_2 + a_3 + b_1 + b_2 + b_3 \quad (2.26)$$

For $a_r, b_r \in \mathbb{Z}$ with $r = 1, 2, 3$, the sum is absolutely convergent provided $a_r + b_r + a_s + b_s \geq 3$ for any pair $r \neq s$, which requires $w \geq 3$. Furthermore, we shall restrict attention to the case where all exponents are non-negative, as is natural from the point of view of string theory.

The space of modular graph forms thus obtained contains forms that are effectively one-loop. Forms with $b_r = 0$ and $a_r \geq 2$ are proportional to holomorphic modular forms G_{2w} . When both exponents of a given momentum vanish, we may use the *algebraic reduction relation* of [13, 14] to relate the form to one-loop forms,

$$\mathcal{C} \begin{bmatrix} a_1 & a_2 & 0 \\ b_1 & b_2 & 0 \end{bmatrix} = \mathcal{C} \begin{bmatrix} a_1 & 0 \\ b_1 & 0 \end{bmatrix} \mathcal{C} \begin{bmatrix} a_2 & 0 \\ b_2 & 0 \end{bmatrix} - (-)^{a_2+b_2} \mathcal{C} \begin{bmatrix} a & 0 \\ b & 0 \end{bmatrix} \quad (2.27)$$

where $a = a_1 + a_2$ and $b = b_1 + b_2$. Finally, when two anti-holomorphic exponents vanish, *holomorphic subgraph reduction* may be used to relate the form to a one-loop form, as will be reviewed in more detail in section 6.

The following proposition provides a systematic decomposition of two-loop modular graph forms into a reduced set of such forms,

Proposition 2.1. *Two-loop modular graph forms with $a_r + a_s + b_r + b_s \geq 3$ for all $r \neq s$ and $a_1, a_2, b_1, b_2 \geq 1$ admit the following decomposition,*

$$\begin{aligned} \mathcal{C} \begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{bmatrix} &= \sum_{k=1}^{a_1} \Lambda_k(a_1, a_2) \sum_{\ell=1}^{b_1} \Lambda_\ell(b_1, b_3) \mathcal{C} \begin{bmatrix} a-k & 0 & k \\ 0 & b-\ell & \ell \end{bmatrix} + (1 \leftrightarrow 2) \\ &+ \sum_{k=1}^{a_1} \Lambda_k(a_1, a_2) \sum_{\ell=1}^{b_3} \Lambda_\ell(b_3, b_1) \mathcal{C} \begin{bmatrix} k & 0 & a-k \\ 0 & b-\ell & \ell \end{bmatrix} + (1 \leftrightarrow 2) \end{aligned} \quad (2.28)$$

where the term $(1 \leftrightarrow 2)$ is obtained from the preceding term by swapping the pairs (a_1, b_1) with (a_2, b_2) leaving (a_3, b_3) unchanged, and Λ is proportional to a binomial coefficient,

$$\Lambda_k(a_1, a_2) = (-)^{a_1+a_2+k} \binom{a_1+a_2-k-1}{a_2-1} \quad (2.29)$$

Odd (resp. even) two-loop modular graph functions admit the same decomposition with the symbol \mathcal{C} replaced by \mathcal{A} (resp. \mathcal{S}) on both sides of the equality.

To prove the proposition, we perform a partial fraction decomposition of the holomorphic factor of the summand in terms of the momentum variable $p_3 = -p_1 - p_2$, and obtain,

$$\frac{1}{p_1^{a_1} p_2^{a_2} p_3^{a_3}} = \sum_{k=1}^{a_1} \frac{\Lambda_k(a_1, a_2)}{p_1^k p_3^{a-k}} + \sum_{k=1}^{a_2} \frac{\Lambda_k(a_2, a_1)}{p_2^k p_3^{a-k}} \quad (2.30)$$

Using the restriction $b_r \geq 0$, the anti-holomorphic factor of the summand multiplying the first sum in (2.30) may be decomposed as follows,

$$\frac{1}{\bar{p}_1^{b_1} \bar{p}_2^{b_2} \bar{p}_3^{b_3}} = \sum_{\ell=1}^{b_1} \frac{\Lambda_\ell(b_1, b_3)}{\bar{p}_1^\ell \bar{p}_2^{b-\ell}} + \sum_{\ell=1}^{b_3} \frac{\Lambda_\ell(b_3, b_1)}{\bar{p}_3^\ell \bar{p}_2^{b-\ell}} \tag{2.31}$$

while the factor multiplying the second term in (2.30) is given by (2.31) with the indices 1 and 2 swapped. The resulting decomposition is then given by (2.28). Symmetrization under $\tau \rightarrow -\bar{\tau}$ then immediately gives the final statement.

Corollary 2.2. *For $a_1 + b_1, a_2 + b_2 \geq 3$, we have the decomposition,*

$$\mathcal{C} \begin{bmatrix} a_1 & a_2 & 0 \\ b_1 & b_2 & 0 \end{bmatrix} = \sum_{k=1}^{a_1} \Lambda_k(a_1, a_2) \mathcal{C} \begin{bmatrix} a-k & k & 0 \\ 0 & b_1 & b_2 \end{bmatrix} + (1 \leftrightarrow 2) \tag{2.32}$$

where $a = a_1 + a_2$.

The proof is an immediate consequence of proposition 2.1 obtained by setting $a_3 = b_3 = 0$.

Corollary 2.3. *For $k, \ell, a-k, b-\ell \geq 1$, and $a+b-k-\ell \geq 3$, the reduced modular graph forms are related by the reflection formula,*

$$\begin{aligned} \mathcal{C} \begin{bmatrix} a-k & k & 0 \\ 0 & \ell & b-\ell \end{bmatrix} &= \sum_{m=1}^{a-k} \Lambda_m(a-k, k) \mathcal{C} \begin{bmatrix} m & a-m & 0 \\ 0 & b-\ell & \ell \end{bmatrix} \\ &+ \sum_{m=1}^k \Lambda_m(k, a-k) \mathcal{C} \begin{bmatrix} m & a-m & 0 \\ \ell & b-\ell & 0 \end{bmatrix} \end{aligned} \tag{2.33}$$

The proof proceeds by partial fraction decomposition of the holomorphic momenta onto p_3 . The modular graph functions appearing on the last line of corollary 2.3 may be expressed in terms of one-loop functions using the algebraic reduction formula of (2.27) and in turn may be expressed in terms of Eisenstein series and their derivatives using (2.21).

3 Poincaré series for two-loop modular graph functions

In this section, we shall construct the Poincaré series for two-loop modular graph functions with respect to the coset $\Gamma_\infty \backslash \Gamma$ with $\Gamma = \text{PSL}(2, \mathbb{Z})$, and outline the generalization of the construction to higher loop orders.

3.1 Poincaré series for two loops

For integer exponents we use proposition 2.1 to recast an arbitrary modular graph function of weight $w = a = b$ as a linear combination of modular graph functions of the form,

$$\mathcal{C}_{u,v;w}(\tau) = \mathcal{C} \begin{bmatrix} u & 0 & w-u \\ 0 & v & w-v \end{bmatrix}(\tau) \tag{3.1}$$

where u, v, w are integers satisfying $1 \leq u, v \leq w - 1$. We furthermore restrict to $u + v > 2$, lest the functions be divergent. These functions satisfy the complex conjugation condition $\mathcal{C}_{u,v;w} = (\mathcal{C}_{v,u;w})^*$. Their Kronecker-Eisenstein sum is given as follows,

$$\mathcal{C}_{u,v;w}(\tau) = \sum_{\substack{m_r, n_r \in \mathbb{Z} \\ (m_r, n_r) \neq (0,0)}} \frac{\tau_2^w}{\pi^w} \left(\frac{m_2\tau + n_2}{m_1\tau + n_1} \right)^u \left(\frac{m_2\bar{\tau} + n_2}{m_3\bar{\tau} + n_3} \right)^v \frac{\delta_{m,0}\delta_{n,0}}{|m_2\tau + n_2|^{2w}} \quad (3.2)$$

where $m = m_1 + m_2 + m_3$, $n = n_1 + n_2 + n_3$ and the Kronecker $\delta_{m,0}\delta_{n,0}$ restricts the sum to contributions for which $m = n = 0$.

We shall obtain the Poincaré series for a generalization of the functions $\mathcal{C}_{u,v;w}$ where u, v are positive integers but w is analytically continued to \mathbb{C} . This generalization will be useful when we evaluate Petersson inner products of modular graph functions.

Theorem 3.1. *The Poincaré series for $\mathcal{C}_{u,v;w}(\tau)$ with respect to $\Gamma_\infty \backslash \Gamma$ for $u, v \in \mathbb{N}$ with $u + v > 2$, and $w \in \mathbb{C}$ with $\text{Re}(w) > 1 + \frac{1}{2} \max(u, v)$, is absolutely convergent and given by,*

$$\mathcal{C}_{u,v;w}(\tau) = \sum_{g \in \Gamma_\infty \backslash \Gamma} \Lambda_{u,v;w}(g\tau) \quad (3.3)$$

where the seed function $\Lambda_{u,v;w}(\tau)$ is given by,

$$\begin{aligned} \Lambda_{u,v;w}(\tau) &= \ell_w (4\pi\tau_2)^w + (-)^{u+v} \Lambda'_{u,v;w}(\tau) \\ \ell_w &= \sum_{k=0}^{[u/2]} \frac{4(-)^{u+v} \binom{u+v-2k-1}{v-1}}{(2\pi)^{2w}} \zeta(2k)\zeta(2w-2k) + (u \leftrightarrow v) \\ \Lambda'_{u,v;w}(\tau) &= \sum_{m \neq 0} \sum_{\mu \in \mathbb{Z}} \sum_{n \neq 0} \frac{\tau_2^w}{\pi^w} \frac{(-)^u n^{u+v}}{|n|^{2w} (m\tau + \mu)^u (m\bar{\tau} + \mu + n)^v} \end{aligned} \quad (3.4)$$

We shall prove theorem 3.1 with the help of two lemmas, of which the first is standard [42].

Lemma 3.2. *For every pair $(m_2, n_2) \in \mathbb{Z}^2 \setminus \{(0,0)\}$ there exists a unique pair $(0, n)$ and a unique $g \in \Gamma_\infty \backslash \Gamma$, such that we have the following matrix relation,*

$$\begin{pmatrix} m_2 & n_2 \\ 0 & n \end{pmatrix} = (0 \ n)g \quad g = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \quad \alpha, \beta, \gamma, \delta \in \mathbb{Z} \quad (3.5)$$

with $\alpha\delta - \beta\gamma = 1$ and $n = \pm \text{gcd}(m_2, n_2)$. The unique solution is given by $\gamma = m_2/n$ and $\delta = n_2/n$ such that $\delta > 0$ if $n_2 \neq 0$ and $\gamma > 0$ if $n_2 = 0$.

To prove lemma 3.2, we show that the equations $m_2 = n\gamma$, $n_2 = n\delta$, and $\alpha\delta - \beta\gamma = 1$ have a unique solution given the conditions of the lemma. Since $(m_2, n_2) \neq 0$ and $\text{gcd}(\gamma, \delta) = 1$, we have $n = \pm \text{gcd}(m_2, n_2)$ where the greatest common divisor is defined to be positive. The sign may be fixed by using $g \in \Gamma$ which allows us to choose $\delta > 0$ if $n_2 \neq 0$ and $\gamma > 0$ if $n_2 = 0$. Thus γ and δ are determined uniquely. The group Γ_∞ is given by,

$$\Gamma_\infty = \left\{ \begin{pmatrix} 1 & \nu \\ 0 & 1 \end{pmatrix}, \nu \in \mathbb{Z} \right\} \quad (3.6)$$

Acting to the right on $(0, n)$ leaves $(0, n)$ invariant. Acting to the left on g transforms $\alpha \rightarrow \alpha + \nu\gamma$ and $\beta \rightarrow \beta + \nu\delta$ for $\nu \in \mathbb{Z}$ mapping all solutions of the equation $\alpha\delta - \beta\gamma = 1$ for given γ, δ , into one another. Therefore, the coset element $g \in \Gamma_\infty \backslash \Gamma$ is unique. This completes the proof of lemma 3.2.

Lemma 3.3. *The following Poincaré series representation is absolutely convergent² for $a_i \in \mathbb{R}$ with $a_i + a_j > 1$ for all $1 \leq i \neq j \leq 3$,*

$$C_{a_1, a_2, a_3}(\tau) = \mathcal{C} \begin{bmatrix} a_1 & a_2 & a_3 \\ a_1 & a_2 & a_3 \end{bmatrix}(\tau) = \frac{(2\pi)^{2a} c_a}{2\zeta(2a)} E_a(\tau) + \sum_{g \in \Gamma_\infty \backslash \Gamma} \lambda_{a_1, a_2, a_3}(g\tau) \quad (3.7)$$

$a = a_1 + a_2 + a_3$. The modular graph function C_{a_1, a_2, a_3} was defined in (2.25). The seed function $\lambda_{a_1, a_2, a_3}(\tau)$ is given by,

$$\lambda_{a_1, a_2, a_3}(\tau) = \sum_{m, n \neq 0} \sum_{\mu \in \mathbb{Z}} \frac{\tau_2^a}{\pi^a n^{2a_2} |m\tau + \mu|^{2a_1} |m\tau + \mu + n|^{2a_3}} \quad (3.8)$$

and c_a is independent of τ and was given in equation (1.20) of [11].

To prove lemma 3.3, we use the results and the notations of lemma 3.2 to obtain,

$$\frac{|m_2\tau + n_2|^2}{\tau_2} = \frac{n^2}{\tau_2'} \quad \frac{m_2\tau + n_2}{m_r\tau + n_r} = \frac{n}{m_r'\tau' + n_r'} \quad \tau' = g\tau = \frac{\alpha\tau + \beta}{\gamma\tau + \delta} \quad (3.9)$$

where $(m_r, n_r) \neq (0, 0)$ for $r = 1, 3$, $n \neq 0$, and subject to the conditions $m_1' + m_3' = 0$, and $n_1' + n + n_3' = 0$. Parametrizing these variables by n , $m_1' = -m_3' = m$, $n_1' = \mu$, and $n_3' = -n - \mu$, and substituting these results into the Kronecker-Eisenstein sum which defines C_{a_1, a_2, a_3} in (2.25), we prove the Poincaré series representation of lemma 3.3. To prove that the Poincaré series is absolutely convergent, we use the fact that for $a_i \in \mathbb{R}$, each term in the Kronecker-Eisenstein sum defining C_{a_1, a_2, a_3} in (2.25) is real and positive. Recasting this sum in the form of a Poincaré series simply amounts to a rearrangement of the infinite series, which is always permitted by Tonelli's theorem since all terms are positive. This completes the proof of lemma 3.3.

To prove the Poincaré series representation of theorem 3.1, we use lemma 3.2 and the decomposition formula (3.9) of the Kronecker-Eisenstein sum into orbits under $\Gamma_\infty \backslash \Gamma$ to derive (3.4), in parallel with the derivation of λ in lemma 3.3. To prove absolute convergence of the Poincaré series (3.3), we bound the series as follows,

$$\left| \mathcal{C}_{u, v; w} - \frac{(2\pi)^{2w} \ell_w}{2\zeta(2w)} E_w \right| \leq \sum_{g \in \Gamma_\infty \backslash \Gamma} \lambda_{a_1, a_2, a_3}(g\tau) \quad (3.10)$$

where $\lambda_{a_1, a_2, a_3}(\tau)$ was defined in (3.8) and a_1, a_2, a_3 are given in terms of u, v, w by $a_1 = \frac{1}{2}u$, $a_3 = \frac{1}{2}v$, $a_2 = \text{Re}(w) - a_1 - a_3$. The left-hand side of (3.10) is the Poincaré series over $\Lambda'_{u, v; w}(\tau)$. Since the assumptions of theorem 3.1 include $u + v > 2$ and $\text{Re}(w) > 1 + \frac{1}{2} \max(u, v)$, it follows that $a_i + a_j > 1$ and by lemma 3.3 the series in $\lambda_{a_1, a_2, a_3}(\tau)$ is absolutely convergent. This completes the proof of theorem 3.1.

²We thank Axel Kleinschmidt and Daniele Dorigoni for bringing their work on Poincaré series of modular graph functions in [43, 44] to our attention, and for questions on convergence that led the authors to the proof of absolute convergence included here.

3.2 Calculating the seed function for integer w

Throughout this paper we shall use the following partial fraction decomposition formula,

$$\frac{1}{(\mu+x)^u(\mu+y)^v} = \sum_{k=1}^u \frac{(-)^v \binom{u+v-k-1}{u-k}}{(\mu+x)^k(x-y)^{u+v-k}} + \sum_{k=1}^v \frac{(-)^u \binom{u+v-k-1}{v-k}}{(\mu+y)^k(y-x)^{u+v-k}} \quad (3.11)$$

for $u, v \in \mathbb{N}$. We shall now derive an explicit formula for the seed function $\Lambda_{u,v;w}(\tau)$. Its first contribution involves the coefficient ℓ_w which is given by the $m = 0$ term,

$$\ell_w = \frac{(-)^v}{(2\pi)^{2w}} \sum_{n \neq 0} \sum_{\mu \neq 0, -n} \frac{1}{n^{2w-u-v} \mu^u (\mu+n)^v} \quad (3.12)$$

The summation over μ in (3.12) may be carried out using the partial fraction decomposition of the μ -dependent factors with $x = 0$ and $y = n$ in (3.11). For integer w , the remaining sum over n gives even ζ -values resulting in the formula for ℓ_w in (3.4). We may express the even zeta-values $\zeta(2k)$ in terms of Bernoulli numbers B_{2k} using the relation,

$$\zeta(2k) = \frac{1}{2} (2\pi)^{2k} (-)^{k+1} \frac{B_{2k}}{(2k)!} \quad (3.13)$$

and obtain the following equivalent formula,

$$\ell_w = \sum_{k=0}^{[u/2]} \binom{u+v-2k-1}{v-1} \frac{(-)^{u+v+w} B_{2k} B_{2w-2k}}{(2k)! (2w-2k)!} + (u \leftrightarrow v) \quad (3.14)$$

This expression agrees with the result $(-)^w c_w$ found for even u and v in [11], and generalizes that result for all u, v . The second contribution Λ' is evaluated using the following lemma.

Lemma 3.4. *For integer w , the function $\Lambda'_{u,v;w}(\tau)$ is given by,*

$$\Lambda'_{u,v;w}(\tau) = 2 \frac{(-\tau_2)^w}{\pi^w} \sum_{k=1}^u \binom{u+v-k-1}{v-1} \sum_{m=1}^{\infty} \Phi_{2w-u-v;u+v-k}(2m\tau_2) \varphi_k(q^m) + (u \leftrightarrow v)^* \quad (3.15)$$

where $q = e^{2\pi i \tau}$ and the notation $(u \leftrightarrow v)^*$ stands for the complex conjugate of the preceding term in which u and v have been swapped. The functions φ_k and $\Phi_{a;b}$ are defined for integer k, a, b with $k \geq 2$ and $a + b \geq 2$ by the following infinite sums,

$$\varphi_k(e^{2\pi iz}) = \sum_{\mu \in \mathbb{Z}} \frac{i^k}{(z + \mu)^k} \quad \Phi_{a;b}(z) = \sum_{n \neq 0} \frac{(-i)^{a+b}}{n^a (n - iz)^b} \quad (3.16)$$

while for $k = 1$ one has $\varphi_1(q) = \pi \frac{1+q}{1-q}$. Explicit formulas for φ_k will be given in (3.19) and (3.20) and for $\Phi_{a;b}$ in (3.21).

The powers of i are included to give the functions simple conjugation properties,

$$\begin{aligned} \overline{\varphi_k(e^{2\pi iz})} &= \varphi_k(e^{-2\pi i \bar{z}}) & \overline{\Phi_{a;b}(z)} &= \Phi_{a;b}(\bar{z}) \\ \varphi_k(e^{-2\pi iz}) &= (-)^k \varphi_k(e^{2\pi iz}) & \Phi_{a;b}(-z) &= (-)^{a+b} \Phi_{a;b}(z) \end{aligned} \quad (3.17)$$

In particular, the functions φ_k and $\Phi_{a;b}$ are real functions of their respective argument. The proof of lemma 3.4 proceeds by first computing the sum over $\mu \in \mathbb{Z}$ using the standard partial fraction decomposition formula of (3.11) with $u, v \in \mathbb{N}$, $x = m\tau$, and $y = m\bar{\tau} + n$, and expressing the result of the summation in terms of φ_k ,

$$\sum_{\mu \in \mathbb{Z}} \frac{(-)^v}{(m\tau + \mu)^u (m\bar{\tau} + \mu + n)^v} = \sum_{k=1}^u \frac{(-i)^k \binom{u+v-k-1}{v-1}}{(2mi\tau_2 - n)^{u+v-k}} \varphi_k(q^m) + (u \leftrightarrow v)^* \quad (3.18)$$

Importantly, the factor $\varphi_k(q^m)$ is independent of n which allows us to express the sum over m in terms of the function $\Phi_{a;b}(2m\tau_2)$ defined above, and this gives the expression in (3.15).

3.3 Evaluating the functions φ_k and $\Phi_{a;b}(z)$

The functions $\varphi_k(q)$ for $k \geq 2$ may be expressed as derivatives of the function $\varphi_1(q)$,

$$\varphi_k(q) = \frac{(-i)^{k-1}}{\Gamma(k)} \frac{\partial^{k-1}}{\partial z^{k-1}} \varphi_1(q) \quad \varphi_1(q) = \pi \frac{1+q}{1-q} \quad (3.19)$$

Their Fourier series expansion for $|q| < 1$ is obtained as follows,

$$\varphi_k(q) = \pi \delta_{k,1} + \frac{(2\pi)^k}{\Gamma(k)} \sum_{p=1}^{\infty} p^{k-1} q^p \quad (3.20)$$

To evaluate the function $\Phi_{a;b}(z)$ for integer $a, b \geq 1$ we perform first the sum over n , using the partial fraction decomposition formula (3.11) for $\mu = n, x = 0, y = -iz, u = a, v = b$, together with the definition of the function φ_k . We find,

$$\Phi_{a;b}(z) = \sum_{\alpha=0}^{[a/2]} \frac{(-)^{a+\alpha} 2\zeta(2\alpha) \binom{a+b-2\alpha-1}{\beta-1}}{z^{a+b-2\alpha}} + \sum_{\beta=1}^b \frac{(-)^a \binom{a+b-\beta-1}{a-1} \varphi_\beta(e^{-2\pi z})}{z^{a+b-\beta}} \quad (3.21)$$

The contribution from $\alpha = 0$ in the sum over α arises from the subtraction required to exclude the $m = 0$ term when recasting the sum over n in terms of the function φ_β . Despite the appearance of poles at $z = 0$ in the individual terms of the sum in (3.21), the function $\Phi_{a;b}(z)$ is analytic near $z = 0$ and, for $a, b \geq 1$ with z in the unit disc $|z| < 1$, is given by the following Taylor expansion,

$$\Phi_{a;b}(z) = -(2\pi)^{a+b} \sum_{k=0}^{\infty} \frac{\Gamma(k+b) B_{a+b+k}}{\Gamma(b)\Gamma(a+b+k+1)k!} (-2\pi z)^k \quad (3.22)$$

The B_{a+b+k} vanish for $a+b+k$ odd since we have $a+b+k \geq 2$. The expression (3.22) confirms the earlier observation that $\Phi_{a;b}(z)$ is a real function of z with parity $(-)^{a+b}$.

We stress that both φ_k and $\Phi_{a;b}$ are elementary functions of their argument.

3.4 Analytic continuation in w

The multiple summation for the seed function in theorem 3.1 is absolutely convergent for $u, v \in \mathbb{N}$, $\text{Re}(2w-u) > 2$, and $\text{Re}(2w-v) > 2$, and the result may be analytically continued in w to all of \mathbb{C} minus some poles. For $w \in \mathbb{C} \setminus \mathbb{N}$, the decomposition of lemma 3.4 in terms of elementary functions $\Phi_{a,b}$ is no longer available. Instead we have,

$$\begin{aligned} \Lambda'_{u,v;w} &= 2 \frac{\tau_2^w}{\pi^w} \sum_{k=1}^u \binom{u+v-k-1}{v-1} \sum_{m=1}^{\infty} \varphi_k(q^m) \Upsilon_{w,k,u+v}(2m\tau_2) \\ &\quad + 2 \frac{\tau_2^w}{\pi^w} \sum_{k=1}^v \binom{u+v-k-1}{u-1} \sum_{m=1}^{\infty} \varphi_k(\bar{q}^m) \Upsilon_{w,k,u+v}(2m\tau_2) \end{aligned} \quad (3.23)$$

where Υ is given by,

$$\Upsilon_{w,k,\ell}(z) = \sum_{n \neq 0} \frac{i^k n^\ell}{|n|^{2w} (n - iz)^{\ell-k}} \quad (3.24)$$

For integer w we recover the expressions given in (3.4), but for arbitrary $w \in \mathbb{C}$ we can no longer use partial fraction decomposition to simplify Υ . Its Taylor series expansion,

$$\Upsilon_{w,k,\ell} = \sum_{m=\lceil (k+1)/2 \rceil}^{\infty} \frac{2(-)^m \Gamma(\ell - 2k + 2m)}{\Gamma(\ell - k) \Gamma(2m + 1 - k)} \zeta(2w + 2m - 2k) z^{2m-k} \quad (3.25)$$

is valid for all $w \in \mathbb{C}$.

3.5 Higher loops

We shall generalize the construction of Poincaré series to higher loops and focus on the case of dihedral modular graphs functions whose Kronecker-Eisenstein sum is given by,

$$\mathcal{C} \begin{bmatrix} a_1 & \cdots & a_R \\ b_1 & \cdots & b_R \end{bmatrix} = \sum_{p_1, \dots, p_R \in \Lambda'} \frac{\tau_2^w \delta_{p_1 + \dots + p_R, 0}}{\pi^w p_1^{a_1} \cdots p_R^{a_R} \bar{p}_1^{b_1} \cdots \bar{p}_R^{b_R}} \quad (3.26)$$

Here, the number of loops is $R - 1$ and we have $w = a = b$ with a, b defined in (2.1). We single out any one of the momentum edges, say $p_R = m_R \tau + n_R$, and apply lemma 3.2 to the pair (m_R, n_R) . In matrix notation, we thus recast the pair as follows,

$$(m_R \quad n_R) = (0 \quad n)g \quad g = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \quad \alpha, \beta, \gamma, \delta \in \mathbb{Z} \quad (3.27)$$

with $\alpha\delta - \beta\gamma = 1$ and $n = \pm \text{gcd}(m_R, n_R)$. The unique solution is given by $\gamma = m_R/n$ and $\delta = n_R/n$ such that $\delta > 0$ if $n_R \neq 0$ and $\gamma > 0$ if $n_R = 0$. By generalizing the arguments used in the two-loop case, we thus have,

$$\mathcal{C} \begin{bmatrix} a_1 & \cdots & a_R \\ b_1 & \cdots & b_R \end{bmatrix} (\tau) = \sum_{g \in \Gamma_\infty \setminus \text{PSL}(2, \mathbb{Z})} \Lambda \begin{bmatrix} a_1 & \cdots & a_R \\ b_1 & \cdots & b_R \end{bmatrix} (g\tau) \quad (3.28)$$

The seed function Λ is given by,

$$\Lambda \begin{bmatrix} a_1 & \cdots & a_R \\ b_1 & \cdots & b_R \end{bmatrix} (\tau) = \sum_{p_1, \dots, p_{R-1} \in \Lambda'} \sum_{n \neq 0} \frac{\tau_2^w}{\pi^w n^{a_R + b_R}} \frac{\delta_{p_1 + \dots + p_{R-1} + n, 0}}{p_1^{a_1} \cdots p_{R-1}^{a_{R-1}} \bar{p}_1^{b_1} \cdots \bar{p}_{R-1}^{b_{R-1}}} \quad (3.29)$$

Effectively the sum over p_R in \mathcal{C} is replaced by a sum over $p_R = (0 \ n)$ with $n \neq 0$ in Λ .

4 Fourier series for two-loop modular graph functions

In this section we shall evaluate the Fourier series expansion of an arbitrary two-loop modular graph function with integer exponents. As in the previous section we use proposition 2.1 to reduce this calculation to evaluation of the Fourier series of the reduced modular graph functions $\mathcal{C}_{u,v,w}(\tau)$, defined in (3.1), for $u, v, w \in \mathbb{N}$. We require $u + v \geq 3$, $2w - u \geq 3$, and $2w - v \geq 3$ to ensure convergence of the Kronecker-Eisenstein series which define $\mathcal{C}_{u,v,w}$ in (3.2), and these conditions require $w \geq 3$. The Fourier decomposition of $\mathcal{C}_{u,v,w}(\tau)$ is given by the following theorem.

Theorem 4.1. *The two-loop modular graph function $\mathcal{C}_{u,v,w}$ with integer exponents $u, v, w \in \mathbb{N}$ admits the following Fourier series expansion,*

$$\mathcal{C}_{u,v,w}(\tau) = \mathcal{L}_{u,v,w}(\tau_2) + \sum_{N=1}^{\infty} \mathcal{Q}_{u,v,w}^{(N)}(\tau_2)(q\bar{q})^N + \sum_{N=1}^{\infty} \left(\mathcal{F}_{u,v,w}^{(N)}(\tau_2)q^N + \mathcal{F}_{v,u,w}^{(N)}(\tau_2)\bar{q}^N \right) \quad (4.1)$$

Here, the functions occurring in the constant Fourier mode, $\mathcal{L}_{u,v,w}(\tau_2)$ and $\mathcal{Q}_{u,v,w}^{(N)}(\tau_2)$, are real-valued Laurent polynomials in τ_2 . The functions $\mathcal{F}_{u,v,w}^{(N)}(\tau_2)$ occurring in the non-constant Fourier modes are real-valued functions which have an expansion in powers of $q\bar{q}$,

$$\mathcal{F}_{u,v,w}^{(N)}(\tau_2) = F_{u,v,w}^{(N)}(\tau_2) + \sum_{L=1}^{\infty} G_{u,v,w}^{(N,L)}(\tau_2)(q\bar{q})^L \quad (4.2)$$

where $F_{u,v,w}^{(N)}(\tau_2)$ and $G_{u,v,w}^{(N,L)}(\tau_2)$ are real-valued Laurent polynomials in τ_2 . The degrees of these Laurent polynomials are given as follows,

$$\begin{aligned} \deg \mathcal{L}_{u,v,w} &= (w, 1 - w) \\ \deg \mathcal{Q}_{u,v,w}^{(N)} &= (w - 2, w - \beta_+ - 1) \\ \deg F_{u,v,w}^{(N)} &= (w - 1, w - \ell_+ - \gamma_+) \\ \deg G_{u,v,w}^{(N,L)} &= (w - 2, w - \ell_+ - \beta_+) \end{aligned} \quad (4.3)$$

where β_+, ℓ_+ , and γ_+ are defined as

$$\begin{aligned} \beta_+ &= \max(w + |u - v| - 1, u + v - 1) \\ \ell_+ &= \max(w - u, u) \\ \gamma_+ &= \max(u + v, 2w - u - v - \epsilon) \end{aligned} \quad (4.4)$$

Explicit formulas for these Laurent polynomials will be given in subsequent sections.

Corollary 4.2. *An immediate corollary of theorem 4.1 is obtained for odd two-loop modular graph functions with integer exponents defined by $\mathcal{A}_{u,v;w}(\tau) = \mathcal{C}_{u,v;w}(\tau) - \mathcal{C}_{v,u;w}(\tau)$. Their Fourier expansion is given by,*

$$\mathcal{A}_{u,v;w}(\tau) = \sum_{N=1}^{\infty} \left(\mathcal{F}_{u,v;w}^{(N)}(\tau_2) - \mathcal{F}_{v,u;w}^{(N)}(\tau_2) \right) (q^N - \bar{q}^N) \tag{4.5}$$

so that $\mathcal{A}_{u,v;w}(\tau)$ is a cuspidal function with exponential decay at the cusp.

4.1 Decomposition of the Kronecker-Eisenstein sum

To prove theorem 4.1 and calculate the coefficient functions in the Fourier series (4.1), we start from the Kronecker-Eisenstein sum representation of $\mathcal{C}_{u,v;w}$, given by,

$$\mathcal{C}_{u,v;w} = \sum_{(m_r, n_r)}' \frac{\tau_2^w \delta_{m_1+m_2+m_3,0} \delta_{n_1+n_2+n_3,0}}{\pi^w (m_1\tau + n_1)^u (m_2\bar{\tau} + n_2)^v (m_3\tau + n_3)^{w-u} (m_3\bar{\tau} + n_3)^{w-v}} \tag{4.6}$$

and decompose the sum according to the vanishing of the summation variables m_r ,

$$\mathcal{C}_{u,v;w} = \sum_{k=0}^4 \mathcal{C}_{u,v;w}^{(k)} \tag{4.7}$$

The individual terms correspond to the following assignments of m_r and n_r ,

| | | | | |
|-----------------------------|--------------|-------------------|---------------|-------|
| $\mathcal{C}_{u,v;w}^{(0)}$ | $m_i = 0$ | $n_i \neq 0$ | $i = 1, 2, 3$ | |
| $\mathcal{C}_{u,v;w}^{(1)}$ | $m_1 = 0$ | $m_2, m_3 \neq 0$ | $n_1 \neq 0$ | |
| $\mathcal{C}_{u,v;w}^{(2)}$ | $m_2 = 0$ | $m_3, m_1 \neq 0$ | $n_2 \neq 0$ | |
| $\mathcal{C}_{u,v;w}^{(3)}$ | $m_3 = 0$ | $m_1, m_2 \neq 0$ | $n_3 \neq 0$ | |
| $\mathcal{C}_{u,v;w}^{(4)}$ | $m_i \neq 0$ | | $i = 1, 2, 3$ | (4.8) |

We shall show that the Fourier series decompositions of the functions $\mathcal{C}_{u,v;w}^{(k)}$ may be computed in terms of the functions $\Phi_{a;b}$ and φ_k defined in (3.16). The calculation of $\mathcal{C}_{u,v;w}^{(0)}$ was already carried out when we evaluated the coefficient ℓ_w in (3.12), and the result is given by,

$$\mathcal{C}_{u,v;w}^{(0)} = \ell_w (4\pi\tau_2)^w \tag{4.9}$$

with ℓ_w given explicitly in the second equation of (3.4). The remaining functions $\mathcal{C}_{u,v;w}^{(k)}$ are considerably more involved and are the focus of the subsequent subsections.

4.2 Calculation of $\mathcal{C}_{u,v;w}^{(1)}$ and $\mathcal{C}_{u,v;w}^{(2)}$

The function $\mathcal{C}_{u,v;w}^{(2)}$ is related to $\mathcal{C}_{u,v;w}^{(1)}$ by swapping the summation variables (m_1, n_1) with (m_2, n_2) or equivalently by simultaneous complex conjugation and swapping u and v ,

$$\mathcal{C}_{u,v;w}^{(2)}(\tau) = \mathcal{C}_{v,u;w}^{(1)}(\tau)^* \tag{4.10}$$

an operation that will be denoted by $(u \leftrightarrow v)^*$ throughout. We begin by evaluating $\mathcal{C}_{u,v;w}^{(1)}$, and express the sum in terms of the independent variables $m = m_3$, $n = n_3$, and n_1 ,

$$\mathcal{C}_{u,v;w}^{(1)} = \frac{\tau_2^w}{\pi^w} \sum_{m \neq 0} \sum_{n_1 \neq 0} \sum_n \frac{(-)^v}{n_1^u (m\bar{\tau} + n + n_1)^v (m\tau + n)^{w-u} (m\bar{\tau} + n)^{w-v}} \quad (4.11)$$

It is natural to perform first the summation over n . Since the denominator has three different factors involving n , we need to perform a double partial fraction decomposition. Performing first the partial fraction decomposition on the last two factors for the variable n we find,

$$\mathcal{C}_{u,v;w}^{(1)} = \frac{\tau_2^w}{\pi^w} (-)^{u+v} \sum_{m \neq 0} \left(\sum_{k=1}^{w-u} \frac{\binom{2w-u-v-k-1}{w-u-k}}{(2m\tau_2)^{2w-u-v-k}} K_{u,v;k} + \sum_{k=1}^{w-v} \frac{\binom{2w-u-v-k-1}{w-v-k}}{(2m\tau_2)^{2w-u-v-k}} L_{u,v;k} \right) \quad (4.12)$$

where the functions K and L are given by,

$$\begin{aligned} K_{u,v;k} &= \sum_{n_1 \neq 0} \sum_n \frac{(-i)^{u+v-k}}{n_1^u (m\bar{\tau} + n + n_1)^v (m\tau + n)^k} \\ L_{u,v;k} &= \sum_{n_1 \neq 0} \sum_n \frac{(-i)^{u+v+k}}{n_1^u (m\bar{\tau} + n + n_1)^v (m\bar{\tau} + n)^k} \end{aligned} \quad (4.13)$$

Throughout, the dependence of $K_{u,v;k}$ and $L_{u,v;k}$ on m and τ will be understood but not exhibited. The factors of i have been inserted to make them real functions of their arguments.

To compute $K_{u,v;k}$, we carry out a partial fraction decomposition in n , and then sum over n in terms of the function φ_k defined in (3.16). The sum over n_1 may then be carried out in terms of the functions $\Phi_{a;b}$ defined in (3.16), and we find,

$$K_{u,v;k} = \sum_{\ell=1}^k \binom{v+k-\ell-1}{k-\ell} \Phi_{u,v+k-\ell}(2m\tau_2) \varphi_\ell(q^m) + (v \leftrightarrow k)^* \quad (4.14)$$

To compute $L_{u,v;k}$, we carry out a partial fraction decomposition in n and express the sum over n in terms of the functions φ_k ,

$$L_{u,v;k} = (-i)^{u+v-k} \sum_{n_1 \neq 0} \left(\sum_{\ell=1}^v \frac{(-i)^{-\ell} \binom{v+k-\ell-1}{v-\ell}}{n_1^{u+v+k-\ell}} \varphi_\ell(\bar{q}^m) + \sum_{\ell=1}^k \frac{(-i)^\ell \binom{v+k-\ell-1}{k-\ell}}{n_1^{u+v+k-\ell}} \varphi_\ell(\bar{q}^m) \right) \quad (4.15)$$

The sum over n_1 vanishes unless $u+v+k-\ell$ is even. Thus we change summation variables from ℓ to $u+v+k-\ell = 2j$, so that the sum becomes,

$$(-)^k L_{u,v;k} = \sum_{j=\lceil \frac{u+k+1}{2} \rceil}^{\lceil \frac{u+v+k-1}{2} \rceil} 2(-)^j \binom{2j-u-1}{k-1} \zeta(2j) \varphi_{u+v+k-2j}(\bar{q}^m) + (-)^{u+v+k} (v \leftrightarrow k) \quad (4.16)$$

Note that the $\ell = 1$ contribution, which is given by the $j = \lceil \frac{u+v+k-1}{2} \rceil$ contribution in the above sum, cancels exactly so that every term has a non-constant Fourier mode.

Collecting both contributions $\mathcal{C}_{u,v;w}^{(1)} + \mathcal{C}_{u,v;w}^{(2)}$, we find,

$$\mathcal{C}_{u,v;w}^{(1)} + \mathcal{C}_{u,v;w}^{(2)} = \sum_{m \neq 0} \sum_{k=1}^{w-u} \frac{(-)^{u+v} \tau_2^w \binom{2w-u-v-k-1}{w-u-k}}{\pi^w (2m\tau_2)^{2w-u-v-k}} \left(K_{u,v;k} + L_{v,u;k}^* \right) + (u \leftrightarrow v)^* \quad (4.17)$$

The functions $K_{u,v;k}$ and $L_{u,v;k}$ involve φ_k , $\Phi_{a;b}$, and factors that are power behaved in τ_2 . As will be shown in the subsequent section, the infinite sum over m may be performed for the terms that are purely power behaved in τ_2 . For the exponential terms the values of m will label the powers in q and \bar{q} and, for a given assignment of powers of q and \bar{q} , the sums over m will reduce to finite sums.

4.3 Calculation of $\mathcal{C}_{u,v;w}^{(3)}$

Expressing the sum in terms of the independent summation variables $m = m_1$, $n = n_3$, and n_1 , this contribution becomes,

$$\mathcal{C}_{u,v;w}^{(3)} = \frac{\tau_2^w}{\pi^w} \sum_{m \neq 0} \sum_{n \neq 0} \sum_{n_1} \frac{(-)^v}{(m\tau + n_1)^u (m\bar{\tau} + n_1 + n)^v n^{2w-u-v}} \quad (4.18)$$

Carrying out the partial fraction decomposition in n_1 , summing over n_1 in terms of the function φ_k , and expressing the sum over n in terms of the function $\Phi_{a;b}$, we find,

$$\mathcal{C}_{u,v;w}^{(3)} = \frac{\tau_2^w}{\pi^w} \sum_{k=1}^u (-)^{u+v+w} \binom{u+v-k-1}{u-k} \sum_{m \neq 0} \Phi_{2w-u-v;u+v-k}(2m\tau_2) \varphi_k(q^m) + (u \leftrightarrow v)^* \quad (4.19)$$

4.4 Calculation of $\mathcal{C}_{u,v;w}^{(4)}$

For $\mathcal{C}_{u,v;w}^{(4)}$ none of the summation variables m_r vanish. We shall use independent continuous variables to abbreviate the m -dependence by letting $m_1\tau \rightarrow \alpha$, $m_2\bar{\tau} \rightarrow \beta$, and $m_3\tau \rightarrow \gamma$, and recast the sum over m_r in terms of a function $\Omega_{u,v;w}$ of the continuous variables α, β, γ ,

$$\mathcal{C}_{u,v;w}^{(4)} = \sum_{m_1, m_2, m_3 \neq 0} \frac{\tau_2^w}{\pi^w} \delta_{m_1+m_2+m_3, 0} \Omega_{u,v;w} \left(m_1\tau, m_2\bar{\tau}, m_3\tau, m_3\bar{\tau} \right) \quad (4.20)$$

where the function Ω is defined by,

$$\Omega_{u,v;w}(\alpha, \beta, \gamma, \bar{\gamma}) = \sum_{n_1, n_2, n_3} \frac{\delta_{n_1+n_2+n_3, 0}}{(\alpha + n_1)^u (\beta + n_2)^v (\gamma + n_3)^{w-u} (\bar{\gamma} + n_3)^{w-v}} \quad (4.21)$$

The partial fraction decomposition of the last two factors in the denominator with respect to n_3 may be expressed in terms of a family of functions $\Psi_{u,v,k}$ defined by,

$$\Psi_{u,v,k}(\alpha, \beta, \gamma) = \sum_{n_1, n_2, n_3} \frac{\delta_{n_1+n_2+n_3, 0}}{(\alpha + n_1)^u (\beta + n_2)^v (\gamma + n_3)^k} \quad (4.22)$$

The function $\Psi_{u,v,k}(\alpha, \beta, \gamma)$ is invariant under all six permutations of the pairs (u, α) , (v, β) , and (k, γ) . In terms of Ψ , the function Ω may be expressed as follows,

$$\begin{aligned} \Omega_{u,v;w}(\alpha, \beta, \gamma, \bar{\gamma}) &= \sum_{k=1}^{w-u} \frac{(-)^{w+v} \binom{2w-u-v-k-1}{w-u-k}}{(\gamma - \bar{\gamma})^{2w-u-v-k}} \Psi_{u,v,k}(\alpha, \beta, \gamma) \\ &+ \sum_{k=1}^{w-v} \frac{(-)^{w+v+k} \binom{2w-u-v-k-1}{w-v-k}}{(\gamma - \bar{\gamma})^{2w-u-v-k}} \Psi_{u,v,k}(\alpha, \beta, \bar{\gamma}) \end{aligned} \quad (4.23)$$

To calculate the function Ψ , we use the following observation,

$$\Psi_{u,v,k}(\alpha, \beta, \gamma) = \frac{(-)^{u+v+k-1}}{\Gamma(u)\Gamma(v)\Gamma(k)} \partial_\alpha^{u-1} \partial_\beta^{v-1} \partial_\gamma^{k-1} \Psi_{1,1,1}(\alpha, \beta, \gamma) \quad (4.24)$$

$\Psi_{1,1,1}$ is readily evaluated by partial fraction decomposition and summation in the variables n_1 and n_2 , and we find,

$$\Psi_{1,1,1}(\alpha, \beta, \gamma) = -\frac{\varphi_1(e^{2\pi i\alpha})\varphi_1(e^{2\pi i\beta}) + \varphi_1(e^{2\pi i\beta})\varphi_1(e^{2\pi i\gamma}) + \varphi_1(e^{2\pi i\gamma})\varphi_1(e^{2\pi i\alpha}) + \pi^2}{\alpha + \beta + \gamma} \quad (4.25)$$

The successive derivatives may be obtained using a trinomial expansion for Leibniz's rule, and we find the following expression,

$$\begin{aligned} \Psi_{u,v;k}(\alpha, \beta, \gamma) = & -\frac{\pi^2 \binom{u+v+k-3}{u-1, v-1, k-1}}{(\alpha + \beta + \gamma)^{u+v+k-2}} \\ & + \sum_{a=1}^u \sum_{b=1}^v \frac{(-i)^{a+b} \binom{u+v+k-a-b-1}{u-a, v-b, k-1}}{(\alpha + \beta + \gamma)^{u+v+k-a-b}} \varphi_a(e^{2\pi i\alpha}) \varphi_b(e^{2\pi i\beta}) \\ & + \sum_{b=1}^v \sum_{c=1}^k \frac{(-i)^{b+c} \binom{u+v+k-b-c-1}{u-1, v-b, k-c}}{(\alpha + \beta + \gamma)^{u+v+k-b-c}} \varphi_b(e^{2\pi i\beta}) \varphi_c(e^{2\pi i\gamma}) \\ & + \sum_{c=1}^k \sum_{a=1}^u \frac{(-i)^{c+a} \binom{u+v+k-c-a-1}{u-a, v-1, k-c}}{(\alpha + \beta + \gamma)^{u+v+k-c-a}} \varphi_a(e^{2\pi i\alpha}) \varphi_c(e^{2\pi i\gamma}) \end{aligned} \quad (4.26)$$

where we use the following notation for the trinomial coefficients,

$$\binom{a+b+c}{a, b, c} = \frac{(a+b+c)!}{a!b!c!} \quad (4.27)$$

Substituting the expression for $\Psi_{u,v,k}$ into Ω and substituting the original values for the continuous variables $\alpha = m_1\tau$, $\beta = m_2\bar{\tau}$, and $\gamma = m_3\tau$, we find,

$$\begin{aligned} \Omega_{u,v;w} = & \sum_{k=1}^{w-u} \sum_{a=1}^u \sum_{b=1}^v \frac{(-)^{b+v} \binom{2w-u-v-k-1}{w-u-k} \binom{u+v+k-a-b-1}{u-a, v-b, k-1}}{(-m_2)^{u+v+k-a-b} m_3^{2w-u-v-k} (2\tau_2)^{2w-a-b}} \varphi_a(q^{m_1}) \varphi_b(\bar{q}^{m_2}) \\ & + \sum_{k=1}^{w-u} \sum_{b=1}^v \sum_{c=1}^k \frac{(-)^{b+v} \binom{2w-u-v-k-1}{w-u-k} \binom{u+v+k-b-c-1}{u-1, v-b, k-c}}{(-m_2)^{u+v+k-b-c} m_3^{2w-u-v-k} (2\tau_2)^{2w-b-c}} \varphi_b(\bar{q}^{m_2}) \varphi_c(q^{m_3}) \\ & + \sum_{k=1}^{w-u} \sum_{c=1}^k \sum_{a=1}^u \frac{(-)^v \binom{2w-u-v-k-1}{w-u-k} \binom{u+v+k-c-a-1}{u-a, v-1, k-c}}{(-m_2)^{u+v+k-c-a} m_3^{2w-u-v-k} (2\tau_2)^{2w-c-a}} \varphi_a(q^{m_1}) \varphi_c(q^{m_3}) \\ & + \sum_{k=1}^{w-u} \frac{(-)^v \pi^2 \binom{2w-u-v-k-1}{w-u-k} \binom{u+v+k-3}{u-1, v-1, k-1}}{(-m_2)^{u+v+k-2} m_3^{2w-u-v-k} (2\tau_2)^{2w-2}} \\ & + ([u, m_1, a] \leftrightarrow [v, m_2, b])^* \end{aligned} \quad (4.28)$$

where the conjugation instruction $([u, m_1, a] \leftrightarrow [v, m_2, b])^*$ applies to the entire expression and leaves w, c, m_3 unchanged. As was the case already for the functions $\mathcal{C}_{u,v;w}^{(i)}$, and as we

shall show explicitly in subsequent sections, the infinite sums over m_r for $r = 1, 2, 3$ may be performed for the terms that are purely power behaved in τ_2 . For the exponential terms the values of m_r will control the powers in q and \bar{q} and, for a given assignment of powers of q and \bar{q} , the sums over m_r will reduce to finite sums.

5 The Fourier coefficient functions

In this section, we shall present the results for all the Fourier modes of $\mathcal{C}_{u,v;w}$ in theorem 4.1. The details of the calculations of the Laurent polynomial $\mathcal{L}_{u,v;w}(\tau_2)$ will be relegated to appendices A and B. Likewise, the details of the calculations of the exponential contributions, including the Laurent polynomials $\mathcal{Q}_{u,v;w}^{(N)}$, $F_{u,v;w}^{(N)}$, and $G_{u,v;w}^{(N,L)}$, will be relegated to appendix C. Various coefficients in the Laurent polynomials $F_{u,v;w}^{(N)}$ and $G_{u,v;w}^{(N,L)}$ involve rational numbers given by lengthy expressions of finite sums and will be presented in appendix D. In the present section, we shall summarize all of these results.

5.1 Decomposition of the functions φ_k and $\Phi_{a;b}$

To extract the Fourier coefficient functions from the formulas for $C_{u,v;w}(\tau)$ computed in the previous section, we decompose the elementary functions φ_k and $\Phi_{a;b}$ into parts which are purely Laurent polynomial in τ_2 and parts which are exponential,

$$\begin{aligned} \varphi_k(q^m) &= (2\pi)^k \varepsilon(m)^k \left(\frac{1}{2} \delta_{k,1} + \hat{\varphi}_k(q^{|m|}) \right) \\ \Phi_{a;b}(2m\tau_2) &= \varepsilon(m)^{a+b} \left(\Phi_{a;b}^{(0)}(2|m|\tau_2) + \Phi_{a;b}^{(1)}(2|m|\tau_2) \right) \end{aligned} \tag{5.1}$$

where the sign function $\varepsilon(m)$ is defined by,

$$\varepsilon(m) = \begin{cases} +1 & \text{for } m > 0 \\ 0 & \text{for } m = 0 \\ -1 & \text{for } m < 0 \end{cases} \tag{5.2}$$

The functions appearing in (5.1) are given as follows,

$$\begin{aligned} \hat{\varphi}_k(q^{|m|}) &= \frac{1}{\Gamma(k)} \sum_{p=1}^{\infty} p^{k-1} q^{p|m|} \\ \Phi_{a;b}^{(0)}(2|m|\tau_2) &= 2 \sum_{\alpha=0}^{[a/2]} \frac{(-)^{a+\alpha} \zeta(2\alpha) \binom{a+b-2\alpha-1}{b-1}}{(2|m|\tau_2)^{a+b-2\alpha}} + \frac{(-)^a \pi \binom{a+b-2}{a-1}}{(2|m|\tau_2)^{a+b-1}} \\ \Phi_{a;b}^{(1)}(2|m|\tau_2) &= \sum_{\beta=1}^b \frac{(-)^a \Gamma(a+b-\beta) (2\pi)^\beta \hat{\varphi}_\beta(e^{-4\pi|m|\tau_2})}{\Gamma(b-\beta+1)\Gamma(a) (2|m|\tau_2)^{a+b-\beta}} \end{aligned} \tag{5.3}$$

We have taken this opportunity to expose the dependence on the sign of the summation variable m for all functions involved.

5.2 The Laurent polynomial $\mathcal{L}_{u,v;w}$

The Laurent polynomial $\mathcal{L}_{u,v;w}$ of $\mathcal{C}_{u,v;w}$ is given by the following theorem.

Theorem 5.1. *The Laurent polynomial $\mathcal{L}_{u,v;w}$ of $\mathcal{C}_{u,v;w}$ is given as follows,*

$$\mathcal{L}_{u,v;w}(\tau_2) = \ell_w(4\pi\tau_2)^w + \sum_{k=0}^{w-2} \ell_{2k-w+1} \frac{\zeta(2w-2k-1)}{(4\pi\tau_2)^{w-2k-1}} + \frac{\ell_{2-w}}{(4\pi\tau_2)^{w-2}} \quad (5.4)$$

The coefficient $\ell_w \in \mathbb{Q}$ arises solely from $\mathcal{C}_{u,v;w}^{(0)}$ and was given in (3.4). The coefficients $\ell_{2k-w+1} \in \mathbb{Q}$ arise from $\mathcal{C}_{u,v;w}^{(i)}$ with $i = 1, 2, 3$ and are given by,

$$\begin{aligned} \ell_{2k-w+1} = & 2\theta\left(\left[\frac{u}{2}\right] - k\right) \frac{(-)^{v+1} B_{2k} \binom{2w-2k-2}{w-u-1} \binom{u+v-1-2k}{u-2k}}{(2k)!} + (u \leftrightarrow v) \\ & + 2\theta\left(\left[\frac{2w-u-v}{2}\right] - k\right) \frac{(-)^{w+1} B_{2k} \binom{2w-2k-2}{2w-u-v-2k} \binom{u+v-2}{v-1}}{(2k)!} \end{aligned} \quad (5.5)$$

where B_{2k} are the Bernoulli numbers and the symmetrization $u \leftrightarrow v$ applies only to the first line. The Heaviside θ -function is defined such that $\theta(x) = 1$ for $x \geq 0$ and zero otherwise. The coefficient ℓ_{2-w} arises from $\mathcal{C}_{u,v;w}^{(i)}$ with $i = 1, 2, 3, 4$ and is given as follows,

$$\begin{aligned} \ell_{2-w} = & \zeta(2w-2) \binom{u+v-2}{u-1} \left[(-)^v \binom{2w-3}{w-u-1} + \frac{1}{2} (-)^w \binom{2w-3}{u+v-2} \right] \\ & + 2(-)^v \sum_{k=u+v+1}^{w+v} \binom{2w-k-1}{w+v-k} \frac{\Gamma(k-2) \zeta(k-2, 2w-k)}{\Gamma(u)\Gamma(v)\Gamma(k-u-v)} + (u \leftrightarrow v) \end{aligned} \quad (5.6)$$

where the symmetrization $(u \leftrightarrow v)$ applies to the entire expression. The combination of multiple zeta values in the second term and even zeta values in the first may be simplified and gives ℓ_{2-w} as a bilinear combination of odd zeta values whose total weight is $2w-2$,

$$\ell_{2-w} = \sum_{k=1}^{w-3} \lambda_k \zeta(2k+1) \zeta(2w-2k-3) \quad \lambda_k \in \mathbb{Q} \quad (5.7)$$

with the coefficients λ_k given in proposition 5.2.

The double zeta value $\zeta(s, t)$ in the first expression for ℓ_{2-w} is defined by,

$$\zeta(s, t) = \sum_{m,n=1}^{\infty} \frac{1}{(m+n)^s n^t} \quad (5.8)$$

We note that the validity of the form of the expression given for ℓ_{2-w} in (5.7) was proven for the two-loop modular graph functions $C_{a,b,c}$ in [11], and may be proven by the same methods in the case of the functions $\mathcal{C}_{u,v;w}$. However, the expressions for the coefficients λ_k can be obtained only upon assuming the validity of a conjecture. The coefficients in the bilinear combination of odd zeta values given in conjecture 1.4 of [11] was obtained with the help of an identity between rational numbers given in conjecture 6.2 of that paper, which was verified to high order by MAPLE. Applying conjecture 6.2 of [11] to the expression for ℓ_{2-w} , we obtain the following expression for the coefficients λ_k .

Proposition 5.2. (Obtained by assuming the validity of conjecture 6.2 of [11].)

The coefficients λ_k in the Laurent series for $\mathcal{C}_{u,v,w}$ are given as follows,

$$\begin{aligned}
 \lambda_k = & (-)^w \delta_{w,v+1} \frac{\theta(w-z-1-\epsilon)\theta\left(\left[\frac{w-u}{2}\right]-w+z+1\right)\Gamma(2w-3)}{\Gamma(u)\Gamma(v)\Gamma(2w-u-v-1)} \\
 & + 2(-)^v \frac{\theta(w-k-3+\epsilon)\theta(k-z+1-\epsilon)\theta\left(\left[\frac{w-u}{2}\right]+z-k-1\right)\Gamma(2w-2k-3)\Gamma(2k+1)}{\Gamma(w+v-2k-2)\Gamma(w-v)\Gamma(u)\Gamma(v)\Gamma(2k-u-v+3)} \\
 & - (-)^v \sum_{m=\epsilon}^{\left[\frac{w-u}{2}\right]} \frac{\theta(w-z-m-2+\epsilon)\Gamma(2w-2z-2m-1)}{\Gamma(w-u-2m+\epsilon)\Gamma(w-v)\Gamma(u)\Gamma(v)\Gamma(2m+1-\epsilon)} \\
 & \quad \times \sum_{n=2m}^{2w-2z-3} \frac{E_{n-2m}(0)\Gamma(2k+1)\Gamma(2z+n-1)}{\Gamma(2w-2z-n-1)\Gamma(2k-2w+2z+n+3)\Gamma(n-2m+1)} \\
 & + (u \leftrightarrow v)
 \end{aligned} \tag{5.9}$$

where $z = [(u+v)/2]$, $\epsilon = u+v \pmod{2}$, and $E_n(0)$ are Euler polynomials evaluated at 0.

The Euler polynomials $E_n(t)$ (not to be confused with the Eisenstein series $E_s(\tau)$) may be defined by the following generating function,

$$\frac{2e^{xt}}{e^x+1} = \sum_{n=0}^{\infty} E_n(t) \frac{x^n}{n!} \tag{5.10}$$

The proof of theorem 5.1 is given in appendix A, while the proof of proposition 5.2, assuming the validity of conjecture 6.2 of [11], is given in appendix B.

5.3 Generalized divisor sum functions

In the calculation of non-constant exponential contributions to $\mathcal{C}_{u,v,w}$ to which we next turn, we shall encounter a generalization of the standard divisor functions $\sigma_s(N) = \sum_{0 < n|N} n^s$. We introduce these generalized divisor sums now. For $M, N \in \mathbb{N}$ and $A, B, C \in \mathbb{Z}$, we introduce the following generalized divisor function,

$$V_{A,B,C}(M, N) = \sum_{\substack{m|M \\ m \neq 0}} \sum_{\substack{n|N \\ n \neq 0, -m}} \frac{\varepsilon(m)\varepsilon(n)}{m^{A-1}n^{B-1}(m+n)^C} \tag{5.11}$$

In contrast to the standard divisor sum, the summation here is carried out over both positive and negative divisors m, n . The function $V_{A,B,C}(M, N)$ vanishes when $A+B+C$ is an odd integer since the summand is then odd under the reversal of the signs of both m and n . To account for this property in a systematic manner, we introduce the function,

$$\mathfrak{J}_n = \frac{1}{2}(1 + (-)^n) \tag{5.12}$$

which vanishes for n odd and equals 1 for n even. A more explicit formula for $V_{A,B,C}(M, N)$ may be obtained by separating the contributions from positive and negative m, n ,

$$V_{A,B,C}(M, N) = \sum_{0 < m|M} \frac{2\mathfrak{J}_{A+B+C}}{m^{A-1}} \left(\sum_{0 < n|N} \frac{1}{n^{B-1}(m+n)^C} + \sum_{\substack{0 < n|N \\ n \neq m}} \frac{(-)^B}{n^{B-1}(m-n)^C} \right) \tag{5.13}$$

5.4 The exponential part of the constant Fourier mode $\mathcal{Q}_{u,v;w}^{(N)}$

We now proceed to the calculation of the exponential part of the constant Fourier mode. To obtain this, we retain the contributions with identical powers of q and \bar{q} in $\mathcal{C}_{u,v;w}$, namely all terms of the form $(q\bar{q})^N$. The calculation of the exponential contributions will be carried out in appendix C, and the contributions to $\mathcal{Q}_{u,v;w}^{(N)}$ are organized in appendix D. The result may be stated in the form of the following theorem.

Theorem 5.3. The exponential part of the constant Fourier mode of $\mathcal{C}_{u,v;w}$ is given by,

$$\begin{aligned} \mathcal{Q}_{u,v;w}^{(N)}(\tau_2) &= \sum_{\beta=1}^{w-u+v-1} \frac{N^{\beta-1} (J_{u,v;w}^{(1)}(\beta, N) + J_{u,v;w}^{(3)}(\beta, N))}{\Gamma(\beta)(4\pi\tau_2)^{w-\beta-1}} \\ &+ \sum_{\beta=1}^{u+v-1} \frac{N^{\beta-1} J_{u,v;w}(\beta, N)}{\Gamma(\beta)(4\pi\tau_2)^{w-\beta-1}} + (u \leftrightarrow v) \end{aligned} \quad (5.14)$$

where the symmetrization in u, v applies to both lines. The coefficients are all rational functions, and are given by,

$$\begin{aligned} J_{u,v;w}^{(1)}(\beta, N) &= 2(-)^v \sigma_{2-2w}(N) \sum_{k=1}^{w+v} \binom{2w-k-1}{w+v-k} \binom{k-\beta-2}{u-1} \binom{k-u-2}{v-1} \\ &\quad \times [\theta(\beta-v)\theta(k-\beta-u-1) + \theta(v-\beta-1)\theta(k-u-v-1)] \\ J_{u,v;w}^{(2)}(\beta, N) &= \sum_{k=u+v+1}^{w+v} \sum_{a=\max(1, \beta-v+1)}^{\min(\beta, u)} \binom{k-\beta-2}{u-a, v+a-\beta-1, k-u-v-1} \\ &\quad \times (-)^{a+v} \binom{\beta-1}{\beta-a} \binom{2w-k-1}{w+v-k} V_{a, k-a, 2w-k}(N, N) \\ J_{u,v;w}^{(3)}(\beta, N) &= \sum_{c=\max(1, \beta-v+1)}^{\min(w-u, \beta)} \sum_{k=u+v}^{w+v-c} \binom{k+c-\beta-2}{u-1, v-\beta+c-1, k-u-v} \binom{2w-k-c-1}{w+v-k-c} \\ &\quad \times (-)^v \binom{\beta-1}{\beta-c} \left(4\mathfrak{J}_k \sigma_{1-k}(N) \sigma_{1-2w+k}(N) - 2\sigma_{2-2w}(N) \right) \\ J_{u,v;w}(\beta, N) &= J_{u,v;w}^{(2)}(\beta, N) + (-)^w \sigma_{2-2w}(N) \binom{2w-\beta-2}{u+v-\beta-1} \binom{u+v-2}{u-1} \end{aligned} \quad (5.15)$$

The functions $V_{A,B,C}(M, N)$ and \mathfrak{J}_n appearing above were defined in subsection 5.3.

5.5 The non-constant Fourier modes $F_{u,v;w}^{(N)}$ and $G_{u,v;w}^{(N,L)}$

The full expressions for the non-constant Fourier modes $G_{u,v;w}^{(N,L)}$ and $F_{u,v;w}^{(N)}$ are more involved than those of $\mathcal{L}_{u,v;w}$ and $\mathcal{Q}_{u,v;w}^{(N)}$. They are obtained in appendix D, with the final result summarized in the following theorem.

Theorem 5.4. The non-constant Fourier modes $G_{u,v;w}^{(N,L)}$ and $F_{u,v;w}^{(N)}$ are given by

$$\begin{aligned} G_{u,v;w}^{(N,L)}(\tau_2) &= \sum_{k=k_-}^{k_+} \sum_{\ell=1}^{\ell_+} \sum_{\beta=1}^{\beta_+} \frac{\mathcal{W}_{u,v;w}^{k,\ell,\beta}(N, L)}{(4\pi\tau_2)^{w-\ell-\beta}} \\ F_{u,v;w}^{(N)}(\tau_2) &= \sum_{k=k_-}^{k_+} \sum_{\ell=1}^{\ell_+} \left[\frac{\mathcal{M}_{u,v;w}^{k,\ell}(N)}{(4\pi\tau_2)^{w-\ell-1}} + \sum_{\gamma=0}^{\gamma_+} \frac{\mathcal{H}_{u,v;w}^{k,\ell,\beta}(N)}{(4\pi\tau_2)^{w-\ell-\gamma}} \right] \end{aligned} \quad (5.16)$$

where

$$\begin{aligned}
 k_- &= 1 + u + v \\
 k_+ &= \max(w + u, w + v) \\
 \ell_+ &= \max(w - u, u) \\
 \beta_+ &= \max(w + |u - v| - 1, u + v - 1) \\
 \gamma_+ &= \max(u + v, 2w - u - v - \epsilon)
 \end{aligned} \tag{5.17}$$

and $\epsilon = u + v \pmod{2}$. The coefficients $\mathcal{W}_{u,v;w}^{k,\ell,\beta}(N, L)$ are given in (D.18), while the coefficients $\mathcal{H}_{u,v;w}^{k,\ell,\beta}(N)$ are defined implicitly by (D.29). Both are rational numbers for all integer-valued arguments and indices. The function $\mathcal{M}_{u,v;w}^{k,\ell}(N)$ is shown in (D.26) and gives rational multiples of odd zeta values.

This completes the calculation of the full Fourier expansion for general two-loop modular graph functions, all of which may be constructed from $\mathcal{C}_{u,v;w}$. In the following subsection we illustrate these results by means of an explicit example.

5.6 An example: $\mathcal{C}_{2,1,1}$

We now illustrate our results for the familiar case of two-loop modular graph functions $\mathcal{C}_{a,b,c}$. To utilize the results of the previous sections, we must first recast these modular graph functions in terms of the basis $\mathcal{C}_{u,v;w}$. One finds for example

$$\mathcal{C}_{2,1,1} = \mathcal{C}_{2,2;4} - \frac{3}{2}(\mathcal{C}_{2,3;4} + \mathcal{C}_{3,2;4}) \tag{5.18}$$

It is known that $\mathcal{C}_{2,1,1}$ has the following Laurent polynomial [14],

$$\mathcal{C}_{2,1,1}^{\mathcal{L}} = \frac{2y^4}{14175} + \frac{\zeta(3)}{45}y + \frac{5\zeta(5)}{12y} - \frac{\zeta(3)^2}{4y^2} + \frac{9\zeta(7)}{16y^3} \tag{5.19}$$

with $y = \pi\tau_2$. Using Mathematica, one verifies that theorem 5.1 reproduces this result,

$$\mathcal{L}_{2,2;4} - \frac{3}{2}(\mathcal{L}_{2,3;4} + \mathcal{L}_{3,2;4}) = \mathcal{C}_{2,1,1}^{\mathcal{L}} \tag{5.20}$$

The exponential part of the Fourier series of $\mathcal{C}_{2,1,1}$ can be obtained by exploiting the following differential equation,

$$(\Delta - 2)\mathcal{C}_{2,1,1} = 9E_4 - E_2^2 \tag{5.21}$$

as well as the known Fourier expansion (2.23) of the non-holomorphic Eisenstein series. Let us define the coefficients of the Fourier expansion as $\mathcal{C}_{2,1,1}^{(M,N)}$, such that,

$$\mathcal{C}_{2,1,1}(\tau) = \sum_{M,N=0}^{\infty} \mathcal{C}_{2,1,1}^{(M,N)}(\tau_2) q^M \bar{q}^N \tag{5.22}$$

We begin by obtaining the exponential part of the constant Fourier mode, denoted by $\mathcal{Q}^{(N)}$ in (4.1). The only contribution of the form $(q\bar{q})^N$ to the right-hand side of (5.21)

comes from E_2^2 , as can be seen from (2.23). Using the latter formula gives the following differential equation for $C_{2,1,1}^{(N,N)}$,

$$(\tau_2^2 \partial_{\tau_2}^2 - 2) \left(C_{2,1,1}^{(N,N)}(\tau_2)(q\bar{q})^N \right) = -8N^2 \sigma_{-3}(N)^2 P_2(4\pi N \tau_2)^2 (q\bar{q})^N \quad (5.23)$$

Restricting to solutions involving only powers of τ_2 , one finds

$$C_{2,1,1}^{(N,N)} = -8 \frac{\sigma_{-3}(N)^2}{(4\pi\tau_2)^2} \quad (5.24)$$

In other words, we expect from (5.18) that

$$\mathcal{Q}_{2,2;4}^{(N)}(\tau_2) - \frac{3}{2} \left(\mathcal{Q}_{2,3;4}^{(N)}(\tau_2) + \mathcal{Q}_{3,2;4}^{(N)}(\tau_2) \right) = -8 \frac{\sigma_{-3}(N)^2}{(4\pi\tau_2)^2} \quad (5.25)$$

Using Mathematica, one may check that this is indeed the result given by theorem 5.3.

One may now similarly proceed to obtain the non-constant contributions. For example, the Laplace equation (5.21) together with appropriate boundary conditions yields the following results,

$$\begin{aligned} C_{2,1,1}^{(1,0)} &= \frac{y}{45} + \frac{1}{3} + \frac{11}{12y} + \frac{9}{8y^2} - \frac{\zeta(3)}{2y^2} + \frac{9}{16y^3} \\ C_{2,1,1}^{(2,0)} &= \frac{y}{40} + \frac{31}{16} + \frac{385}{128y} + \frac{1033}{512y^2} - \frac{9\zeta(3)}{16y^2} + \frac{1161}{2048y^3} \\ C_{2,1,1}^{(2,1)} &= -\frac{9}{16y^2} \end{aligned} \quad (5.26)$$

One may check that these are consistent with the results of theorem 5.4 for $F^{(1)}$, $F^{(2)}$, and $G^{(1,1)}$ respectively, and that the first line is consistent with equation (5.7) of [4].

6 The space of odd two-loop modular functions

In this section, we shall study the space \mathfrak{A}_w of odd two-loop modular graph functions of weight w . They are cuspidal functions with exponential decay at the cusp. Using holomorphic subgraph reduction and the sieve algorithm studied in [13–15], we shall exhibit a subspace of \mathfrak{A}_w consisting of functions which may be expressed in terms of Eisenstein series, construct two other linearly independent subspaces, and use these results to give a lower bound on the dimension of \mathfrak{A}_w . Finally, we shall show that \mathfrak{A}_w is trivial for $w \leq 4$ and that the lower bound is saturated for $5 \leq w \leq 11$.

6.1 Odd two-loop modular graph functions

Odd two-loop modular graph functions may be obtained from general two-loop modular graph functions by taking their parity odd part,

$$\mathcal{A} \begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{bmatrix} = \mathcal{C} \begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{bmatrix} - \mathcal{C} \begin{bmatrix} b_1 & b_2 & b_3 \\ a_1 & a_2 & a_3 \end{bmatrix} \quad (6.1)$$

where the total exponents a, b , defined by,

$$a = a_1 + a_2 + a_3 \quad b = b_1 + b_2 + b_3 \tag{6.2}$$

are equal to one another and the weight w is given by $w = a = b$. We shall impose the following restrictions in order to obtain a space on which differential operators, such as the Laplace operator, act consistently,

$$\mathfrak{A}_w = \left\{ \mathcal{A} \begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{bmatrix}, \left\{ \begin{array}{l} a_r, b_r \geq 0, \quad a_r + a_s + b_r + b_s \geq 3 \text{ for } r \neq s \\ \text{at most one } a_r \text{ and at most one } b_r \text{ vanishes} \end{array} \right\} \right\} \tag{6.3}$$

The following theorem is an immediate consequence of the structure of the Fourier series for two-loop modular graph functions given in the preceding section, and in particular follows from the reality of the Laurent polynomial $\mathcal{L}_{u,v;w}$.

Theorem 6.1. *All odd two-loop modular graph functions in \mathfrak{A}_w are cuspidal functions.*

The exponential suppression at the cusp of odd modular graph functions allows us to introduce the Petersson inner product on the space $\mathfrak{A} = \bigoplus_w \mathfrak{A}_w$, which is defined by,

$$\langle \mathcal{A}_1 | \mathcal{A}_2 \rangle = \int_{\mathcal{M}} d\mu \mathcal{A}_1(\tau)^* \mathcal{A}_2(\tau) \quad d\mu = \frac{i}{2\tau_2^2} d\tau \wedge d\bar{\tau} \tag{6.4}$$

for $\mathcal{A}_1, \mathcal{A}_2 \in \mathfrak{A}$ and where \mathcal{M} is a fundamental domain $\mathcal{M} = \mathcal{H}/\text{PSL}(2, \mathbb{Z})$.

Using proposition 2.1 all odd two-loop modular graph functions may be expressed as linear combinations of the following functions, for which we adopt a convenient notation,

$$\mathcal{A}_{u,v;w} = -\mathcal{A}_{v,u;w} = \mathcal{A} \begin{bmatrix} u & 0 & w-u \\ 0 & v & w-v \end{bmatrix} \tag{6.5}$$

Without loss of generality, we restrict the range of parameters to $1 \leq u < v \leq w - 1$. This restriction gives a trivial upper bound on the dimension $\dim \mathfrak{A}_w \leq \frac{1}{2}(w-1)(w-2)$. However, many linear relations exist between the functions of (6.5), and one readily shows $\mathcal{A}_{1,2;3} = \mathcal{A}_{1,2;4} = \mathcal{A}_{1,3;4} = \mathcal{A}_{2,3;4} = 0$ so that

$$\dim \mathfrak{A}_3 = \dim \mathfrak{A}_4 = 0 \tag{6.6}$$

To investigate the spaces \mathfrak{A}_w with $w \geq 5$, we shall use holomorphic subgraph reduction and the sieve algorithm, which we review in the next two subsections.

6.2 Holomorphic subgraph reduction

A systematic *sieve algorithm* was developed in [13, 14] to prove identities between modular graph forms. The key ingredient is the use of the Cauchy-Riemann operator $\nabla = 2i\tau_2^2 \partial_{\bar{\tau}}$ to relate identities between modular graph forms to identities between holomorphic Eisenstein series, using *holomorphic subgraph reduction*.

Applying the Cauchy-Riemann operator to an odd modular graph function will produce a modular graph form. Thus, we shall need to work on a larger space, of two-loop modular

graph forms given by the Kronecker-Eisenstein sums of (2.25). For independent total exponents $a, b \geq 2$, we define the spaces,

$$\mathcal{V}_{(a,b)} = \left\{ \mathcal{C}^+ \begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{bmatrix}, \left\{ \begin{array}{l} a_r, b_r \geq 0, \quad a_r + a_s + b_r + b_s \geq 3 \text{ for } r \neq s \\ \text{at most one } a_r \text{ and at most one } b_r \text{ vanishes} \end{array} \right\} \right\} \quad (6.7)$$

while for $a = 1$ or $b = 1$, we define the spaces as follows,

$$\mathcal{V}_{(a,1)} = \left\{ \mathcal{C}^+ \begin{bmatrix} a & 0 \\ 1 & 0 \end{bmatrix}, \quad a \geq 5 \right\} \quad \mathcal{V}_{(1,b)} = \left\{ \mathcal{C}^+ \begin{bmatrix} 1 & 0 \\ b & 0 \end{bmatrix}, \quad b \geq 5 \right\} \quad (6.8)$$

The restriction that at most one a_r and at most one b_r is allowed to vanish provides a self-consistent truncation, and guarantees that the Laplace operator maps $\mathcal{V}_{(a,a)}$ to itself [13, 14]. The spaces $\mathcal{V}_{(a,b)}$ for $a, b \geq 2$ and $a + b \geq 6$ also contain one-loop modular graph functions and products of one-loop modular graph functions as was shown in (2.27).

The operator ∇ acts as follows on an arbitrary two-loop modular graph form $\mathcal{C}^+ \in \mathcal{V}_{(a,b)}$,

$$\nabla \mathcal{C}^+ \begin{bmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{bmatrix} = \sum_{i=1}^3 a_i \mathcal{C}^+ \begin{bmatrix} a_i + 1 & a_{i'} & a_{i''} \\ b_i - 1 & b_{i'} & b_{i''} \end{bmatrix} \quad (6.9)$$

where (i, i', i'') is a cyclic permutation of $(1, 2, 3)$. The operator ∇ maps $\mathcal{V}_{(a,b)}$ to forms of weight $(a + 1, b - 1)$, but these forms do not necessarily belong to $\mathcal{V}_{(a+1,b-1)}$. Indeed, an exponent with value -1 can occur in the entry i of the lower row of exponents when the corresponding exponent b_i vanishes. Given the definition of $\mathcal{V}_{(a,b)}$, this means that the other two lower exponents $b_{i'}, b_{i''}$ are non-zero so that the momentum conservation identities of (2.4) can be used to convert the modular form with a negative entry into modular forms whose entries are all non-negative. These modular forms, however, still do not necessarily belong to $\mathcal{V}_{(a+1,b-1)}$ since two zeros may appear in the lower row. This is the point where *holomorphic subgraph reduction* enters, as the Kronecker-Eisenstein sum now contains a holomorphic subgraph sum which, for the case of two-loops, may be reduced as follows,

$$\begin{aligned} (-)^{a_0} \mathcal{C}^+ \begin{bmatrix} a_1 & a_2 & a_3 \\ 0 & 0 & b \end{bmatrix} &= \sum_{k=2}^{[a_1/2]} \binom{a_0 - 1 - 2k}{a_1 - 2k} \mathcal{G}_{2k} \mathcal{C}^+ \begin{bmatrix} a - 2k & 0 \\ b & 0 \end{bmatrix} + (a_1 \leftrightarrow a_2) \\ &- \binom{a_0}{a_1} \mathcal{C}^+ \begin{bmatrix} a & 0 \\ b & 0 \end{bmatrix} + \binom{a_0 - 2}{a_1 - 1} \left\{ \mathcal{G}_2 \mathcal{C}^+ \begin{bmatrix} a - 2 & 0 \\ b & 0 \end{bmatrix} + \mathcal{C}^+ \begin{bmatrix} a - 1 & 0 \\ b - 1 & 0 \end{bmatrix} \right\} \end{aligned} \quad (6.10)$$

where we have used the notation $a_0 = a_1 + a_2$. The form \mathcal{G}_{2k} is defined by $\mathcal{G}_{2k}(\tau) = (\tau_2)^{2k} G_{2k}(\tau)$ for $k \geq 2$ while $\mathcal{G}_2 = \tau_2^2 G_2$ is the non-holomorphic modular covariant weight two Eisenstein series. It was shown in [13, 14] that ∇ applied to any form in $\mathcal{V}_{(a,b)}$ produces linear combinations of modular graph forms in which the last two terms on the right side in (6.10) cancel, so that \mathcal{G}_2 never appears in the range $\nabla \mathcal{V}_{(a,b)}$.

6.3 The sieve algorithm

The sieve algorithm, developed in [13], can be stated simply and explicitly for two-loop graphs. Holomorphic subgraph reduction shows that the range $\nabla\mathcal{V}_{(a,b)}$ contains modular graph forms of weight $(a+1, b-1)$ which do not belong to $\mathcal{V}_{(a+1,b-1)}$. Those modular graph forms belong to the space $\mathfrak{C}_{(a+1,b-1)}$ specified by the following lemma.³

Lemma 6.2. *For $a-b \in 2\mathbb{Z}$ and $a, b \geq 2$ the following sum is direct,*

$$\mathfrak{C}_{(a,b)} = \bigoplus_{k=2}^{\lfloor a/2 \rfloor} \left\{ \mathcal{G}_{2k} \mathcal{C}^+ \begin{bmatrix} a-2k & 0 \\ b & 0 \end{bmatrix} \right\} \quad (6.11)$$

We shall prove the lemma by showing that the asymptotics near the cusp, given by a Laurent series up to exponential corrections, are linearly independent. The Laurent series in τ_2 may be obtained by combining the asymptotics of (2.23) with the first equation in (2.21) when $a \geq b$, and with the second equation of (2.21) when $a \leq b$. The result may be combined into the following expression which is valid in both cases,

$$\mathcal{C}^+ \begin{bmatrix} a & 0 \\ b & 0 \end{bmatrix} = \nu_a \tau_2^a + \nu_b \tau_2^{1-b} + \mathcal{O}(e^{-2\pi\tau_2}) \quad (6.12)$$

where $\nu_a, \nu_b \neq 0$. The asymptotics of $\mathcal{G}_{2k} = (\tau_2)^{2k} G_{2k}$ is given by τ_2^{2k} in view of (2.22), so that the asymptotics of the term with summation index k in (6.11) is proportional to $\nu'_a \tau_2^a + \nu'_b \tau_2^{1+2k-b}$ where $\nu'_a, \nu'_b \neq 0$. The linear independence of the terms in τ_2^{1+2k-b} then shows linear independence of the full functions, which proves the lemma.

6.3.1 The sieve

From the definition of $\mathfrak{C}_{(a,b)}$ it is clear that $\mathcal{V}_{(a,b)} \cap \mathfrak{C}_{(a,b)} = 0$, so that ∇ acts as follows,

$$\nabla : \mathcal{V}_{(a,b)} \rightarrow \mathcal{V}_{(a+1,b-1)} \oplus \mathfrak{C}_{(a+1,b-1)} \quad (6.13)$$

We define an ordered set of subspaces of $\mathfrak{C}_{(a,b)}$, or sieve,

$$\mathcal{V}_{(a,b)} \supset \mathcal{V}_{(a,b)}^{(1)} \supset \mathcal{V}_{(a,b)}^{(2)} \supset \dots \supset \mathcal{V}_{(a,b)}^{(b-1)} \quad (6.14)$$

by the following iterative procedure. Starting with $n=1$, we define $\mathcal{V}_{(a,b)}^{(1)}$ to be the maximal subspace of $\mathcal{V}_{(a,b)}$ whose range under ∇ has vanishing component along $\mathfrak{C}_{(a+1,b-1)}$,

$$\nabla : \mathcal{V}_{(a,b)}^{(1)} \rightarrow \mathcal{V}_{(a+1,b-1)} \quad (6.15)$$

The process may be repeated to define $\mathcal{V}_{(a+1,b-1)}^{(1)}$ to be the maximal subspace of $\mathcal{V}_{(a+1,b-1)}$ on which the range of ∇ has vanishing component along $\mathfrak{C}_{(a+2,b-2)}$ by,

$$\nabla : \mathcal{V}_{(a+1,b-1)}^{(1)} \rightarrow \mathcal{V}_{(a+2,b-2)} \quad (6.16)$$

³The space $\mathcal{V}_{(a,b)}^0$ used in [13] will be denoted by $\mathfrak{C}_{(a,b)}$ in this paper for the sake of greater clarity.

In turn the space $\mathcal{V}_{(a+1,b-1)}^{(1)}$ allows us to define $\mathcal{V}_{(a,b)}^{(2)}$ as the maximal subspace of $\mathcal{V}_{(a,b)}^{(1)}$ on which the range of ∇ is entirely inside $\mathcal{V}_{(a+1,b-1)}^{(1)}$ so that the range of ∇^2 on $\mathcal{V}_{(a,b)}^{(2)}$ has vanishing component along $\mathfrak{E}_{(a+2,b-2)}$,

$$\nabla : \mathcal{V}_{(a,b)}^{(2)} \rightarrow \mathcal{V}_{(a+1,b-1)}^{(1)} \quad \nabla^2 : \mathcal{V}_{(a,b)}^{(2)} \rightarrow \mathcal{V}_{(a+2,b-2)} \quad (6.17)$$

For the general case, we continue the iterative process by defining $\mathcal{V}_{(a,b)}^{(n)}$ to be the maximal subspace of $\mathcal{V}_{(a,b)}^{(n-1)}$ on which the range of ∇^n has zero component along $\mathfrak{E}_{(a+n,b-n)}$,

$$\nabla^n : \mathcal{V}_{(a,b)}^{(n)} \rightarrow \mathcal{V}_{(a+n,b-n)} \quad (6.18)$$

The process ends when $n = b - 1$ because it follows from the definition (6.7) that $\mathcal{V}_{(a,1)}$ vanishes for even a and is one-dimensional for odd a generated by $\nabla^{w-1}E_w$ with $2w - 1 = a$.

6.3.2 Direct sum decomposition

Of fundamental importance in the application of the sieve algorithm are the difference spaces $\mathcal{U}_{(a,b)}^{(n)}$ defined by the following direct sum decompositions,

$$\begin{aligned} \mathcal{V}_{(a,b)} &= \mathcal{U}_{(a,b)}^{(1)} \oplus \mathcal{V}_{(a,b)}^{(1)} \\ \mathcal{V}_{(a,b)}^{(n-1)} &= \mathcal{U}_{(a,b)}^{(n)} \oplus \mathcal{V}_{(a,b)}^{(n)} \end{aligned} \quad 2 \leq n \leq b - 1 \quad (6.19)$$

Therefore, we have,

$$\begin{aligned} \nabla^k \mathcal{V}_{(a,b)}^{(n-1)} &\subset \mathcal{V}_{(a+k,b-k)}^{(n-1-k)} & k \leq n - 1 \\ \nabla^n \mathcal{V}_{(a,b)}^{(n-1)} &\subset \mathcal{V}_{(a+n,b-n)} \oplus \nabla^n \mathcal{U}_{(a,b)}^{(n)} \end{aligned} \quad (6.20)$$

These relations do not define the elements in the spaces $\mathcal{U}_{(a,b)}^{(n)}$ uniquely, but we achieve uniqueness by requiring,

$$\nabla^n \mathcal{U}_{(a,b)}^{(n)} \subset \mathfrak{E}_{(a+n,b-n)} \quad (6.21)$$

Thus, the subspaces $\mathcal{U}_{(a,b)}^{(n)}$ collect the obstruction to ∇ mapping to $\mathcal{V}_{(a,b)}$ spaces. For the special case of *modular graph functions* with $a = b = w$ the sieve reduces to,

$$\mathcal{V}_{(w,w)} \supset \mathcal{V}_{(w,w)}^{(1)} \supset \mathcal{V}_{(w,w)}^{(2)} \supset \dots \supset \mathcal{V}_{(w,w)}^{(w-1)} \quad (6.22)$$

The Eisenstein series E_w belongs to each space in the sieve $E_w \in \mathcal{V}_{(w,w)}^{(n)}$ for all $0 \leq n \leq w - 1$.

6.4 Odd modular graph functions from Eisenstein series

An important subspace of odd two-loop modular graph functions of weight w is constructed from the following two-loop modular graph functions of weight $w = a_1 + a_2 = b_1 + b_2$,

$$\mathcal{A} \begin{bmatrix} a_1 & a_2 & 0 \\ b_1 & b_2 & 0 \end{bmatrix} = \mathcal{C} \begin{bmatrix} a_1 & a_2 & 0 \\ b_1 & b_2 & 0 \end{bmatrix} - \mathcal{C} \begin{bmatrix} b_1 & b_2 & 0 \\ a_1 & a_2 & 0 \end{bmatrix} \quad (6.23)$$

Convergence of the sums which define the modular graph functions in (2.25) requires $a_1 + b_1 \geq 3$ and $a_2 + b_2 \geq 3$. Using the decomposition of corollary 2.2, these functions are linear combinations of the functions $\mathcal{A}_{u,v,w}$ with the range for u, v defined in (6.5). Applying the algebraic reduction formulas of (2.27) to \mathcal{A} , we find,

$$\mathcal{A} \begin{bmatrix} a_1 & a_2 & 0 \\ b_1 & b_2 & 0 \end{bmatrix} = \mathcal{C} \begin{bmatrix} a_1 & 0 \\ b_1 & 0 \end{bmatrix} \mathcal{C} \begin{bmatrix} a_2 & 0 \\ b_2 & 0 \end{bmatrix} - \mathcal{C} \begin{bmatrix} b_1 & 0 \\ a_1 & 0 \end{bmatrix} \mathcal{C} \begin{bmatrix} b_2 & 0 \\ a_2 & 0 \end{bmatrix} \quad (6.24)$$

If $a_1 + b_1$ is an odd integer, and thus $a_2 + b_2$ is also odd, each factor on the right side of (6.24) vanishes and the resulting \mathcal{A} is zero. Assuming now that $a_1 + b_1$ is even and, without loss of generality, that $a_1 \geq b_1$, we define the following combinations,

$$\begin{aligned} a_1 + b_1 &= 2w_1 & a_1 - b_1 &= 2k \\ a_2 + b_2 &= 2w_2 & b_2 - a_2 &= 2k \end{aligned} \quad (6.25)$$

where $k \geq 0$, and $w = w_1 + w_2$ with $w_1, w_2 \geq 2$. We use the expressions of (2.21) for one-loop modular graph functions in terms of derivatives of Eisenstein series to simplify \mathcal{A} as follows,

$$\mathcal{A} \begin{bmatrix} a_1 & a_2 & 0 \\ b_1 & b_2 & 0 \end{bmatrix} = \frac{\Gamma(w_1)\Gamma(w_2)}{\Gamma(w_1+k)\Gamma(w_2+k)} \mathcal{P}_k(w_1, w_2) \quad (6.26)$$

where the function \mathcal{P} is given as follows,

$$\mathcal{P}_k(w_1, w_2) = \tau_2^{-2k} \left(\nabla^k E_{w_1} \bar{\nabla}^k E_{w_2} - \nabla^k E_{w_2} \bar{\nabla}^k E_{w_1} \right) \quad (6.27)$$

Manifestly, the function $\mathcal{P}_k(w_1, w_2)$ vanishes for $k = 0$ and is odd under swapping w_1 and w_2 . Thus we shall assume $k \geq 1$ and $w_1 > w_2$. We have $\mathcal{A} \in \mathfrak{A}_w$ whenever none of the exponents a_1, a_2, b_1, b_2 vanishes or, in this case, we have $\mathcal{P}_k(w_1, w_2) \in \mathfrak{A}_w$ whenever $k + 1 \leq w_2 < w_1$. We define the corresponding subspace as follows,

$$\mathfrak{A}_w^{(1)} = \left\{ \mathcal{P}_k(w_1, w_2) \text{ with } w = w_1 + w_2 \text{ and } 1 \leq k < w_2 < w_1 \right\} \quad (6.28)$$

Note that $\mathcal{P}_{w_2}(w_1, w_2)$ does not belong to \mathfrak{A}_w but instead belongs to $\mathfrak{C}_{(w,w)}$ defined in (6.11).

6.5 The spaces $\mathfrak{A}_w^{(2)}$ and $\mathfrak{A}_w^{(3)}$

We now introduce two further subspaces $\mathfrak{A}_w^{(2)}, \mathfrak{A}_w^{(3)} \subset \mathfrak{A}_w$, defined as follows,

$$\begin{aligned} \mathfrak{A}_w^{(2)} &= \left\{ \mathcal{A}_{u,u+1;w} \text{ with } 1 \leq u \leq \left\lfloor \frac{w-3}{2} \right\rfloor \right\} \\ \mathfrak{A}_w^{(3)} &= \left\{ \mathcal{A}_{u,u+1;w} \text{ with } \left\lfloor \frac{w-1}{2} \right\rfloor \leq u \leq w-5 \right\} \end{aligned} \quad (6.29)$$

The following subsections will rely on the following theorem, proven in appendix E.

Theorem 6.3. *The spaces $\mathfrak{A}_w^{(i)}$, $i = 1, 2, 3$ are linearly independent.*

6.6 Bounds on the dimension of \mathfrak{A}_w

The construction of the subspaces $\mathfrak{A}_w^{(1)}$, $\mathfrak{A}_w^{(2)}$, and $\mathfrak{A}_w^{(3)}$, and theorem 6.3 allow us to put a lower bound on $\dim \mathfrak{A}_w$. Together with the upper bound given after (6.5), we have,

Theorem 6.4. *The dimension of the space \mathfrak{A}_w for $w \geq 5$ is bounded by*

$$\sum_{i=1}^3 \dim \mathfrak{A}_w^{(i)} \leq \dim \mathfrak{A}_w \leq \frac{1}{2}(w-1)(w-2) \tag{6.30}$$

where

$$\dim \mathfrak{A}_w^{(1)} = \sum_{w_2=2}^{\lfloor \frac{w-1}{2} \rfloor} (w_2 - 1) = \frac{1}{2} \left\lfloor \frac{w-1}{2} \right\rfloor \left\lfloor \frac{w-3}{2} \right\rfloor \tag{6.31}$$

and

$$\dim \mathfrak{A}_w^{(2)} = \left\lfloor \frac{w-3}{2} \right\rfloor \quad \dim \mathfrak{A}_w^{(3)} = \begin{cases} w-5 - \lfloor \frac{w-3}{2} \rfloor & w \geq 8 \\ 0 & \text{otherwise} \end{cases} \tag{6.32}$$

Explicit computation shows that this lower bound is saturated for $w \leq 11$, while for $w \geq 12$ there are additional contributions. We find the following values for $\dim \mathfrak{A}_w$ for $w \leq 12$,

$$\begin{array}{lll} \dim \mathfrak{A}_5 = 2 & \dim \mathfrak{A}_6 = 2 & \dim \mathfrak{A}_7 = 5 \\ \dim \mathfrak{A}_8 = 6 & \dim \mathfrak{A}_9 = 10 & \dim \mathfrak{A}_{10} = 11 \\ \dim \mathfrak{A}_{11} = 16 & \dim \mathfrak{A}_{12} = 18 & \end{array} \tag{6.33}$$

In the next subsection we illustrate this explicit computation for the simplest case of \mathfrak{A}_5 .

6.7 Constructing a basis for $\dim \mathfrak{A}_5$

To make the discussion of this section more concrete, we illustrate here the construction of a basis for \mathfrak{A}_5 using holomorphic subgraph reduction and the sieve algorithm. By definition (6.3), the space \mathfrak{A}_5 is generated by the following six functions,

$$\mathcal{A}_{u,v;5} \quad 1 \leq u < v \leq 4 \tag{6.34}$$

The unique weight five \mathcal{P} -function $\mathcal{P}_1(2,3)$ is a linear combination of the above functions. We shall now use the sieve algorithm to construct all linear relations between the functions $\mathcal{A}_{u,v;w}$. To this end we apply ∇ repeatedly until we produce a modular form $\mathcal{G}_{2k} = \tau_2^{2k} G_{2k}$ proportional to the holomorphic Eisenstein series G_{2k} for $k \geq 2$. Applying ∇ once, we obtain,

$$\nabla \mathcal{A}_{1,2;5}, \nabla \mathcal{A}_{2,3;5} \in \mathcal{V}_{(6,4)} \tag{6.35}$$

as well as

$$\begin{aligned}
 \nabla \mathcal{A}_{1,3;5} - 3 \mathcal{G}_4 C^+ \begin{bmatrix} 2 & 0 \\ 4 & 0 \end{bmatrix} &\in \mathcal{V}_{(6,4)} \\
 \nabla \mathcal{A}_{1,4;5} - 3 \mathcal{G}_4 C^+ \begin{bmatrix} 2 & 0 \\ 4 & 0 \end{bmatrix} &\in \mathcal{V}_{(6,4)} \\
 \nabla \mathcal{A}_{2,4;5} - 3 \mathcal{G}_4 C^+ \begin{bmatrix} 2 & 0 \\ 4 & 0 \end{bmatrix} &\in \mathcal{V}_{(6,4)} \\
 \nabla \mathcal{A}_{3,4;5} + 3 \mathcal{G}_4 C^+ \begin{bmatrix} 2 & 0 \\ 4 & 0 \end{bmatrix} &\in \mathcal{V}_{(6,4)}
 \end{aligned} \tag{6.36}$$

Retaining $\mathcal{A}_{1,4;5}$ as a first basis function of \mathfrak{A}_5 , we take linear combinations $\mathcal{A}_{1,3;5} - \mathcal{A}_{1,4;5}$, $\mathcal{A}_{2,4;5} - \mathcal{A}_{1,4;5}$, and $\mathcal{A}_{3,4;5} + \mathcal{A}_{1,4;5}$ whose image under ∇ is in $\mathcal{V}_{(6,4)}$ in view of (6.36). Applying ∇^2 to these functions, and ∇ to the forms in (6.35), we obtain,

$$\begin{aligned}
 \nabla^2(\mathcal{A}_{1,3;5} - \mathcal{A}_{1,4;5}) + 6 \mathcal{G}_4 E_3 &\in \mathcal{V}_{(7,3)} \\
 \nabla^2(\mathcal{A}_{2,4;5} - \mathcal{A}_{1,4;5}) + 6 \mathcal{G}_4 E_3 &\in \mathcal{V}_{(7,3)} \\
 \nabla^2(\mathcal{A}_{3,4;5} + \mathcal{A}_{1,4;5}) + 6 \mathcal{G}_4 E_3 &\in \mathcal{V}_{(7,3)} \\
 \nabla^2 \mathcal{A}_{1,2;5} + 6 \mathcal{G}_4 E_3 &\in \mathcal{V}_{(7,3)} \\
 \nabla^2 \mathcal{A}_{2,3;5} + 18 \mathcal{G}_4 E_3 &\in \mathcal{V}_{(7,3)}
 \end{aligned} \tag{6.37}$$

Retaining $\mathcal{A}_{1,2;5}$ as a second basis vector of \mathfrak{A}_5 (which is independent of $\mathcal{A}_{1,4;5}$ by the sieve algorithm), we take linear combinations of all the other double derivative expressions to eliminate the $\mathcal{G}_4 E_3$ term, and to obtain combinations which belong to $\mathcal{V}_{(7,3)}$. The further application of ∇ produces the following results for $k = 3, 4$,

$$\begin{aligned}
 \nabla^k(\mathcal{A}_{1,3;5} - \mathcal{A}_{1,4;5} - \mathcal{A}_{1,2;5}) &\in \mathcal{V}_{(5+k,5-k)} \\
 \nabla^k(\mathcal{A}_{2,4;5} - \mathcal{A}_{1,4;5} - \mathcal{A}_{1,2;5}) &\in \mathcal{V}_{(5+k,5-k)} \\
 \nabla^k(\mathcal{A}_{3,4;5} + \mathcal{A}_{1,4;5} - \mathcal{A}_{1,2;5}) &\in \mathcal{V}_{(5+k,5-k)} \\
 \nabla^k(\mathcal{A}_{2,3;5} - 3\mathcal{A}_{1,2;5}) &\in \mathcal{V}_{(5+k,5-k)}
 \end{aligned} \tag{6.38}$$

By inspection of its definition in (6.7), the space $\mathcal{V}_{(9,1)}$, which enters above for $k = 4$, is one-dimensional and generated by $\nabla^4 E_5$. However, E_5 is even and thus the left side of each line in (6.38) must vanish for $k = 4$. Each equation above then states that $\nabla^4 \mathcal{A} = 0$ for the corresponding \mathcal{A} . Lemma 1 of [13] implies in each case that \mathcal{A} must be constant. Since there are no constant odd functions, \mathcal{A} must vanish identically, and we obtain the identities,

$$\begin{aligned}
 \mathcal{A}_{1,3;5} &= \mathcal{A}_{1,2;5} + \mathcal{A}_{1,4;5} & \mathcal{A}_{2,3;5} &= 3\mathcal{A}_{1,2;5} \\
 \mathcal{A}_{2,4;5} &= \mathcal{A}_{1,2;5} + \mathcal{A}_{1,4;5} & \mathcal{A}_{3,4;5} &= \mathcal{A}_{1,2;5} - \mathcal{A}_{1,4;5}
 \end{aligned} \tag{6.39}$$

One may use similar means to show that $\mathcal{P}_1(2,3) = 6\mathcal{A}_{1,4;5}$. The differential equation satisfied by $\mathcal{A}_{1,2;5}$ in the fourth line of (6.37) and by $\mathcal{A}_{1,4;5}$ in the second line of (6.36) imply the linear independence of these functions. Therefore we conclude that $\dim \mathfrak{A}_5 = 2$, and we may take $\mathcal{A}_{1,2;5}$ and $\mathcal{A}_{1,4;5}$ as a basis.

6.8 Speculations on a basis for $w \geq 12$

For weight 12, the dimensions of $\mathfrak{A}_{12}^{(1)}$, $\mathfrak{A}_{12}^{(2)}$, $\mathfrak{A}_{12}^{(3)}$ are respectively 10, 4, and 3, adding up to 17, one fewer than the result of explicit calculation. The missing subspace may be generated, for example, by the function $\mathcal{A}_{4,7;12}$. For weights $w > 12$, no systematic pattern could yet be proven. However, preliminary checks done up to weight 20 using Mathematica indicate that the following space may be a candidate for the missing subspace for higher weights,

$$\mathfrak{A}_w^{(4)} = \left\{ \mathcal{A} \begin{bmatrix} u & 0 & w-u \\ 0 & v & w-v \end{bmatrix} \mid 1 \leq \gamma \leq \gamma_{\max}, \left[\frac{w+1}{2} \right] \leq v \leq w-6 \right\} \quad (6.40)$$

where γ and γ_{\max} are defined as follows,

$$u = \left[\frac{w+1}{2} \right] - 3 + \gamma \quad \gamma_{\max}(v, w) = \min \left\{ w - v - 5, v - \left[\frac{w+1}{2} \right] + 1 \right\} \quad (6.41)$$

Functions in this set would be expected to produce holomorphic Eisenstein series either at order ∇^u or ∇^{w-v} , and it can be shown that only the latter occurs. However, a complete proof of linear independence has remained elusive.

Assuming linear independence, the dimension of the space $\mathfrak{A}_w^{(4)}$ is given by,

$$\dim \mathfrak{A}_w^{(4)} = \sum_{n=6}^{\lfloor w/2 \rfloor} \min \left\{ n - 5, \left[\frac{w}{2} \right] - n + 1 \right\} = \sum_{n=2}^{\lfloor \frac{w-8}{2} \rfloor} \left[\frac{n}{2} \right] \quad (6.42)$$

which would lead to the following full dimension of \mathfrak{A}_w ,

$$\dim \mathfrak{A}_w = \sum_{i=1}^4 \dim \mathfrak{A}_w^{(i)} \quad (6.43)$$

giving up to weight $w \leq 20$ the following speculated predictions,

$$\begin{array}{lll} \dim \mathfrak{A}_{13} = 24 & \dim \mathfrak{A}_{14} = 26 & \dim \mathfrak{A}_{15} = 33 \\ \dim \mathfrak{A}_{16} = 36 & \dim \mathfrak{A}_{17} = 44 & \dim \mathfrak{A}_{18} = 47 \\ \dim \mathfrak{A}_{19} = 56 & \dim \mathfrak{A}_{20} = 60 & \end{array} \quad (6.44)$$

It would be interesting to establish a complete formula for the dimension at all weights.

7 Inner product of modular graph functions

The Petersson inner product $\langle f|g \rangle$ of modular functions f, g is defined by [45],

$$\langle f|g \rangle = \int_{\mathcal{M}} d\mu f(\tau)^* g(\tau) \quad d\mu = \frac{i}{2\tau_2^2} d\tau \wedge d\bar{\tau} \quad (7.1)$$

where \mathcal{M} is the fundamental domain for $\text{PSL}(2, \mathbb{Z})$ in the upper half τ -plane \mathcal{H} . The Petersson inner product defines the space $L^2(\mathcal{M})$ of modular functions which are square

integrable on \mathcal{M} . The Petersson inner product may also be defined for modular forms, but we shall not consider this case here. Clearly, the inner product vanishes when f is an even modular function and g is an odd modular function. Therefore, it suffices to consider the inner product between modular functions which are both even or both odd.

In this section, we shall investigate the Petersson inner product involving one-loop and two-loop modular graph functions, and evaluate the product by applying the Rankin-Selberg-Zagier method [46–48] to the Poincaré and Fourier series obtained in preceding sections (see also [49] for a useful reference in the physics literature). It will be convenient to consider the cases of even and odd modular graph functions separately. Of considerable use will be the action of the Laplace-Beltrami operator on modular graph functions, which we shall summarize in the next subsection.

7.1 The Laplace operator acting on $\mathcal{C}_{u,v;w}$

The Eisenstein series are eigenfunctions of the Laplace operator $\Delta = 4\tau_2^2 \partial_{\bar{\tau}} \partial_{\tau}$ on \mathcal{H} ,

$$\Delta E_s = s(s-1)E_s \tag{7.2}$$

The action of the Laplace operator on two-loop modular graph functions was studied extensively in [4] for a special class of even functions. Here we shall need a generalization to the functions $\mathcal{C}_{u,v;w}$ which include both even and odd functions and is given by,

$$\begin{aligned} \Delta \mathcal{C}_{u,v;w} = & (w^2 + 2uv - uw - vw - w) \mathcal{C}_{u,v;w} + uv \mathcal{C}_{u+1,v+1;w} \\ & + u(2v - w) \mathcal{C}_{u+1,v;w} + v(2u - w) \mathcal{C}_{u,v+1;w} \\ & + u(v - w) \mathcal{C}_{u+1,v-1;w} + v(u - w) \mathcal{C}_{u-1,v+1;w} \end{aligned} \tag{7.3}$$

The indices u, v are integer-valued, but we shall allow $w \in \mathbb{C}$, subject to the convergence conditions given earlier.

The Laplace operator Δ is invariant under parity $\tau \rightarrow -\bar{\tau}$ and (7.3) is invariant under interchange of u and v for fixed w . Therefore, the symmetric and anti-symmetric parts of $\mathcal{C}_{u,v;w}$, respectively denoted $\mathcal{S}_{u,v;w} \in \mathfrak{S}_w$ and $\mathcal{A}_{u,v;w} \in \mathfrak{A}_w$, separately obey (7.3).

The odd two-loop modular graph functions $\mathcal{P}_k(s, t)$ for $k \in \mathbb{N}$ and $s, t \in \mathbb{C}$ defined in (6.26) and expressed in terms of bilinears in derivatives of Eisenstein series in (6.27),

$$\mathcal{P}_k(s, t)(\tau) = \tau_2^{-2k} \left(\nabla^k E_s \bar{\nabla}^k E_t - \nabla^k E_t \bar{\nabla}^k E_s \right) \tag{7.4}$$

satisfy a particularly simple system of Laplace eigenvalue equations given by,

$$\begin{aligned} \Delta \mathcal{P}_k(s, t) = & \mathcal{P}_{k+1}(s, t) + (s^2 + t^2 - s - t - 2k^2) \mathcal{P}_k(s, t) \\ & + (s - k)(t - k)(s + k - 1)(t + k - 1) \mathcal{P}_{k-1}(s, t) \end{aligned} \tag{7.5}$$

The validity of this formula may be verified by direct calculation, and it will be convenient to set $\mathcal{P}_0(s, t) = 0$. A particularly useful property of the system (7.5) is that it allows us to express \mathcal{P}_{k+1} in terms of a linear combination of $\Delta \mathcal{P}_k$ and \mathcal{P}_ℓ with $\ell < k$.

Restricting attention to $s, t \in \mathbb{N}$, the system (7.5) truncates in the following sense. For $1 \leq k < t < s$, the functions $\mathcal{P}_k(s, t)$ belong to the space $\mathfrak{A}_w^{(1)}$, but $\mathcal{P}_t(s, t)$ is no longer

an element of $\mathfrak{A}_w^{(1)}$ because it may be reduced to a combination of holomorphic Eisenstein series. Truncating the system to $1 \leq k < t < s$ and treating the function $\mathcal{P}_t(s, t)$ as an inhomogeneous term, we find the following system of differential equations,

$$\Delta \mathcal{P}_k(s, t) - \sum_{\ell=1}^{t-1} M_{k\ell} \mathcal{P}_\ell(s, t) = \delta_{k,t-1} \mathcal{P}_t(s, t) \tag{7.6}$$

The entries of the matrix M are given by (7.5) and its spectrum obeys the theorem below.

Theorem 7.1. *The eigenvalues of the matrix M have multiplicity one and are found to be,*

$$(s + t - 2n)(s + t - 1 - 2n) \qquad n = 1, \dots, t - 1 \tag{7.7}$$

The theorem is a special case of a result which was proven in section 5.3 of [14].

7.2 Petersson inner product on odd modular graph functions

Odd modular graph functions do not exist at one loop order. The space of odd two-loop modular graph functions is denoted $\mathfrak{A} = \bigoplus_w \mathfrak{A}_w$ and is the direct sum of the spaces \mathfrak{A}_w of functions of weight w . In view of theorem 6.1 all odd two-loop modular graph functions are cuspidal functions with exponential decay at the cusp so that $\mathfrak{A} \subset L^2(\mathcal{M})$. The Petersson inner product between any pair of odd modular graph functions is convergent and may be calculated in terms of Poincaré and Fourier series by Rankin-Selberg methods.

In this section we shall investigate the Petersson inner product between odd two-loop modular graph functions and show how the product is evaluated concretely between $\mathcal{A}_{u,v;w}$ and $\mathcal{P}_k(s, t)$. The Poincaré series of $\mathcal{A}_{u,v;w}(\tau)$ with respect to $\Gamma_\infty \backslash \text{PSL}(2, \mathbb{Z})$ is given by,

$$\mathcal{A}_{u,v;w}(\tau) = \sum_{g \in \Gamma_\infty \backslash \text{PSL}(2, \mathbb{Z})} \Lambda_{u,v;w}^A(g\tau) \tag{7.8}$$

where $\Lambda_{u,v;w}^A(\tau) = \Lambda_{u,v;w}(\tau) - \Lambda_{v,u;w}(\tau)$ and $\Lambda_{u,v;w}(\tau)$ is given in equation (3.4) of theorem 3.1. The Fourier series of $\mathcal{A}_{u,v;w}(\tau)$ is given in (4.5). Using standard Rankin-Selberg, we have,

$$\langle \mathcal{A}_{u_1,v_1;w_1} | \mathcal{A}_{u_2,v_2;w_2} \rangle = 2 \sum_{N=1}^{\infty} \int_0^{\infty} \frac{d\tau_2}{\tau_2^2} \mathcal{F}_{u_1,v_1;w_1}^{(N)}(\tau_2) \int_0^1 d\tau_1 (\bar{q}^N - q^N) \Lambda_{u_2,v_2;w_2}^A(\tau) \tag{7.9}$$

For $w_2 \in \mathbb{C}$, we use equation (3.23) to express the seed function and carry out the integral over τ_1 to obtain the theorem below.

Theorem 7.2. *The inner product between two odd modular graph functions $\mathcal{A}_{u_1,v_1;w_1}$ with Fourier coefficients \mathcal{F} and $\mathcal{A}_{u_2,v_2;w_2}$ with Poincaré series seed Υ , is given by,*

$$\begin{aligned} \langle \mathcal{A}_{u_1,v_1;w_1} | \mathcal{A}_{u_2,v_2;w_2} \rangle &= 8 \sum_{k=1}^u \binom{u_2 + v_2 - k - 1}{v_2 - 1} \sum_{N=1}^{\infty} \sum_{0 < m | N} \frac{(2\pi)^k N^{k-1}}{\Gamma(k) m^{k-1}} \int_0^{\infty} d\tau_2 \tau_2^{w_2-2} \\ &\times e^{-4\pi N \tau_2} \mathcal{F}_{u_1,v_1;w_1}^{(N)}(\tau_2) \Upsilon_{w_2,k,u_2+v_2}(2m\tau_2) - (u \leftrightarrow v) \end{aligned} \tag{7.10}$$

The integral over τ_2 is absolutely convergent for sufficiently large $\text{Re}(w_2)$.

7.2.1 The inner product of \mathcal{P} with \mathcal{A}

The evaluation simplifies for the special case of the odd modular graph functions $\mathcal{P}_k(s, t)$. Consider the Petersson inner product of $\mathcal{P}_k(s, t)$ with $\mathcal{A}_{u,v;w}$ given by,

$$\langle \mathcal{P}_k(s, t) | \mathcal{A}_{u,v;w} \rangle = \int_{\mathcal{M}} d\mu \mathcal{P}_k(s, t)(\tau) \mathcal{A}_{u,v;w}(\tau) \quad (7.11)$$

The inner product with functions $\mathcal{P}_k(s, t)$ for $k > 1$ may be expressed in terms of inner products involving only $\mathcal{P}_1(s, t)$ with the help of the Laplace equations for both functions, and the self-adjointness of the Laplace operator on the space of odd modular graph functions,

$$\langle \Delta \mathcal{P}_k(s, t) | \mathcal{A}_{u,v;w} \rangle = \langle \mathcal{P}_k(s, t) | \Delta \mathcal{A}_{u,v;w} \rangle \quad (7.12)$$

For any $k \geq 1$ and fixed s, t , we abbreviate $\mathcal{P}_k = \mathcal{P}_k(s, t)$ and obtain the following recursion relations on the index k ,

$$\begin{aligned} \langle \mathcal{P}_{k+1} | \mathcal{A}_{u,v;w} \rangle &= uv \langle \mathcal{P}_k | \mathcal{A}_{u+1,v+1;w} \rangle \\ &\quad - (s-k)(t-k)(s+k-1)(t+k-1) \langle \mathcal{P}_{k-1} | \mathcal{A}_{u,v;w} \rangle \\ &\quad \{ w^2 + 2uv - w(1+u+v) - s^2 - t^2 + s+t + 2k^2 \} \langle \mathcal{P}_k | \mathcal{A}_{u,v;w} \rangle \\ &\quad + u(2v-w) \langle \mathcal{P}_k | \mathcal{A}_{u+1,v;w} \rangle + v(2u-w) \langle \mathcal{P}_k | \mathcal{A}_{u,v+1;w} \rangle \\ &\quad + u(v-w) \langle \mathcal{P}_k | \mathcal{A}_{u+1,v-1;w} \rangle + v(u-w) \langle \mathcal{P}_k | \mathcal{A}_{u-1,v+1;w} \rangle \end{aligned} \quad (7.13)$$

which proves the assertion.

To evaluate the Petersson inner product $\langle \mathcal{P}_1(s, t) | \mathcal{A}_{u,v;w} \rangle$ we use the expression for $\mathcal{P}_1(s, t)$ in terms of Eisenstein series (6.27). We express the Eisenstein series E_s in terms of its Poincaré series and express E_t in terms of its Fourier series expansion (2.19). We shall keep $s \in \mathbb{C}$ but restrict $t \in \mathbb{N}$. Finally, we use the fact that $\mathcal{A}_{u,v;w}$ is cuspidal and unfold the Poincaré series using standard Rankin-Selberg,

$$\begin{aligned} \langle \mathcal{P}_1(s, t) | \mathcal{A}_{u,v;w} \rangle &= \frac{16 s \zeta(2s)}{\pi^{s-1} \Gamma(t)} \sum_{k=0}^{t-1} \frac{\Gamma(t+k)}{(4\pi)^k \Gamma(t-k) k!} \sum_{N=1}^{\infty} N^{t-k} \sigma_{1-2t}(N) \\ &\quad \times \int_0^{\infty} d\tau_2 \tau_2^{s-k-1} \int_0^1 d\tau_1 (\bar{q}^N - q^N) \mathcal{A}_{u,v;w}(\tau) \end{aligned} \quad (7.14)$$

The Fourier series decomposition of $\mathcal{A}_{u,v;w}$, given in (4.5), then produces the theorem below.

Theorem 7.3. *The inner product of $\mathcal{P}_1(s, t)$ with the odd modular graph function $\mathcal{A}_{u,v;w}$ whose Fourier coefficients are $\mathcal{F}_{u,v;w}^{(N)} - \mathcal{F}_{v,u;w}^{(N)}$ is given as follows,*

$$\begin{aligned} \langle \mathcal{P}_1(s, t) | \mathcal{A}_{u,v;w} \rangle &= \frac{32 s \zeta(2s)}{\pi^{s-1} \Gamma(t)} \sum_{k=0}^{t-1} \frac{\Gamma(t+k)}{(4\pi)^k \Gamma(t-k) k!} \sum_{N=1}^{\infty} N^{t-k} \sigma_{1-2t}(N) \\ &\quad \times \int_0^{\infty} d\tau_2 \tau_2^{s-k-1} e^{-4\pi N \tau_2} \left(\mathcal{F}_{u,v;w}^{(N)}(\tau_2) - \mathcal{F}_{v,u;w}^{(N)}(\tau_2) \right) \end{aligned} \quad (7.15)$$

The integral over τ_2 is absolutely convergent for sufficiently large $\text{Re}(s)$.

Explicit formulas may be obtained in terms of the coefficients $\mathcal{W}_{u,v;w}^{k,\ell,\beta}(N,L)$, $\mathcal{M}_{u,v;w}^{k,\ell}(N)$, and $\mathcal{H}_{u,v;w}^{k,\ell,\beta}(N)$ of the Laurent polynomials which define $\mathcal{F}_{u,v;w}^{(N)}$ using theorem 5.4. The integral over τ_2 of a term proportional to τ_2^ν in these Laurent polynomials is given by,

$$\int_0^\infty d\tau_2 \tau_2^{s-k+\nu-1} e^{-4\pi N\tau_2} = \frac{\Gamma(s-k+\nu)}{(4\pi N)^{s-k+\nu}} \tag{7.16}$$

which shows that the sum over N will converge absolutely for $\text{Re}(s)$ sufficiently large.

7.3 Petersson inner product on even modular graph functions

Even modular graph functions at one-loop order consist of non-holomorphic Eisenstein series E_s . The space of even modular graph functions at two-loop order will be denoted $\mathfrak{S} = \bigoplus_w \mathfrak{S}_w$ and is the direct sum of the spaces \mathfrak{S}_w of functions of weight w . Even modular graph functions, either at one or two loops, generically grow as positive powers of τ_2 near the cusp, and are not in $L^2(\mathcal{M})$. Zagier has extended the use of the Rankin-Selberg method to functions of power-growth near the cusp in terms of “renormalized” Petersson integrals [48]. For applications to string theory, however, it is more useful to consider the regularized integrals defined on the cut-off domain

$$\mathcal{M}_L = \mathcal{M} \cap \{\tau_2 < L\} \tag{7.17}$$

7.3.1 Producing even cuspidal functions from E_s and $\mathcal{C}_{u,v;w}$

We begin by defining the operator Δ_k in terms of the Laplace-Beltrami operator Δ mapping the space of modular functions into itself by,

$$\Delta_k = \prod_{\ell=1}^k (\Delta - \ell(\ell-1)) \qquad \Delta = \tau_2^2 (\partial_{\tau_1}^2 + \partial_{\tau_2}^2) \tag{7.18}$$

An alternative expression for Δ_k may be obtained in terms of the first order operators,

$$\begin{aligned} \nabla &= +2i\tau_2^2 \partial_\tau & \nabla &: (0, n) \rightarrow (0, n-2) \\ \bar{\nabla} &= -2i\tau_2^2 \partial_{\bar{\tau}} & \bar{\nabla} &: (n, 0) \rightarrow (n-2, 0) \end{aligned} \tag{7.19}$$

where (m, n) is modular weight. The operator Δ_k satisfies,

$$\Delta_k = \bar{\nabla}^k \tau_2^{-2k} \nabla^k = \nabla^k \tau_2^{-2k} \bar{\nabla}^k \tag{7.20}$$

We have $\Delta_1 = \Delta$, and its action on a monomial τ_2^s is given by,

$$\Delta_k \tau_2^s = \lambda_k(s) \tau_2^s \qquad \lambda_k(s) = \prod_{\ell=1-k}^k (s-\ell) \tag{7.21}$$

The following lemma follows from the observation that the operator Δ_w annihilates an arbitrary Laurent polynomial in τ_2 of degrees $(w, 1-w)$.

Lemma 7.4. *The modular functions $\Delta_w(E_{w_1}E_{w_2})$ with $w_1 + w_2 \leq w$, and $\Delta_w \mathcal{C}_{u,v;w_1}$ for $w_1 \leq w$ are cuspidal functions.*

Lemma 7.4 is a special case of a much more general lemma which we include below.

Lemma 7.5. *An arbitrary genus-one modular graph function \mathcal{C} of weight w has a Laurent polynomial of degree $(w, 1 - w)$ and an associated cuspidal function $\Delta_w \mathcal{C}$ whose integral is given in terms of the coefficient \mathfrak{c}_1 of τ_2 in its Laurent polynomial by the following formula,*

$$\int_{\mathcal{M}} d\mu \Delta_w \mathcal{C} = (-)^w w! (w - 1)! \mathfrak{c}_1 \quad (7.22)$$

The statement that a modular graph function of weight w has a Laurent polynomial of degree $(w, 1 - w)$ was proven long ago in [6], so that we have,

$$\mathcal{C}(\tau) = \sum_{k=1-w}^w \mathfrak{c}_k \tau_2^k + \mathcal{O}(e^{-2\pi\tau_2}) \quad (7.23)$$

In view of (7.21) we have $\Delta_w \tau_2^k = 0$ for all $1 - w \leq k \leq w$. It follows that $\Delta_w \mathcal{C}$ is a cuspidal function with exponential decay at the cusp. The integral of the cuspidal function $\Delta_w \mathcal{C}$ reduces to the contribution localized at the cusp only. Expressing the integral as a limit of the integral over the cutoff domain \mathcal{M}_L defined in (7.17), we see that it reduces to a contribution from the boundary of \mathcal{M}_L ,

$$\int_{\mathcal{M}} d\mu \Delta_w \mathcal{C} = \lim_{L \rightarrow \infty} \int_{\mathcal{M}_L} d\mu \Delta_w \mathcal{C} = \lim_{L \rightarrow \infty} \int_0^1 d\tau_1 \left(\partial_{\tau_2} \Delta'_w \mathcal{C} \right) \Big|_{\tau_2=L} \quad (7.24)$$

where the operator Δ'_w is defined by,

$$\Delta'_w = \prod_{\ell=2}^w \left(\Delta - \ell(\ell - 1) \right) \quad (7.25)$$

We have $\Delta'_w \tau_2^k = 0$ for all $k \neq 0, 1$ in the range $1 - w \leq k \leq w$. For the remaining terms, $k = 0, 1$, we see that $\Delta'_w 1$ is a constant, which does not contribute to (7.24), and $\Delta'_w \tau_2 = (-)^{w-1} w! (w - 1)! \tau_2$ with the help of which (7.22) is readily established.

7.3.2 Calculation of the regularized inner product of E_s with $\mathcal{C}_{u,v;w}$

Consider a two-loop modular graph function $\mathcal{C}_{u,v;w}(\tau)$ of weight w . Its Laurent polynomial has degree $(w, 1 - w)$. We wish to evaluate the integral,

$$\mathfrak{J}_{u,v;w}(s, L) = \int_{\mathcal{M}_L} d\mu E_s(\tau) \mathcal{C}_{u,v;w}(\tau) \quad (7.26)$$

by relating it to the following integral,

$$I_{u,v;w}(s) = \int_{\mathcal{M}} d\mu E_s(\tau) \Delta_w \mathcal{C}_{u,v;w}(\tau) \quad (7.27)$$

In view of lemma 7.4, the function $\Delta_w \mathcal{C}_{u,v;w}$ is cuspidal and the integral $I_{u,v;w}(s)$ is therefore absolutely convergent for sufficiently large $\text{Re}(s)$. The integral $I_{u,v;w}(s)$ is readily evaluated

by standard Rankin-Selberg in terms of the constant Fourier mode of $\mathcal{C}_{u,v;w}$, whose Laurent polynomial part cancels out, and we are thus left with,

$$I_{u,v;w}(s) = \frac{2\zeta(2s)}{\pi^s} \sum_{N=1}^{\infty} \int_0^{\infty} d\tau_2 \tau_2^{s-2} \Delta_w \left(\mathcal{Q}_{u,v;w}^{(N)}(\tau_2) e^{-4\pi N\tau_2} \right) \quad (7.28)$$

The integral is convergent for sufficiently large $\text{Re}(s)$, and we may use the self-adjointness of Δ_w to move Δ_w onto τ_2^{s-2} to obtain the following final expression,

$$I_{u,v;w}(s) = \frac{2\zeta(2s)\lambda_w(s-2)}{\pi^s} \sum_{N=1}^{\infty} \int_0^{\infty} d\tau_2 \tau_2^{s-2} \mathcal{Q}_{u,v;w}^{(N)}(\tau_2) e^{-4\pi N\tau_2} \quad (7.29)$$

The expression for the Laurent polynomial coefficient functions $\mathcal{Q}_{u,v;w}^{(N)}(\tau_2)$ of the exponential part of the constant Fourier mode was given in (5.14) of theorem 5.3.

To work out the relation between the integrals $\mathfrak{J}_{u,v;w}(s, L)$ and $I_{u,v;w}(s)$ we start from,

$$\lambda_w(s) \mathfrak{J}_{u,v;w}(s, L) = \int_{\mathcal{M}_L} d\mu (\Delta_w E_s(\tau)) \mathcal{C}_{u,v;w}(\tau) \quad (7.30)$$

We use formula (7.20) and carry out successive integrations by parts making sure to collect all the contributions from the boundary of \mathcal{M}_L at $\tau_2 = L$, and we derive the following relation for two arbitrary modular functions f, g ,

$$\begin{aligned} & \int_{\mathcal{M}_L} d\mu (\Delta_w f) g - \int_{\mathcal{M}_L} d\mu f (\Delta_w g) \\ &= \sum_{k=0}^{w-1} (-)^k \int_0^1 d\tau_1 \left[(\bar{\nabla}^{w-k-1} \tau_2^{-2w} \nabla^w f) \bar{\nabla}^k g + (\nabla^{w-k-1} \tau_2^{-2w} \bar{\nabla}^w g) \nabla^k f \right] \Big|_{\tau_2=L} \end{aligned} \quad (7.31)$$

Substituting $f = E_s$ and $g = \mathcal{C}_{u,v;w}$, evaluating Δ_w on E_s , and partitioning the integration domain \mathcal{M} in $I_{u,v;w}$ into \mathcal{M}_L and its complement, gives the theorem below.

Theorem 7.6. *The regularized inner product integral $\mathfrak{J}_{u,v;w}(s, L)$ is given in terms of the convergent integral $I_{u,v;w}(s)$ by,*

$$\begin{aligned} \lambda_w(s) \mathfrak{J}_{u,v;w}(s, L) &= I_{u,v;w}(s) - \int_L^{\infty} \frac{d\tau_2}{\tau_2^2} \int_0^1 d\tau_1 E_s(\Delta_w \mathcal{C}_{u,v;w}) \\ &+ \sum_{k=0}^{w-1} (-)^k \int_0^1 d\tau_1 \left[(\bar{\nabla}^{w-k-1} \tau_2^{-2w} \nabla^w E_s) \bar{\nabla}^k \mathcal{C}_{u,v;w} \right. \\ &\quad \left. + (\nabla^{w-k-1} \tau_2^{-2w} \bar{\nabla}^w \mathcal{C}_{u,v;w}) \nabla^k E_s \right] \Big|_{\tau_2=L} \end{aligned} \quad (7.32)$$

Up to corrections of order $\mathcal{O}(e^{-4\pi L})$ the second term on the right side may be neglected, while in the remaining sum we may replace E_s and $\mathcal{C}_{u,v;w}$ by their respective Laurent polynomial parts thereby resulting in a finite sum of powers of L .

7.4 Summations over N

The calculation of Petersson inner products for both odd-odd or even-even arrangements of modular graph functions involves infinite-range summations, for which we shall now provide some useful formulas. We begin by recalling the well-known results given in [50],

$$\sum_{N=1}^{\infty} \frac{\sigma_a(N)}{N^s} = \zeta(s)\zeta(s-a)$$

$$\sum_{N=1}^{\infty} \frac{\sigma_a(N)\sigma_b(N)}{N^s} = \frac{\zeta(s)\zeta(s-a)\zeta(s-b)\zeta(s-a-b)}{\zeta(2s-a-b)} \quad (7.33)$$

We shall also need sums involving the generalized divisor function $V_{A,B,C}(M, N)$ defined for $A, B, C \in \mathbb{Z}$ and $M, N \in \mathbb{N}$ in (5.11). We shall assume that $A + B + C$ is even, since otherwise the sum vanishes, and we compute by manner of example the following sum which is required in the integration of the constant Fourier mode,

$$W_{A,B,C}(s) = \sum_{N=1}^{\infty} \frac{1}{N^s} V_{A,B,C}(N, N) \quad (7.34)$$

We choose $\text{Re}(s)$ large enough so that the sum is absolutely convergent. Substituting the definition of V into the summand, we obtain,

$$W_{A,B,C}(s) = \sum_{N=1}^{\infty} \frac{1}{N^s} \sum_{\substack{m,n|N \\ m,n,m+n \neq 0}} \frac{\varepsilon(m)\varepsilon(n)}{m^{A-1}n^{B-1}(m+n)^C} \quad (7.35)$$

Both positive and negative m and n contribute to the sum. Denoting by $k = \text{gcd}(m, n) > 0$ the greatest positive common divisor of m and n , we may decompose m, n as follows,

$$m = k\mu \quad n = k\nu \quad \text{gcd}(\mu, \nu) = 1 \quad \nu \neq -\mu \quad (7.36)$$

Since m and n both divide N , clearly k must divide N , and we write $N = kM$ with $M > 0$. The summations over k and M are now independent of the summations over μ and ν and may be carried out in terms of the ζ -function,

$$W_{A,B,C}(s) = \zeta(s)\zeta(s+A+B+C-2) \sum_{\substack{\text{gcd}(\mu,\nu)=1 \\ \mu,\nu,\mu+\nu \neq 0}} \frac{\varepsilon(\mu)\varepsilon(\nu)}{\mu^{A-1}\nu^{B-1}(\mu+\nu)^C} \quad (7.37)$$

Rescaling $\mu \rightarrow m = k\mu$ and $\nu \rightarrow n = k\nu$ for $k \in \mathbb{N}$ and then summing over k allows us to recover a simplified sum in m and n without divisor conditions,

$$W_{A,B,C}(s) = \frac{\zeta(s)\zeta(s+A+B+C-2)}{\zeta(A+B+C-2)} \sum_{m \neq 0} \sum_{n \neq 0, -m} \frac{\varepsilon(m)\varepsilon(n)}{m^{A-1}n^{B-1}(m+n)^C} \quad (7.38)$$

Since the summand is invariant under $(m, n) \rightarrow (-m, -n)$ we sum over $m > 0$ upon including a factor of 2. Furthermore, for fixed m , the sum over n is given by the function $S_{B-1,C}(m)$, which is defined and evaluated in equation in (C.15) of appendix C.4,

$$W_{A,B,C}(s) = \frac{2\zeta(s)\zeta(s+A+B+C-2)}{\zeta(A+B+C-2)} \sum_{m=1}^{\infty} \frac{S_{B-1,C}(m)}{m^{A-1}} \quad (7.39)$$

Evaluating the sums over m with the help of the formulas given in appendix C.4, we find,

$$\begin{aligned}
 (-)^{B-1} \sum_{m=1}^{\infty} \frac{S_{B-1,C}(m)}{m^{A-1}} &= \sum_{j=3}^{B-1} (-)^j \binom{B+C-j-2}{C-1} \zeta_{\text{sv}}(j) \zeta(A+B+C-2-j) \\
 &+ \sum_{j=3}^C \binom{B+C-j-2}{B-2} \zeta_{\text{sv}}(j) \zeta(A+B+C-2-j) \\
 &- \binom{B+C-1}{B-1} \zeta(A+B+C-2) \\
 &- 2 \sum_{j=1}^C \binom{B+C-j-2}{B-2} \zeta(A+B+C-2-j, j) \quad (7.40)
 \end{aligned}$$

Note that in the first two lines above, the second ζ -factor is an odd zeta-value since the first factor is non-zero only when j is odd, and by assumption $A+B+C-2$ is even.

7.5 Example: the inner product of E_s with $\Delta_4 C_{2,1,1}$

In this final subsection, we shall evaluate the Petersson inner product of E_s with $\Delta_4 C_{2,1,1}$,

$$f(s) = \int_{\mathcal{M}} d\mu E_s \Delta_4 C_{2,1,1} \quad (7.41)$$

Lemma 7.4 guarantees that $\Delta_4 C_{2,1,1}$ is a cuspidal function so that the above integral is absolutely convergent for sufficiently large $\text{Re}(s)$, and may be analytically continued to a meromorphic function in \mathbb{C} . We shall evaluate $f(s)$ in two different ways. First, by expressing E_s as a Poincaré series for the coset $\Gamma_{\infty} \backslash \Gamma$ and evaluating $f(s)$ in terms of an integral over the constant Fourier mode of $\Delta_4 C_{2,1,1}$. The latter is obtained from the expression for the constant Fourier mode of $C_{2,1,1}$ in subsection 5.6. Second, by using the differential equation for $C_{2,1,1}$ and Zagier's integral formula for the product of three Eisenstein series [48].

7.5.1 Calculation by Poincaré and Fourier series

With the help of the Poincaré series representation for E_s , we may express $f(s)$ in terms of an integral of the constant Fourier mode of $\Delta_4 C_{2,1,1}$,

$$f(s) = c_s \int_0^{\infty} d\tau_2 \tau_2^{s-2} \int_0^1 d\tau_1 \Delta_4 C_{2,1,1} \quad (7.42)$$

where the asymptotics of the Eisenstein series is expressed as follows,

$$E_s(\tau) = c_s \tau_2^s + \tilde{c}_s \tau_2^{1-s} + \mathcal{O}(e^{-2\pi\tau_2}), \quad c_s = \frac{2\zeta(2s)}{\pi^s}, \quad \tilde{c}_s = \frac{2\Gamma(s - \frac{1}{2})\zeta(2s-1)}{\Gamma(s)\pi^{s-\frac{1}{2}}} \quad (7.43)$$

Using the expression for the constant Fourier mode of $C_{2,1,1}$ given in (5.22) and (5.24), and the absolute convergence of the integral for sufficiently large $\text{Re}(s)$ to interchange the sum and integration, we find,

$$f(s) = -8c_s \sum_{N=1}^{\infty} \sigma_{-3}(N)^2 \int_0^{\infty} d\tau_2 \tau_2^{s-2} \Delta_4 \left(\frac{e^{-4\pi N\tau_2}}{(4\pi\tau_2)^2} \right) \quad (7.44)$$

Since the integrand falls off exponentially near the cusp, we may integrate Δ_4 by parts for sufficiently large $\text{Re}(s)$ which brings out a factor of the function $\lambda_4(s)$ defined in (7.21). Carrying out the remaining integral over τ_2 we have,

$$f(s) = -8\lambda_4(s) c_s \frac{\Gamma(s-3)}{(4\pi)^{s-1}} \sum_{N=1}^{\infty} \frac{\sigma_{-3}(N)^2}{N^{s-3}} \tag{7.45}$$

Using Ramanujan’s formula on the second line of (7.33) for $a = b = -3$ and the expression for c_s gives the following result,

$$f(s) = -32 \lambda_4(s) \frac{\Gamma(s-3)}{(2\pi)^{2s-1}} \zeta(s)^2 \zeta(s+3) \zeta(s-3) \tag{7.46}$$

We note that $f(s)$ has a simple pole at $s = 1$, whose residue gives the integral of the cuspidal function $\Delta_4 C_{2,1,1}$ by Rankin-Selberg.

The value of the residue may be obtained from (7.46) and equals $-16\pi\zeta(3)/5$, which also equals $-4!3!c_1$ where c_1 is the coefficient of the τ_2 -term in the Laurent expansion of $C_{2,1,1}$ given in (5.19). This result is in agreement with the general formula (7.22) of theorem 7.5 for the integral of such cuspidal functions for the special case of $\mathcal{C} = C_{2,1,1}$.

7.5.2 Calculation by Zagier’s integral for triple product of Eisenstein series

In the second calculation, we use the differential equation for $C_{2,1,1}$ in (5.21) and $\Delta E_4 = 12E_4$ to recast $f(s)$ as follows,

$$f(s) = - \int_{\mathcal{M}} d\mu E_s \Delta(\Delta - 6)(\Delta - 12)E_2^2 \tag{7.47}$$

We cannot integrate by parts over the domain \mathcal{M} because the Eisenstein series have polynomial growth at the cusp. Hence we shall consider the integral over a cut-off domain \mathcal{M}_L , introduced in (7.17), for arbitrary $L \gg 1$,

$$f(s) = \lim_{L \rightarrow \infty} f_L(s) \quad f_L(s) = - \int_{\mathcal{M}_L} d\mu E_s \Delta(\Delta^2 - 18\Delta + 72)E_2^2 \tag{7.48}$$

We may now evaluate this integral via theorem 7.6. In fact, the current example is simple enough that we may rederive the result of (7.32) explicitly as follows. Integrating (7.48) by parts while keeping track of the boundary contributions at $\tau_2 = L$, we find,

$$f_L(s) = \int_0^1 d\tau_1 \left[\mathfrak{F} \partial_{\tau_2} E_s - E_s \partial_{\tau_2} \mathfrak{F} \right]_{\tau_2=L} - \frac{\lambda_4(s)}{(s+1)(s-2)} \int_{\mathcal{M}_L} d\mu E_s E_2^2 \tag{7.49}$$

where \mathfrak{F} is given by,

$$\mathfrak{F} = \left((\Delta - 6)(\Delta - 12) + s(s-1)(\Delta - 18) + s^2(s-1)^2 \right) E_2^2 \tag{7.50}$$

The power-behaved terms in the combination \mathfrak{F} are τ_2^4 , τ_2 and τ_2^{-2} , while E_s has the power-behaved terms τ_2^s and τ_2^{1-s} . Thus, the power-behaved terms in the first term in (7.49) are given by a linear combination of L^{s+3} , L^s , L^{s-3} , L^{4-s} , L^{1-s} , and L^{-2-s} .

The evaluation of the integral over \mathcal{M}_L in (7.49) was given in [48], and takes the form,

$$\int_{\mathcal{M}_L} d\mu E_s E_2^2 = c_s c_2^2 \frac{L^{s+3}}{s+3} + 2 c_s c_2 \tilde{c}_2 \frac{L^s}{s} + c_s \tilde{c}_s^2 \frac{L^{s-3}}{s-3} + (s \rightarrow 1-s) \quad (7.51)$$

$$+ \frac{32 \Gamma(s-3)(s+1)(s-2)}{(2\pi)^{2s-1}} \zeta(s+3) \zeta(s-3) \zeta(s)^2 + \mathcal{O}(e^{-2\pi L})$$

where the instruction to add the contribution from $s \rightarrow 1-s$ applies only to the first line. Omitting contributions to $f_L(s)$ which are exponentially suppressed as a function of L , using the Laurent polynomials of E_2 and E_s to evaluate the power-behaved terms of \mathfrak{F} , we readily establish that the first integral in (7.49) precisely cancels all the power-behaved terms in the contribution from the integral in (7.51). The remaining term on the second line of (7.51) equals the result (7.46) computed using Poincaré and Fourier series and Rankin-Selberg.

A Proof of theorem 5.1

To evaluate the Laurent polynomial $\mathcal{L}_{u,v;w}$ and thereby prove theorem 5.1, we decompose $\mathcal{L}_{u,v;w}$ into contributions $\mathcal{L}_{u,v;w}^{(k)}$ from $\mathcal{C}_{u,v;w}^{(k)}$ for $k = 0, 1, 2, 3, 4$, so that,

$$\mathcal{L}_{u,v;w} = \sum_{k=0}^4 \mathcal{L}_{u,v;w}^{(k)} \quad (A.1)$$

To obtain $\mathcal{L}_{u,v;w}^{(k)}$, we decompose the functions φ_k and $\Phi_{a;b}$ entering $\mathcal{C}_{u,v;w}^{(k)}$ with the help of the decomposition formulas (5.1) and (5.3) and retain for $\mathcal{L}_{u,v;w}^{(k)}$ only the contributions proportional to $\hat{\varphi}_k$ and $\Phi_{a;b}^{(0)}$. Clearly we have,

$$\mathcal{L}_{u,v;w}^{(0)} = \mathcal{C}_{u,v;w}^{(0)} = \ell_w (4\pi\tau_2)^w \quad (A.2)$$

with ℓ_w given in (3.4), which produces the first term in (5.4).

A.1 Calculation of $\mathcal{L}_{u,v;w}^{(1)} + \mathcal{L}_{u,v;w}^{(2)}$

No contributions to $\mathcal{L}_{u,v;w}^{(1)} + \mathcal{L}_{u,v;w}^{(2)}$ arise from the terms involving $L_{u,v;k}$ since this function has only exponential contributions. The contribution from the function $K_{u,v;k}$ reduces to

$$K_{u,v;k} = 2\pi \binom{v+k-2}{v-1} \Phi_{u;v+k-1}^{(0)} (2|m|\tau_2) \varepsilon(m)^{u+v+k} + \mathcal{O}(e^{-2\pi\tau_2}) \quad (A.3)$$

where $\Phi_{u;v+k-1}^{(0)}$ was given in (5.3). The sum over m may be carried out in terms of even and odd ζ -values, and we obtain,

$$\mathcal{L}_{u,v;w}^{(1)} + \mathcal{L}_{u,v;w}^{(2)} = \sum_{k=1}^{w-u} \sum_{\alpha=0}^{\lfloor u/2 \rfloor} \frac{4 \binom{-}{v+\alpha} \binom{2w-u-v-k-1}{w-u-k} \binom{u+v+k-2-2\alpha}{v-1, k-1, u-2-2\alpha}}{(2\pi)^{2\alpha} (4\pi\tau_2)^{w-1-2\alpha}} \zeta(2\alpha) \zeta(2w-2\alpha-1)$$

$$+ \sum_{k=1}^{w-u} \frac{\binom{-}{v} \binom{2w-u-v-k-1}{w-u-k} \binom{v+k-2}{v-1} \binom{u+v+k-3}{u-1}}{(4\pi\tau_2)^{w-2}} \zeta(2w-2) + (u \leftrightarrow v) \quad (A.4)$$

Symmetrization ($u \leftrightarrow v$) applies to the entire expression. The sum over k in the first line may be performed using a variant of Gauss' formula, valid for $c \in \mathbb{N}$ and $a, b \in \mathbb{C}$,

$$\sum_{k=1}^{c-1} \frac{\Gamma(a-k)\Gamma(b+k)}{\Gamma(c-k)\Gamma(k)} = \frac{\Gamma(b+1)\Gamma(a+1-c)\Gamma(a+b)}{\Gamma(c-1)\Gamma(a+b+2-c)} \quad (\text{A.5})$$

and we obtain,

$$\begin{aligned} \mathcal{L}_{u,v;w}^{(1)} + \mathcal{L}_{u,v;w}^{(2)} &= 4 \sum_{\alpha=0}^{\lfloor u/2 \rfloor} \frac{(-)^{v+\alpha} \zeta(2\alpha) \zeta(2w-2\alpha-1) \binom{2w-2\alpha-2}{w-u-1} \binom{u+v-1-2\alpha}{v-1}}{(2\pi)^{2\alpha} (4\pi\tau_2)^{w-1-2\alpha}} \\ &\quad + \frac{(-)^v}{(4\pi\tau_2)^{w-2}} \zeta(2w-2) \binom{u+v-2}{u-1} \binom{2w-3}{w-u-1} + (u \leftrightarrow v) \end{aligned} \quad (\text{A.6})$$

where the addition of ($u \leftrightarrow v$) again applies to the entire preceding expression. The first term contributes to ℓ_{2k-w+1} in (5.5) while the second contributes to ℓ_{2-w} in (5.6).

A.2 Calculation of $\mathcal{L}_{u,v;w}^{(3)}$

The contribution $\mathcal{L}_{u,v;w}^{(3)}$ is given by,

$$\mathcal{L}_{u,v;w}^{(3)} = 2\pi \frac{\tau_2^w}{\pi^w} (-)^{u+v+w} \binom{u+v-2}{v-1} \sum_{m \neq 0} \Phi_{2w-u-v;u+v-1}^{(0)}(2|m|\tau_2) \quad (\text{A.7})$$

Carrying out the sum over m in terms of even and odd zeta values gives,

$$\begin{aligned} \mathcal{L}_{u,v;w}^{(3)} &= 4 \binom{u+v-2}{v-1} \sum_{\alpha=0}^{\lfloor (2w-u-v)/2 \rfloor} \frac{(-)^{w+\alpha} \zeta(2\alpha) \zeta(2w-2\alpha-1) \binom{2w-2\alpha-2}{u+v-2}}{(2\pi)^{2\alpha} (4\pi\tau_2)^{w-1-2\alpha}} \\ &\quad + (-)^w \binom{u+v-2}{v-1} \binom{2w-3}{u+v-2} \frac{\zeta(2w-2)}{(4\pi\tau_2)^{w-2}} \end{aligned} \quad (\text{A.8})$$

The first term contributes to ℓ_{2k-w+1} in (5.5) while the second contributes to ℓ_{2-w} in (5.6).

A.3 Calculation of $\mathcal{L}_{u,v;w}^{(4)}$

The contribution $\mathcal{L}_{u,v;w}^{(4)}$ arises from the fourth term in Ω of (4.28), as well as from the remaining terms with $a = b = c = 1$. Collecting these terms up to exponential contributions,

$$\begin{aligned} \Omega_{u,v;w} &= \sum_{k=u+v+1}^{w+v} \frac{(-)^v \pi^2 \binom{2w-k-1}{w+v-k} \binom{k-3}{u-1, v-1, k-u-v-1} (\varepsilon(m_1) - \varepsilon(m_2)) (\varepsilon(m_1) + \varepsilon(m_3))}{(-m_2)^{k-2} m_3^{2w-k} (2\tau_2)^{2w-2}} \\ &\quad + \sum_{k=u+v+1}^{w+u} \frac{(-)^u \pi^2 \binom{2w-k-1}{w+u-k} \binom{k-3}{u-1, v-1, k-u-v-1} (\varepsilon(m_2) - \varepsilon(m_1)) (\varepsilon(m_2) + \varepsilon(m_3))}{(-m_1)^{k-2} m_3^{2w-k} (2\tau_2)^{2w-2}} \end{aligned} \quad (\text{A.9})$$

Summing now over m_1, m_2, m_3 to obtain $\mathcal{L}_{u,v;w}^{(4)}$, we use the symmetry under the simultaneous sign reversal of m_1, m_2, m_3 to set $m_1 > 0$ upon including an overall factor of 2. In the first sum, we then need $m_3 > 0$ and set $-m_2 = m_1 + m_3$, while in the second sum m_1

and m_2 are interchanged. The sums over m_1 and m_3 in the first term and over m_2 and m_3 in the second term give the multiple zeta values defined in (5.8),

$$\mathcal{L}_{u,v;w}^{(4)} = 2(-)^v \sum_{k=u+v+1}^{w+v} \frac{\binom{2w-k-1}{w+v-k} \binom{k-3}{u-1, v-1, k-u-v-1}}{(4\pi\tau_2)^{w-2}} \zeta(k-2, 2w-k) + (u \leftrightarrow v) \quad (\text{A.10})$$

This contribution accounts for the entire multiple zeta value part of ℓ_{2-w} in (5.6).

B Proof of proposition 5.2

We start from the expression obtained for ℓ_{2-w} in theorem 5.1, and use a key result of [11] that expresses the odd-odd MZVs in terms of even-even MZVs plus a function \mathcal{T} which is a bilinear combination of odd zeta values with rational coefficients. For $N \geq 1$, we have,

$$\begin{aligned} \zeta(2M-1, 2N+1) &= -\mathcal{T}(M, N) + \zeta(2M-1)\zeta(2N+1) - \zeta(2M+2N) \\ &+ \sum_{n=0}^{N-1} \frac{E_{2n+1}(0)\Gamma(2M+2n)}{(2n+1)!\Gamma(2M-1)} \zeta(2M+2n, 2N-2n) \\ &- \sum_{n=0}^{N-1} \frac{E_{2n+1}(0)\Gamma(2M+2n)}{(2n+1)!\Gamma(2M-1)} \left(\zeta(2M+2n)\zeta(2N-2n) - \zeta(2M+2N) \right) \end{aligned} \quad (\text{B.1})$$

Here $E_n(0)$ is the Euler polynomial evaluated at zero argument. For $N \geq 1$, the function $\mathcal{T}(M, N)$ evaluates as follows,

$$\begin{aligned} \mathcal{T}(M, N) &= \sum_{\alpha=1}^{M+N-2} \zeta(2\alpha+1)\zeta(2M+2N-2\alpha-1) \sum_{n=0}^{2N-1} \frac{1}{2} E_n(0) \binom{2\alpha}{2N-n} \binom{2M+n-2}{n} \\ &- \sum_{\alpha=1}^{M+N-1} \zeta(2\alpha)\zeta(2M+2N-2\alpha) \sum_{n=0}^{2N-1} \frac{1}{2} E_n(0) \binom{2\alpha-1}{2N-n} \binom{2M+n-2}{n} \end{aligned} \quad (\text{B.2})$$

Eliminating all odd-odd MZVs from ℓ_{2-w} using MAPLE for $w \leq 18$ and the above formulas, we find that ℓ_{2-w} is given by a bilinear sum of odd zeta values, with integer coefficients λ_k ,

$$\ell_{2-w} = \sum_{k=1}^{w-3} \lambda_k \zeta(2k+1)\zeta(2w-2k-3) \quad (\text{B.3})$$

This result proceeds via the cancellation of the MZVs $\zeta(u+v+k-2, 2w-u-v-k)$ for each value of k for which $u+v+k$ is even, obtained by eliminating all odd-odd MZVs using (B.1). The cancellation takes place as if the even-even MZVs were independent variables, even though they do obey the Euler relation,

$$\zeta(s, t) + \zeta(t, s) = \zeta(s)\zeta(t) - \zeta(s+t) \quad (\text{B.4})$$

and are thus not necessarily independent. Below we shall exhibit the formulas required for the cancellation separately for $u+v$ even or odd.

For $u + v = 2z$ even, the contributions with even-even MZVs are obtained from the even k contributions in (5.5) and are given by,

$$X_{u,v;w}^e = 2(-)^v \sum_{k=1}^{\lfloor \frac{w-u}{2} \rfloor} \binom{2w-u-v-2k-1}{w-u-2k} \binom{u+v+2k-3}{u-1, v-1, 2k-1} \times \zeta(2z+2k-2, 2w-2z-2k) + (u \leftrightarrow v) \quad (\text{B.5})$$

while the contributions from eliminating odd-odd MZVs are given by,

$$X_{u,v;w}^{\mathcal{T}} = 2(-)^v \sum_{k=1}^{w-z-1} \sum_{\ell=1}^{2k-1} \theta \left(2 \left\lfloor \frac{w-u}{2} \right\rfloor - 2k + \ell + 1 \right) \zeta(2z+2k-2, 2w-2z-2k) \times \frac{\binom{2w-u-v-2k+\ell-1}{w-u-2k+\ell} \binom{u+v+2k-\ell-3}{u-1, v-1, 2k-\ell-1} \text{E}_\ell(0) \Gamma(u+v+2k-2)}{\Gamma(\ell+1) \Gamma(u+v+2k-\ell-2)} + (u \leftrightarrow v) \quad (\text{B.6})$$

Recognizing the contribution $X_{u,v;w}^e$ as being the same as the $\ell = 0$ part of $X^{\mathcal{T}}$ would be, we see that the cancellation term-by-term in k of the coefficients of the even-even MZVs is equivalent to the cancellation of the following sums,

$$X_{u,v;w}^e + X_{u,v;w}^{\mathcal{T}} = 2 \sum_{k=1}^{w-z-1} Y_{u,v;w,k} \frac{\Gamma(u+v+2k-2)}{\Gamma(u)\Gamma(v)} \zeta(2z+2k-2, 2w-2z-2k) \quad (\text{B.7})$$

with $Y_{u,v;w,k}$ given by,

$$Y_{u,v;w,k} = (-)^v \sum_{\ell=0}^{2k-1} \frac{\theta \left(2 \left\lfloor \frac{w-u}{2} \right\rfloor - 2k + \ell + 1 \right) \text{E}_\ell(0) \Gamma(2w-u-v-2k+\ell)}{\Gamma(w-u-2k+\ell+1) \Gamma(w-v) \Gamma(2k-\ell) \Gamma(\ell+1)} + (u \leftrightarrow v) \quad (\text{B.8})$$

The constraint arising from the Heaviside θ -function is automatically satisfied in view of the first Γ -function in the denominator. We have checked using MAPLE that $Y_{u,v;w,k}$ vanishes for all $w \leq 52$ with $1 \leq u \leq w-2$, $2 \leq v \leq u$, and $1 \leq k \leq w-z-1$. An analytical proof of the vanishing of $Y_{u,v;w,k}$ is an open problem, as was the case with its analogue in [11]. Hopefully, such proof may be achieved using the algorithmic techniques of [51].

It remains to analyze the case of $N = 0$, for which we have

$$\zeta(2M-1, 1) = \frac{1}{2}(2M-1)\zeta(2M) - \frac{1}{2} \sum_{n=1}^{2M-3} \zeta(n+1)\zeta(2M-1-n) \quad (\text{B.9})$$

This contains only bilinears in odd zeta values and terms which belong to $\pi^{2w-2}\mathbb{Q}$. The sum of all terms proportional to $\pi^{2w-2}\mathbb{Q}$ in ℓ_{2-w} are known to cancel by the generalization of theorem 1.2 of [11], and they were verified to vanish by MAPLE. The remaining terms are then all bilinear in odd zeta values and arise from the second term on the first line of (B.1), the first line of contributions to \mathcal{T} in (B.2), and from the term on the second line of (B.9). The coefficients λ_k are then found to be given by the formula in proposition 5.2 for $u + v$ even. A corresponding calculation establishes proposition 5.2 for $u + v$ odd.

C Calculation of exponential contributions

In this section, we shall evaluate the contributions which are exponentially suppressed near the cusp. The key formulas separating the exponential contributions in φ_k and $\Phi_{a,b}$ are given in (5.1) and (5.3). There are no exponential contributions arising from $\mathcal{C}_{u,v,w}^{(0)}$. The exponential contribution arising from $\mathcal{C}_{u,v,w}^{(i)}$ will be denoted by $\mathcal{E}_{u,v,w}^{(i)}$ for $i = 1, 2, 3, 4$.

C.1 Calculation of $\mathcal{E}_{u,v,w}^{(1)} + \mathcal{E}_{u,v,w}^{(2)}$

The exponential contributions $\mathcal{E}_{u,v,w}^{(1)} + \mathcal{E}_{u,v,w}^{(2)}$ arising from the combination $\mathcal{C}_{u,v,w}^{(1)} + \mathcal{C}_{u,v,w}^{(2)}$ given in (4.17) take the following form,

$$\mathcal{E}_{u,v,w}^{(1)} + \mathcal{E}_{u,v,w}^{(2)} = (-)^v \sum_{k=1}^{w-u} \binom{2w-u-v-k-1}{w-u-k} \left(\mathcal{E}_{u,v,w;k}^{(K)} + \bar{\mathcal{E}}_{v,u,w;k}^{(L)} \right) + (u \leftrightarrow v)^* \quad (\text{C.1})$$

The contribution $\mathcal{E}_{u,v,w;k}^{(K)}$ arises from the term involving $K_{u,v;k}$, which was evaluated in (4.14), and may be decomposed as follows,

$$\mathcal{E}_{u,v,w;k}^{(K)} = \sum_{\ell=1}^v \binom{v+k-\ell-1}{v-\ell} \left[\Xi_{u,v;k;\ell}^{(1)} + \Xi_{u,v;k;\ell}^{(2)} + \Xi_{u,v;k;\ell}^{(3)} \right] + (v \leftrightarrow k)^* \quad (\text{C.2})$$

where we have defined

$$\Xi_{u,v;k;\ell}^{(1)} = \delta_{\ell,1} \sum_{\beta=1}^{v+k-1} \frac{\binom{u+v+k-\beta-2}{u-1}}{(4\pi\tau_2)^{w-\beta-1}} \sum_{N=1}^{\infty} \frac{N^{\beta-1}}{\Gamma(\beta)} q^N \bar{q}^N \sigma_{2-2w}(N) \quad (\text{C.3})$$

$$\begin{aligned} \Xi_{u,v;k;\ell}^{(2)} &= 4 \sum_{\alpha=0}^{\lfloor \frac{u}{2} \rfloor} \frac{(-)^{\alpha} \zeta(2\alpha) \binom{u+v+k-\ell-2\alpha-1}{u-2\alpha}}{(2\pi)^{2\alpha} (4\pi\tau_2)^{w-2\alpha-\ell}} \sum_{N=1}^{\infty} \frac{N^{\ell-1}}{\Gamma(\ell)} \bar{q}^N \sigma_{1+2\alpha-2w}(N) \\ &\quad + \frac{\binom{u+v+k-\ell-2}{u-1}}{(4\pi\tau_2)^{w-\ell-1}} \sum_{N=1}^{\infty} \frac{N^{\ell-1}}{\Gamma(\ell)} \bar{q}^N \sigma_{2-2w}(N) \end{aligned}$$

$$\Xi_{u,v;k;\ell}^{(3)} = \sum_{\beta=1}^{v+k-\ell} \frac{2 \binom{u+v+k-\ell-\beta-1}{u-1}}{(4\pi\tau_2)^{w-\beta-\ell}} \sum_{N_1, N_2=1}^{\infty} \frac{N_1^{\beta-1} N_2^{\ell-1}}{\Gamma(\beta)\Gamma(\ell)} q^{N_1} \bar{q}^{N_1+N_2} \sigma_{2-2w}(\gcd(N_1, N_2))$$

The contribution $\mathcal{E}_{u,v,w;k}^{(L)}$ arises from the term involving $L_{u,v;k}$ which was evaluated in (4.16), and is given as follows,

$$\begin{aligned} (-)^k \mathcal{E}_{u,v,w;k}^{(L)} &= \sum_{j=\lfloor \frac{u+k+1}{2} \rfloor}^{\lfloor \frac{u+v+k-1}{2} \rfloor} \frac{4 (-)^{v+j} \binom{2j-u-1}{k-1} \zeta(2j)}{(4\pi\tau_2)^{w-u-v-k} (2\pi)^{2j}} \sum_{N=1}^{\infty} \frac{N^{u+v+k-2j-1} \sigma_{1+2j-2w}(N)}{\Gamma(u+v+k-2j)} \bar{q}^N \\ &\quad + (-)^{u+k} (v \leftrightarrow k) \end{aligned} \quad (\text{C.4})$$

C.2 Calculation of $\mathcal{E}_{u,v,w}^{(3)}$

The exponential contribution $\mathcal{E}_{u,v,w}^{(3)}$ arising from $\mathcal{C}_{u,v,w}^{(3)}$ given in (4.19) takes the form,

$$\mathcal{E}_{u,v,w}^{(3)} = (-)^w \sum_{k=1}^u \binom{u+v-k-1}{u-k} \left[\Pi_{u,v;k}^{(1)} + \Pi_{u,v;k}^{(2)} + \Pi_{u,v;k}^{(3)} \right] + (u \leftrightarrow v)^* \quad (\text{C.5})$$

where we have defined

$$\begin{aligned}
 \Pi_{u,v;k}^{(1)} &= \delta_{k,1} \sum_{\beta=1}^{u+v-1} \frac{\binom{2w-\beta-2}{u+v-\beta-1}}{(4\pi\tau_2)^{w-\beta-1}} \sum_{N=1}^{\infty} \frac{N^{\beta-1}}{\Gamma(\beta)} q^N \bar{q}^N \sigma_{2-2w}(N) \\
 \Pi_{u,v;k}^{(2)} &= \sum_{\alpha=0}^{\lfloor \frac{2w-u-v}{2} \rfloor} \frac{4(-)^\alpha \zeta(2\alpha) \binom{2w-2\alpha-k-1}{u+v-k-1}}{(2\pi)^{2\alpha} (4\pi\tau_2)^{w-k-2\alpha}} \sum_{N=1}^{\infty} \frac{N^{k-1}}{\Gamma(k)} q^N \sigma_{1+2\alpha-2w}(N) \\
 &\quad + \frac{\binom{2w-k-2}{2w-u-v-1}}{(4\pi\tau_2)^{w-k-1}} \sum_{N=1}^{\infty} \frac{N^{k-1}}{\Gamma(k)} q^N \sigma_{2-2w}(N) \\
 \Pi_{u,v;k}^{(3)} &= \sum_{\beta=1}^{u+v-k} \frac{2 \binom{2w-k-\beta-1}{u+v-k-\beta}}{(4\pi\tau_2)^{w-k-\beta}} \sum_{N_1, N_2=1}^{\infty} \frac{N_1^{\beta-1} N_2^{k-1}}{\Gamma(k)\Gamma(\beta)} q^{N_1+N_2} \bar{q}^{N_1} \sigma_{2-2w}(\gcd(N_1, N_2))
 \end{aligned} \tag{C.6}$$

C.3 Calculation of $\mathcal{E}_{u,v;w}^{(4)}$

Recall that $\mathcal{C}_{u,v;w}^{(4)}$ is given by,

$$\mathcal{C}_{u,v;w}^{(4)} = \sum_{m_r \neq 0} \frac{\tau_2^w}{\pi^w} \delta_{m_1+m_2+m_3,0} \Omega_{u,v;w}(m_1\tau, m_2\bar{\tau}, m_3\tau, m_3\bar{\tau}) \tag{C.7}$$

where Ω was given in (4.28). The sum over the m -variables is carried out by partitioning the contributions according to the decomposition of the φ -functions. The terms with two Kronecker δ -symbols have already been counted towards the Laurent series.

The contributions with a single Kronecker δ require the following sums,

$$\begin{aligned}
 \Sigma_1^{(2)}(B, C; a, b) &= \sum_{m_r \neq 0} \frac{(-)^B \delta_{m,0}}{2m_2^B m_3^C} \left(\delta_{a,1} \varepsilon(m_1) \varepsilon(m_2)^b \hat{\varphi}_b(\bar{q}^{|m_2|}) + \delta_{b,1} \varepsilon(m_2) \varepsilon(m_1)^a \hat{\varphi}_a(q^{|m_1|}) \right) \\
 \Sigma_1^{(3)}(B, C; b, c) &= \sum_{m_r \neq 0} \frac{(-)^B \delta_{m,0}}{2m_2^B m_3^C} \left(\delta_{b,1} \varepsilon(m_2) \varepsilon(m_3)^c \hat{\varphi}_c(q^{|m_3|}) + \delta_{c,1} \varepsilon(m_3) \varepsilon(m_2)^b \hat{\varphi}_b(\bar{q}^{|m_2|}) \right) \\
 \Sigma_1^{(4)}(B, C; c, a) &= \sum_{m_r \neq 0} \frac{(-)^B \delta_{m,0}}{2m_2^B m_3^C} \left(\delta_{c,1} \varepsilon(m_3) \varepsilon(m_1)^a \hat{\varphi}_a(q^{|m_1|}) + \delta_{a,1} \varepsilon(m_1) \varepsilon(m_3)^c \hat{\varphi}_c(q^{|m_3|}) \right)
 \end{aligned} \tag{C.8}$$

These contributions are all harmonic in q . Each function vanishes by $m_r \rightarrow -m_r$ symmetry of the summation unless the sum of all four of its arguments is even, so for example in $\Sigma_1^{(2)}(B, C; a, b)$ one must have $B + C + a + b$ even.

The contributions without Kronecker δ require the following sums,

$$\begin{aligned}
 \Sigma_0^{(2)}(B, C; a, b) &= \sum_{m_r \neq 0} \frac{\delta_{m,0}}{(-m_2)^B m_3^C} \varepsilon(m_1)^a \varepsilon(m_2)^b \hat{\varphi}_a(q^{|m_1|}) \hat{\varphi}_b(\bar{q}^{|m_2|}) \\
 \Sigma_0^{(3)}(B, C; b, c) &= \sum_{m_r \neq 0} \frac{\delta_{m,0}}{(-m_2)^B m_3^C} \varepsilon(m_2)^b \varepsilon(m_3)^c \hat{\varphi}_b(\bar{q}^{|m_2|}) \hat{\varphi}_c(q^{|m_3|}) \\
 \Sigma_0^{(4)}(B, C; c, a) &= \sum_{m_r \neq 0} \frac{\delta_{m,0}}{(-m_2)^B m_3^C} \varepsilon(m_3)^c \varepsilon(m_1)^a \hat{\varphi}_c(q^{|m_3|}) \hat{\varphi}_a(q^{|m_1|})
 \end{aligned} \tag{C.9}$$

In terms of these functions, we have,

$$\mathcal{E}_{u,v;w}^{(4)} = \sum_{k=u+v+1}^{w+v} \binom{2w-k-1}{w+v-k} \sum_{i=2,3,4} \sum_{j=0,1} (-)^v \mathcal{R}_{u,v;w,k}^{(i,j)} + (u \leftrightarrow v)^* \quad (\text{C.10})$$

where we have the following expressions for $j = 0, 1$,

$$\begin{aligned} \mathcal{R}_{u,v;w,k}^{(2,j)} &= \sum_{a=1}^u \sum_{b=1}^v \frac{(-)^b \binom{k-a-b-1}{u-a, v-b, k-u-v-1}}{(4\pi\tau_2)^{w-a-b}} \Sigma_j^{(2)}(k-a-b, 2w-k; a, b) \\ \mathcal{R}_{u,v;w,k}^{(3,j)} &= \sum_{b=1}^v \sum_{c=1}^{k-u-v} \frac{(-)^b \binom{k-b-c-1}{u-1, v-b, k-u-v-c}}{(4\pi\tau_2)^{w-b-c}} \Sigma_j^{(3)}(k-b-c, 2w-k; b, c) \\ \mathcal{R}_{u,v;w,k}^{(4,j)} &= \sum_{c=1}^{k-u-v} \sum_{a=1}^u \frac{\binom{k-c-a-1}{u-a, v-1, k-u-v-c}}{(4\pi\tau_2)^{w-c-a}} \Sigma_j^{(4)}(k-c-a, 2w-k; a, c) \end{aligned} \quad (\text{C.11})$$

C.4 Harmonic sums and single-valued zeta-values

The functions $\Sigma_1^{(i)}$ for $i = 2, 3, 4$ may be evaluated in terms of harmonic sums, sums over harmonic sums, and single-valued zeta-values, which we shall briefly discuss first. The basic harmonic sum $H_n(m)$ satisfies the following relations,

$$H_n(m) = \sum_{\ell=1}^m \frac{1}{\ell^n} \quad H_n(m) = H_n(m-1) + \frac{1}{m^n} \quad (\text{C.12})$$

as well as $H_n(0) = 0$ and $H_n(\infty) = \zeta(n)$. The double zeta-value $\zeta(k, n)$ may be expressed in terms of the following sum over harmonic sums,

$$\sum_{m=1}^{\infty} \frac{H_n(m-1)}{m^k} = \zeta(k, n) \quad (\text{C.13})$$

The single-valued ζ -values were introduced in [22], and may be defined as follows,

$$\zeta_{\text{sv}}(n) = \begin{cases} 2\zeta(n) & n \in 2\mathbb{N} + 1 \\ 0 & \text{otherwise} \end{cases} \quad (\text{C.14})$$

As we shall see below, they arise very naturally in the exponential part of $\mathcal{C}_{u,v;w}$. Though we will not need them for our current work, we note in passing that extensions of the single-valued projection to MZVs of higher depth exist as well [22].

We may apply these definitions to evaluating the ubiquitous sum defined by,

$$S_{a,b}(m) = \sum_{n \neq 0, -m} \frac{\varepsilon(n)}{n^a (m+n)^b} \quad (\text{C.15})$$

Partial fraction decomposition in n and summation over n , using the sums,

$$\begin{aligned} \sum_{n \neq 0, -m} \frac{\varepsilon(n)}{n^j} &= \zeta_{\text{sv}}(j) + \frac{(-)^j \varepsilon(m)}{m^j} \quad j \geq 2 \\ \sum_{n \neq 0, -m} \left(\frac{\varepsilon(n)}{m+n} - \frac{\varepsilon(n)}{n} \right) &= -2H_1(m-1) \end{aligned} \quad (\text{C.16})$$

gives the following result,

$$\begin{aligned}
 (-)^a S_{a,b}(m) &= \sum_{j=3}^a \frac{(-)^j \binom{a+b-j-1}{b-1} \zeta_{\text{sv}}(j)}{m^{a+b-j}} + \sum_{j=3}^b \frac{\binom{a+b-j-1}{a-1} \zeta_{\text{sv}}(j)}{m^{a+b-j}} \\
 &+ \frac{\binom{a+b}{a}}{m^{a+b}} - 2 \sum_{j=1}^b \frac{\binom{a+b-j-1}{a-1} H_j(m)}{m^{a+b-j}}
 \end{aligned} \tag{C.17}$$

C.5 Calculation of $\Sigma_1^{(i)}$ for $i = 2, 3, 4$

To compute the sum of the term proportional to $\delta_{a,1}$ in the summand of $\Sigma_1^{(2)}(B, C; a, b)$, given in (C.8), we use $m_r \rightarrow -m_r$ symmetry to choose $m = m_2 > 0$, so that the term becomes,

$$\delta_{a,1}(-)^{B+C} \sum_{m_2=1}^{\infty} \sum_{m_1 \neq 0, -m_2} \frac{\varepsilon(m_1) \hat{\varphi}_b(\bar{q}^{m_2})}{m_2^B (m_1 + m_2)^C} \tag{C.18}$$

The sum over m_1 may be carried out in terms of the function $S_{0,C}(m_2)$ defined in (C.17), and upon setting $N = pm$ and eliminating the sum over p in favor of a sum over N , we find,

$$\delta_{a,1}(-)^{B+C} \sum_{N=1}^{\infty} \frac{N^{b-1}}{\Gamma(b)} \bar{q}^N \sum_{0 < m|N} \frac{S_{0,C}(m)}{m^{B+b-1}} \tag{C.19}$$

For given N , the sum is over a finite number of values of m . For each value of m , the contribution is a sum of a rational number and a rational number times an odd zeta-value. To compute the sum of the term proportional to $\delta_{b,1}$ in the summand of $\Sigma_1^{(2)}(B, C; a, b)$, we use $m_r \rightarrow -m_r$ symmetry to choose $m = m_1 > 0$, so that this term becomes,

$$\delta_{b,1}(-)^{B+C} \sum_{m=1}^{\infty} \sum_{m_2 \neq 0, -m} \frac{\varepsilon(m_2) \hat{\varphi}_a(q^m)}{m_2^B (m + m_2)^C} \tag{C.20}$$

The sum over m_2 may be carried out in terms of $S_{B,C}(m)$ and putting all together, we find,

$$\begin{aligned}
 \Sigma_1^{(2)}(B, C; a, b) &= \delta_{a,1}(-)^{B+C} \sum_{N=1}^{\infty} \frac{N^{b-1}}{\Gamma(b)} \bar{q}^N \sum_{0 < m|N} \frac{S_{0,C}(m)}{m^{B+b-1}} \\
 &+ \delta_{b,1}(-)^{B+C} \sum_{N=1}^{\infty} \frac{N^{a-1}}{\Gamma(a)} q^N \sum_{0 < m|N} \frac{S_{B,C}(m)}{m^{a-1}}
 \end{aligned} \tag{C.21}$$

The computation of $\Sigma_1^{(3)}(B, C; b, c)$ gives,

$$\begin{aligned}
 \Sigma_1^{(3)}(B, C; b, c) &= \delta_{b,1} \sum_{N=1}^{\infty} \frac{N^{c-1}}{\Gamma(c)} q^N \left((-)^B \zeta_{\text{sv}}(B) \sigma_{1-C-c}(N) + \sigma_{1-B-C-c}(N) \right) \\
 &+ \delta_{c,1}(-)^B \sum_{N=1}^{\infty} \frac{N^{b-1}}{\Gamma(b)} \bar{q}^N \left(\zeta_{\text{sv}}(C) \sigma_{1-B-b}(N) + (-)^C \sigma_{1-B-C-b}(N) \right)
 \end{aligned} \tag{C.22}$$

while the computation of $\Sigma_1^{(4)}(B, C; c, a)$ gives,

$$\Sigma_1^{(4)}(B, C; c, a) = \sum_{N=1}^{\infty} q^N \left(\delta_{a,1} \frac{N^{c-1}}{\Gamma(c)} \sum_{0 < m|N} \frac{S_{0,B}(m)}{m^{C+c-1}} + \delta_{c,1} \frac{N^{a-1}}{\Gamma(a)} \sum_{0 < m|N} \frac{S_{C,B}(m)}{m^{a-1}} \right) \tag{C.23}$$

C.6 Calculation of $\Sigma_0^{(i)}$ for $i = 2, 3, 4$

Calculating the functions $\Sigma_0^{(i)}$ for $i = 2, 3, 4$ given in (C.9) involves the generalized divisor functions $V_{A,B,C}(M, N)$ introduced in subsection 5.3 and which we recall here for convenience,

$$V_{A,B,C}(M, N) = \sum_{\substack{m|M \\ m \neq 0}} \sum_{\substack{n|N \\ n \neq 0, -m}} \frac{\varepsilon(m)\varepsilon(n)}{m^{A-1}n^{B-1}(m+n)^C} \quad (\text{C.24})$$

Recall that $V_{A,B,C}(M, N) = 0$ for odd $A + B + C$. To account for this property in a systematic manner, we introduced the function,

$$\mathfrak{J}_n = \frac{1}{2}(1 + (-)^n) \quad (\text{C.25})$$

which vanishes for n odd and equals 1 for n even. A more explicit formula for $V_{A,B,C}(M, N)$ is given in (5.13).

C.6.1 Calculation of $\Sigma_0^{(2)}(B, C; a, b)$

To calculate $\Sigma_0^{(2)}(B, C; a, b)$, we choose independent summation variables m_1, m_2 and expand the $\hat{\varphi}$ -functions using (5.3),

$$\Sigma_0^{(2)}(B, C; a, b) = \sum_{p_1, p_2=1}^{\infty} \sum_{m_2 \neq 0} \sum_{m_1 \neq 0, -m_2} \frac{(-)^{B+C} \varepsilon(m_1)^a \varepsilon(m_2)^b p_1^{a-1} p_2^{b-1}}{m_2^B (m_1 + m_2)^C} \frac{p_1^{a-1} p_2^{b-1}}{\Gamma(a)\Gamma(b)} q^{p_1|m_1|} \bar{q}^{p_2|m_2|} \quad (\text{C.26})$$

Changing variables from (p_1, p_2) to (N_1, N_2) with $N_1 = p_1|m_1|, N_2 = p_2|m_2|$, and we find,

$$\Sigma_0^{(2)}(B, C; a, b) = (-)^{B+C} \sum_{N_1, N_2=1}^{\infty} \frac{N_1^{a-1} N_2^{b-1}}{\Gamma(a)\Gamma(b)} q^{N_1} \bar{q}^{N_2} V_{a, B+b, C}(N_1, N_2) \quad (\text{C.27})$$

C.6.2 Calculation of $\Sigma_0^{(3)}(B, C; b, c)$

Choosing independent summation variables m_2, m_3 and solving for $m_1 = -m_2 - m_3$,

$$\Sigma_0^{(3)}(B, C; b, c) = (-)^B T_{B,b}(\bar{q}) T_{C,c}(q) - 2(-)^b \sum_{m_2=1}^{\infty} \frac{\hat{\varphi}_b(\bar{q}^{m_2}) \hat{\varphi}_c(q^{m_2})}{m_2^{B+C}} \quad (\text{C.28})$$

where $T_{B,b}(q)$ is given by,

$$T_{B,b}(q) = \sum_{m_2 \neq 0} \frac{\varepsilon(m_2)^b \hat{\varphi}_b(q^{|m_2|})}{m_2^B} \quad (\text{C.29})$$

This quantity vanishes unless $B + b$ is even, in which case it may be simplified as follows,

$$T_{B,b}(q) = 2 \mathfrak{J}_{b+B} \sum_{N=1}^{\infty} \frac{N^{b-1}}{\Gamma(b)} q^N \sigma_{1-B-b}(N) \quad (\text{C.30})$$

The last sum may be evaluated by expanding $\hat{\varphi}_k$ using (5.3) and changing summation variables from p_1, p_2 to $N_1 = p_2 m_2$ and $N_2 = p_1 m_2$. Putting all together, we find,

$$\Sigma_0^{(3)}(B, C; b, c) = \sum_{N_1, N_2=1}^{\infty} \frac{N_1^{c-1} N_2^{b-1}}{\Gamma(b)\Gamma(c)} q^{N_1} \bar{q}^{N_2} \left(4(-)^B \mathfrak{J}_{b+B} \mathfrak{J}_{c+C} \sigma_{1-B-b}(N_2) \sigma_{1-C-c}(N_1) - 2(-)^b \sigma_{2-B-C-b-c}(\gcd(N_1, N_2)) \right) \quad (C.31)$$

C.6.3 Calculation of $\Sigma_0^{(4)}(B, C; c, a)$

Choosing independent variables m_1, m_3 and expanding the $\hat{\varphi}$ -functions,

$$\Sigma_0^{(4)}(B, C; c, a) = \sum_{p_1, p_2=1}^{\infty} \sum_{m_1 \neq 0} \sum_{m_3 \neq 0, -m_1} \frac{p_1^{a-1} p_2^{c-1}}{\Gamma(a)\Gamma(c)} \frac{\varepsilon(m_1)^a \varepsilon(m_3)^c}{(m_1 + m_3)^B m_3^C} q^{p_1|m_1| + p_2|m_3|} \quad (C.32)$$

Change variables from p_1, p_2 to $N_1 = p_1|m_1|$ and $N_2 = p_2|m_3|$,

$$\Sigma_0^{(4)}(B, C; c, a) = \sum_{N_1, N_2=1}^{\infty} \frac{N_1^{a-1} N_2^{c-1}}{\Gamma(a)\Gamma(c)} q^{N_1+N_2} V_{a, C+c, B}(N_1, N_2) \quad (C.33)$$

where $V_{A,B,C}$ was defined in (C.24), and takes rational values.

C.7 Calculation of $\mathcal{R}_{u,v;w,k}^{(i,1)}$ for $i = 2, 3, 4$

For $i = 2$ we use $\Sigma_1^{(2)}(B, C; a, b)$ given by (C.21) with $B = k - a - b$, $C = 2w - k$ and thus $B + C = 2w - a - b$. Substituting this result in gives,

$$\begin{aligned} \mathcal{R}_{u,v;w,k}^{(2,1)} &= - \sum_{b=1}^v \frac{\binom{k-b-2}{u-1, v-b, k-u-v-1}}{(4\pi\tau_2)^{w-b-1}} \sum_{N=1}^{\infty} \frac{N^{b-1}}{\Gamma(b)} \bar{q}^N \sum_{0 < m|N} \frac{S_{0, 2w-k}(m)}{m^{k-2}} \\ &+ \sum_{a=1}^u \frac{(-)^a \binom{k-a-2}{u-a, v-1, k-u-v-1}}{(4\pi\tau_2)^{w-a-1}} \sum_{N=1}^{\infty} \frac{N^{a-1}}{\Gamma(a)} q^N \sum_{0 < m|N} \frac{S_{k-a-1, 2w-k}(m)}{m^{a-1}} \end{aligned} \quad (C.34)$$

For $i = 3$ we use $\Sigma_1^{(3)}(B, C; b, c)$ given by (C.21) with $B = k - b - c$, $C = 2w - k$ and thus $B + C = 2w - b - c$. Substituting this result in gives,

$$\begin{aligned} \mathcal{R}_{u,v;w,k}^{(3,1)} &= \sum_{c=1}^{k-u-v} \frac{\binom{k-c-2}{u-1, v-1, k-u-v-c}}{(4\pi\tau_2)^{w-c-1}} \sum_{N=1}^{\infty} \frac{N^{c-1}}{\Gamma(c)} q^N \left(\zeta_{sv}(k-c-1) \sigma_{1-2w+k-c}(N) - \sigma_{2-2w}(N) \right) \\ &+ \sum_{b=1}^v \frac{\binom{k-b-2}{u-1, v-b, k-u-v-1}}{(4\pi\tau_2)^{w-b-1}} \sum_{N=1}^{\infty} \frac{N^{b-1}}{\Gamma(b)} \bar{q}^N \left(\zeta_{sv}(2w-k) \sigma_{2-k}(N) - \sigma_{2-2w}(N) \right) \end{aligned} \quad (C.35)$$

For $i = 4$ we use $\Sigma_1^{(4)}(B, C; c, a)$ given by (C.21) with $B = k - c - a$, $C = 2w - k$ and thus $B + C = 2w - c - a$. Substituting this result in gives,

$$\begin{aligned} \mathcal{R}_{u,v;w,k}^{(4,1)} &= \sum_{c=1}^{k-u-v} \frac{\binom{k-c-2}{u-1, v-1, k-u-v-c}}{(4\pi\tau_2)^{w-c-1}} \sum_{N=1}^{\infty} \frac{N^{c-1}}{\Gamma(c)} q^N \sum_{0 < m|N} \frac{S_{0, k-c-1}(m)}{m^{2w-k+c-1}} \\ &+ \sum_{a=1}^u \frac{\binom{k-a-2}{u-a, v-1, k-u-v-1}}{(4\pi\tau_2)^{w-a-1}} \sum_{N=1}^{\infty} \frac{N^{a-1}}{\Gamma(a)} q^N \sum_{0 < m|N} \frac{S_{2w-k, k-a-1}(m)}{m^{a-1}} \end{aligned} \quad (C.36)$$

C.8 Calculation of $\mathcal{R}_{u,v;w,k}^{(i,0)}$ for $i = 2, 3, 4$

For $i = 2$ we use $\Sigma_1^{(2)}(B, C; a, b)$ given by (C.21) with $B = k - a - b$, $C = 2w - k$ and thus $B + C = 2w - a - b$. Substituting this result in gives,

$$\mathcal{R}_{u,v;w,k}^{(2,0)} = \sum_{a=1}^u \sum_{b=1}^v \frac{(-)^a \binom{k-a-b-1}{u-a, v-b, k-u-v-1}}{(4\pi\tau_2)^{w-a-b}} \sum_{N_1, N_2=1}^{\infty} \frac{N_1^{a-1} N_2^{b-1}}{\Gamma(a)\Gamma(b)} q^{N_1} \bar{q}^{N_2} V_{a, k-a, 2w-k}(N_1, N_2) \quad (\text{C.37})$$

For $i = 3$ we use $\Sigma_1^{(3)}(B, C; b, c)$ given by (C.21) with $B = k - b - c$, $C = 2w - k$ and thus $B + C = 2w - b - c$. Substituting this result in gives,

$$\begin{aligned} \mathcal{R}_{u,v;w,k}^{(3,0)} &= \sum_{b=1}^v \sum_{c=1}^{k-u-v} \frac{\binom{k-b-c-1}{u-1, v-b, k-u-v-c}}{(4\pi\tau_2)^{w-b-c}} \sum_{N_1, N_2=1}^{\infty} \frac{N_1^{c-1} N_2^{b-1}}{\Gamma(b)\Gamma(c)} q^{N_1} \bar{q}^{N_2} \\ &\quad \times \left(4\mathfrak{J}_{k-c} \sigma_{1-k+c}(N_2) \sigma_{1-2w+k-c}(N_1) - 2\sigma_{2-2w}(\text{gcd}(N_1, N_2)) \right) \end{aligned} \quad (\text{C.38})$$

For $i = 4$ we use $\Sigma_1^{(4)}(B, C; c, a)$ given by (C.21) with $B = k - c - a$, $C = 2w - k$ and thus $B + C = 2w - c - a$. Substituting this result in gives,

$$\mathcal{R}_{u,v;w,k}^{(4,0)} = \sum_{c=1}^{k-u-v} \sum_{a=1}^u \frac{\binom{k-c-a-1}{u-a, v-1, k-u-v-c}}{(4\pi\tau_2)^{w-c-a}} \sum_{N_1, N_2=1}^{\infty} \frac{N_1^{a-1} N_2^{c-1}}{\Gamma(a)\Gamma(c)} q^{N_1+N_2} V_{a, 2w-k+c, k-c-a}(N_1, N_2) \quad (\text{C.39})$$

D Fourier coefficients of exponential contributions

In this appendix, we shall use the results of section 4 and appendix C to compute explicitly the exponential contributions to the two-loop modular graph functions $\mathcal{C}_{u,v;w}$ considered in this paper. We begin with the calculation of the exponential contributions to the constant Fourier mode in subsection D.1 and then proceed to evaluating the non-constant Fourier modes in subsections D.2 and D.3.

D.1 Calculation of $\mathcal{Q}_{u,v;w}^{(N)}(\tau_2)$

We begin by obtaining the exponential part of the constant Fourier mode $\mathcal{Q}_{u,v;w}^{(N)}(\tau_2)$. There is no contribution to $\mathcal{Q}_{u,v;w}^{(N)}(\tau_2)$ from $\mathcal{C}_{u,v;w}^{(0)}$. The contribution from $\mathcal{C}_{u,v;w}^{(1)} + \mathcal{C}_{u,v;w}^{(2)}$ is,

$$\begin{aligned} &(-)^v \sum_{k=u+v+1}^{w+v} \sum_{\beta=1}^{k-u-1} \frac{2 \binom{2w-k-1}{w+v-k} \binom{k-\beta-2}{u-1} \binom{k-u-2}{v-1}}{\Gamma(\beta) (4\pi\tau_2)^{w-\beta-1}} \sum_{N=1}^{\infty} N^{\beta-1} q^N \bar{q}^N \sigma_{2-2w}(N) \\ &+ (-)^u \sum_{k=u+v+1}^{w+u} \sum_{\beta=1}^{k-v-1} \frac{2 \binom{2w-k-1}{w+u-k} \binom{k-\beta-2}{v-1} \binom{k-v-2}{u-1}}{\Gamma(\beta) (4\pi\tau_2)^{w-\beta-1}} \sum_{N=1}^{\infty} N^{\beta-1} q^N \bar{q}^N \sigma_{2-2w}(N) \end{aligned} \quad (\text{D.1})$$

while the contribution from $\mathcal{C}_{u,v;w}^{(3)}$ is given by,

$$2(-)^w \sum_{\beta=1}^{u+v-1} \frac{\binom{2w-\beta-2}{u+v-\beta-1} \binom{u+v-2}{u-1}}{\Gamma(\beta) (4\pi\tau_2)^{w-\beta-1}} \sum_{N=1}^{\infty} N^{\beta-1} q^N \bar{q}^N \sigma_{2-2w}(N) \quad (\text{D.2})$$

The contribution from $\mathcal{C}_{u,v;w}^{(4)}$ arises only from $\mathcal{R}_{u,v;w,k}^{(i,0)}$ for $i = 2, 3$ and is given by,

$$\begin{aligned}
 & \sum_{k=u+v+1}^{w+v} \sum_{a=1}^u \sum_{b=1}^v \frac{(-)^{a+v} \binom{k-a-b-1}{u-a, v-b, k-u-v-1} \binom{2w-k-1}{w+v-k}}{(4\pi\tau_2)^{w-a-b}} \sum_{N=1}^{\infty} \frac{N^{a+b-2}}{\Gamma(a)\Gamma(b)} q^N \bar{q}^N V_{a,k-a,2w-k}(N, N) \\
 & + \sum_{k=u+v+1}^{w+v} \sum_{b=1}^v \sum_{c=1}^{k-u-v} \frac{(-)^v \binom{k-b-c-1}{u-1, v-b, k-u-v-c} \binom{2w-k-1}{w+v-k}}{(4\pi\tau_2)^{w-b-c}} \sum_{N=1}^{\infty} \frac{N^{b+c-2}}{\Gamma(b)\Gamma(c)} q^N \bar{q}^N \\
 & \quad \times \left(4\mathfrak{J}_{k-c} \sigma_{1-k+c}(N) \sigma_{1-2w+k-c}(N) - 2\sigma_{2-2w}(N) \right) \\
 & + (u \leftrightarrow v)
 \end{aligned} \tag{D.3}$$

Thus $\mathcal{Q}_{u,v;w}^{(N)}(\tau_2)$, defined in (4.1), is given by,

$$\begin{aligned}
 \mathcal{Q}_{u,v;w}^{(N)}(\tau_2) & = \sigma_{2-2w}(N) \sum_{k=1+u+v}^{w+v} \sum_{\beta=1}^{v+k-1} N^{\beta-1} \frac{2(-)^v \binom{2w-k-1}{w+v-k} \binom{k-\beta-2}{u-1} \binom{k-u-2}{v-1}}{\Gamma(\beta)(4\pi\tau_2)^{w-\beta-1}} \\
 & + \sigma_{2-2w}(N) \sum_{\beta=1}^{u+v-1} N^{\beta-1} \frac{(-)^w \binom{2w-\beta-2}{u+v-\beta-1} \binom{u+v-2}{u-1}}{\Gamma(\beta)(4\pi\tau_2)^{w-\beta-1}} \\
 & + \sum_{k=1+u+v}^{w+v} \sum_{a=1}^u \sum_{b=1}^v \frac{(-)^{a+v} \binom{k-a-b-1}{u-a, v-b, k-u-v-1} \binom{2w-k-1}{w+v-k}}{(4\pi\tau_2)^{w-a-b}} \frac{N^{a+b-2}}{\Gamma(a)\Gamma(b)} V_{a,k-a,2w-k}(N, N) \\
 & + \sum_{k=1+u+v}^{w+v} \sum_{b=1}^v \sum_{c=1}^k \frac{\binom{k-b-c-1}{u-1, v-b, k-u-v-c} \binom{2w-k-1}{w+v-k}}{(4\pi\tau_2)^{w-b-c}} \frac{N^{b+c-2}}{\Gamma(b)\Gamma(c)} \\
 & \quad \times (-)^v \left(4\mathfrak{J}_{k-c} \sigma_{1-k+c}(N) \sigma_{1-2w+k-c}(N) - 2\sigma_{2-2w}(N) \right) \\
 & + (u \leftrightarrow v)
 \end{aligned} \tag{D.4}$$

We may now simplify this as follows. In the first term of (D.4), the summations over k, β may be interchanged and, introducing the function

$$\begin{aligned}
 J_{u,v;w}^{(1)}(\beta, N) & = 2(-)^v \sigma_{2-2w}(N) \sum_{k=1}^{w+v} \binom{2w-k-1}{w+v-k} \binom{k-\beta-2}{u-1} \binom{k-u-2}{v-1} \\
 & \quad \times [\theta(\beta-v)\theta(k-\beta-u-1) + \theta(v-\beta-1)\theta(k-u-v-1)]
 \end{aligned} \tag{D.5}$$

the first line becomes,

$$\sum_{\beta=1}^{w-u+v-1} \frac{N^{\beta-1} J_{u,v;w}^{(1)}(\beta, N)}{\Gamma(\beta)(4\pi\tau_2)^{w-\beta-1}} \tag{D.6}$$

Likewise in the third term of (D.4), we may change variables from b to $\beta = a + b - 1$, and introduce the function,

$$\begin{aligned}
 J_{u,v;w}^{(2)}(\beta, N) & = \sum_{k=u+v+1}^{w+v} \sum_{a=\max(1, \beta-v+1)}^{\min(\beta, u)} \binom{k-\beta-2}{u-a, v+a-\beta-1, k-u-v-1} \\
 & \quad \times (-)^{a+v} \binom{\beta-1}{\beta-a} \binom{2w-k-1}{w+v-k} V_{a,k-a,2w-k}(N, N)
 \end{aligned} \tag{D.7}$$

The third line then becomes,

$$\sum_{\beta=1}^{u+v-1} \frac{N^{\beta-1} J_{u,v;w}^{(2)}(\beta, N)}{\Gamma(\beta)(4\pi\tau_2)^{w-\beta-1}} \quad (\text{D.8})$$

In the fourth term we change variables from b to $\beta = b + c - 1$, and introduce the function,

$$\begin{aligned} J_{u,v;w}^{(3)}(\beta, N) = & \sum_{c=\max(1, \beta-v+1)}^{\min(w-u, \beta)} \sum_{k=u+v}^{w+v-c} \binom{k+c-\beta-2}{u-1, v-\beta+c-1, k-u-v} \binom{2w-k-c-1}{w+v-k-c} \\ & \times (-)^v \binom{\beta-1}{\beta-c} \left(4\mathfrak{J}_k \sigma_{1-k}(N) \sigma_{1-2w+k}(N) - 2\sigma_{2-2w}(N) \right) \end{aligned} \quad (\text{D.9})$$

The fourth term then becomes,

$$\sum_{\beta=1}^{w-u+v-1} \frac{N^{\beta-1} J_{u,v;w}^{(3)}(\beta, N)}{\Gamma(\beta)(4\pi\tau_2)^{w-\beta-1}} \quad (\text{D.10})$$

Assembling all the pieces gives the result quoted in (5.14).

D.2 Calculation of $G_{u,v;w}^{(N,L)}(\tau_2)$

We now obtain the coefficients $G_{u,v;w}^{(N,L)}(\tau_2)$ in the Fourier expansion, defined in (4.2). There are no contributions from $\mathcal{C}_{u,v;w}^{(0)}$. The contribution from $\mathcal{C}_{u,v;w}^{(1)} + \mathcal{C}_{u,v;w}^{(2)}$ is given by,

$$\begin{aligned} 2\sigma_{2-2w}(\gcd(L, N)) \left[(-)^v \sum_{k=1}^{w-u} \sum_{\ell=1}^k \sum_{\beta=1}^{v+k-\ell} \frac{\binom{2w-u-v-k-1}{w-u-k} \binom{v+k-\ell-1}{k-\ell} \binom{u+v+k-\ell-\beta-1}{u-1}}{\Gamma(\ell)\Gamma(\beta)(4\pi\tau_2)^{w-\beta-\ell}} L^{\beta-1} N^{\ell-1} \right. \\ \left. + (-)^u \sum_{k=1}^{w-v} \sum_{\ell=1}^u \sum_{\beta=1}^{u+k-\ell} \frac{\binom{2w-u-v-k-1}{w-v-k} \binom{u+k-\ell-1}{u-\ell} \binom{u+v+k-\ell-\beta-1}{v-1}}{\Gamma(\ell)\Gamma(\beta)(4\pi\tau_2)^{w-\beta-\ell}} L^{\beta-1} N^{\ell-1} \right] \end{aligned} \quad (\text{D.11})$$

The contribution from $\mathcal{C}_{u,v;w}^{(3)}$ is given by,

$$2\sigma_{2-2w}(\gcd(L, N)) (-)^w \sum_{k=1}^u \sum_{\beta=1}^{u+v-k} \frac{\binom{u+v-k-1}{u-k} \binom{2w-k-\beta-1}{u+v-k-\beta}}{\Gamma(k)\Gamma(\beta)(4\pi\tau_2)^{w-k-\beta}} L^{\beta-1} N^{k-1} \quad (\text{D.12})$$

The contributions from $\mathcal{C}_{u,v;w}^{(4)}$ arise from $\mathcal{R}_{u,v;w,k}^{(i,0)}$ for $i = 2, 3$ and are given respectively by,

$$\begin{aligned} \sum_{k=1+u+v}^{w+v} \sum_{a=1}^u \sum_{b=1}^v \frac{(-)^{a+v} \binom{2w-k-1}{w+v-k} \binom{k-a-b-1}{u-a, v-b, k-u-v-1}}{\Gamma(a)\Gamma(b)(4\pi\tau_2)^{w-a-b}} (L+N)^{a-1} L^{b-1} V_{a,k-a,2w-k}(L+N, L) \\ + \sum_{k=1+u+v}^{w+u} \sum_{a=1}^u \sum_{b=1}^v \frac{(-)^{b+u} \binom{2w-k-1}{w+u-k} \binom{k-a-b-1}{u-a, v-b, k-u-v-1}}{\Gamma(a)\Gamma(b)(4\pi\tau_2)^{w-a-b}} (L+N)^{a-1} L^{b-1} V_{b,k-b,2w-k}(L, L+N) \end{aligned} \quad (\text{D.13})$$

and

$$\begin{aligned}
 & \sum_{k=1+u+v}^{w+v} \sum_{b=1}^v \sum_{c=1}^{k-u-v} \frac{\binom{2w-k-1}{w+v-k} \binom{k-b-c-1}{u-1, v-b, k-u-v-c}}{\Gamma(b)\Gamma(c)(4\pi\tau_2)^{w-b-c}} (L+N)^{c-1} L^{b-1} \\
 & \quad \times (-)^v [4\mathfrak{J}_{k-c} \sigma_{1-k+c}(L) \sigma_{1-2w+k-c}(L+N) - 2\sigma_{2-2w}(\gcd(L, L+N))] \\
 & + \sum_{k=1+u+v}^{w+u} \sum_{b=1}^u \sum_{c=1}^{k-u-v} \frac{\binom{2w-k-1}{w+u-k} \binom{k-b-c-1}{v-1, u-b, k-u-v-c}}{\Gamma(b)\Gamma(c)(4\pi\tau_2)^{w-b-c}} (L+N)^{b-1} L^{c-1} \\
 & \quad \times (-)^u [4\mathfrak{J}_{k-c} \sigma_{1-k+c}(L+N) \sigma_{1-2w+k-c}(L) - 2\sigma_{2-2w}(\gcd(L, L+N))] \quad (D.14)
 \end{aligned}$$

The total result can be written in an abridged form as follows,

$$G_{u,v;w}^{(N,L)}(\tau_2) = \sum_{k=k_-}^{k_+} \sum_{\ell=1}^{\ell_+} \sum_{\beta=1}^{\beta_+} \frac{\mathcal{W}_{u,v;w}^{k,\ell,\beta}(N,L)}{(4\pi\tau_2)^{w-\beta-\ell}} \quad (D.15)$$

where

$$\begin{aligned}
 k_- &= 1 + u + v \\
 k_+ &= \max(w + u, w + v) \\
 \ell_+ &= \max(w - u, u) \\
 \beta_+ &= \max(w + |u - v| - 1, u + v - 1) \quad (D.16)
 \end{aligned}$$

To express the coefficients $\mathcal{W}_{u,v;w}^{k,\ell,\beta}(N,L)$ in a form as simple as possible, we shall adopt the convention whereby binomial and trinomial coefficients vanish if any one of their lower entries is a negative integer,

$$\binom{A}{B_1, \dots, B_r} = 0 \quad \text{if} \quad -B_i \in \mathbb{N} \quad (D.17)$$

for any $i = 1, \dots, r$, or if $-A \in \mathbb{N}$. For all integer arguments/indices, the coefficients $\mathcal{W}_{u,v;w}^{k,\ell,\beta}(N,L)$ are rational numbers. They are given by the following lengthy expression,

$$\begin{aligned}
 & \mathcal{W}_{u,v;w}^{k,\ell,\beta}(N,L) = 2L^{\beta-1} N^{\ell-1} \sigma_{2-2w}(\gcd(L, N)) \\
 & \quad \times \left[(-)^v \frac{\binom{2w-k-1}{w+v-k} \binom{k-u-\ell-1}{k-u-v-\ell} \binom{k-\ell-\beta-1}{k-\ell-\beta-u}}{\Gamma(\ell)\Gamma(\beta)} + (-)^u \frac{\binom{2w-k-1}{w+u-k} \binom{k-v-\ell-1}{u-\ell} \binom{k-\ell-\beta-1}{k-\ell-\beta-v}}{\Gamma(\ell)\Gamma(\beta)} \right. \\
 & \quad \left. + (-)^w \delta_{k-u-v,1} \frac{\binom{u+v-\ell-1}{u-\ell} \binom{2w-\ell-\beta-1}{u+v-\ell-\beta}}{\Gamma(\ell)\Gamma(\beta)} \right] \\
 & + L^{\beta-1} (L+N)^{\ell-1} \left[\frac{(-)^{\ell+v} \binom{2w-k-1}{w+v-k} \binom{k-\ell-\beta-1}{u-\ell, v-\beta, k-u-v-1}}{\Gamma(\ell)\Gamma(\beta)} V_{\ell, k-\ell, 2w-k}(L+N, L) \right. \\
 & \quad \left. + \frac{(-)^{\beta+u} \binom{2w-k-1}{w+u-k} \binom{k-\ell-\beta-1}{u-\ell, v-\beta, k-u-v-1}}{\Gamma(\ell)\Gamma(\beta)} V_{\beta, k-\beta, 2w-k}(L, L+N) \right] \\
 & + L^{\beta-1} (L+N)^{\ell-1} \left[\frac{\binom{2w-k-1}{w+v-k} \binom{k-\ell-\beta-1}{u-1, v-\beta, k-u-v-\ell}}{\Gamma(\ell)\Gamma(\beta)} \mathcal{V}_{u,v;w}^{k,\ell}(L, L+N) \right. \\
 & \quad \left. + \frac{\binom{2w-k-1}{w+u-k} \binom{k-\ell-\beta-1}{v-1, u-\ell, k-u-v-\beta}}{\Gamma(\ell)\Gamma(\beta)} \mathcal{V}_{v,u;w}^{k,\beta}(L+N, L) \right] \quad (D.18)
 \end{aligned}$$

where we have defined

$$(-)^v \mathcal{V}_{u,v;w}^{k,\ell}(L, M) = 4 \mathfrak{J}_{k-\ell} \sigma_{1-k+\ell}(L) \sigma_{1-2w+k-\ell}(M) - 2 \sigma_{2-2w}(\gcd(L, M)) \quad (\text{D.19})$$

This gives the result cited in the first line of theorem 5.4.

D.3 Calculation of $F_{u,v;w}^{(N)}(\tau_2)$

We now calculate the coefficients $F_{u,v;w}^{(N)}(\tau_2)$ in the Fourier expansion, defined in (4.2). There are no contributions from $\mathcal{C}_{u,v;w}^{(0)}$. The contribution from $\mathcal{C}_{u,v;w}^{(1)} + \mathcal{C}_{u,v;w}^{(2)}$ is given by,

$$\begin{aligned} F_{u,v;w}^{(N)(12)}(\tau_2) = & (-)^v \sum_{k=1}^{w-u} \sum_{\ell=1}^k \frac{(2w-u-v-k-1)(v+k-\ell-1)}{w-u-k} \frac{\Gamma(k-\ell)}{\Gamma(\ell)} N^{\ell-1} \left[4 \sum_{\alpha=0}^{\lfloor \frac{u}{2} \rfloor} \frac{(-)^\alpha \zeta(2\alpha) \binom{u+v+k-\ell-2\alpha-1}{u-2\alpha}}{(2\pi)^{2\alpha} (4\pi\tau_2)^{w-2\alpha-\ell}} \sigma_{1+2\alpha-2w}(N) \right. \\ & \left. + \frac{\binom{u+v+k-\ell-2}{u-1}}{(4\pi\tau_2)^{w-\ell-1}} \sigma_{2-2w}(N) \right] \\ & + (-)^u \sum_{k=1}^{w-v} \sum_{\ell=1}^u \frac{(2w-u-v-k-1)(u+k-\ell-1)}{w-v-k} \frac{\Gamma(u-\ell)}{\Gamma(\ell)} N^{\ell-1} \left[4 \sum_{\alpha=0}^{\lfloor \frac{u}{2} \rfloor} \frac{(-)^\alpha \zeta(2\alpha) \binom{u+v+k-\ell-2\alpha-1}{v-2\alpha}}{(2\pi)^{2\alpha} (4\pi\tau_2)^{w-2\alpha-\ell}} \sigma_{1+2\alpha-2w}(N) \right. \\ & \left. + \frac{\binom{u+v+k-\ell-2}{v-1}}{(4\pi\tau_2)^{w-\ell-1}} \sigma_{2-2w}(N) \right] \\ & + 4 \sum_{\ell=1}^{w-u} \frac{(-)^{v+u}}{(4\pi\tau_2)^{w-u-v-\ell}} \left[\sum_{j=\lfloor \frac{1+v+\ell}{2} \rfloor}^{\lfloor \frac{u+v+\ell-1}{2} \rfloor} \frac{(-)^{j+\ell} \binom{2w-u-v-\ell-1}{w-u-\ell} \binom{2j-v-1}{\ell-1} \zeta(2j)}{\Gamma(u+v+\ell-2j)} \frac{\zeta(2j)}{(2\pi)^{2j}} N^{u+v+\ell-2j-1} \sigma_{1+2j-2w}(N) \right. \\ & \left. + (-)^v (u \leftrightarrow \ell) \right] \quad (\text{D.20}) \end{aligned}$$

Note that $(u \leftrightarrow \ell)$ applies only to the portion in brackets on the penultimate line.

The contribution from $\mathcal{C}_{u,v;w}^{(3)}$ is

$$F_{u,v;w}^{(N)(3)}(\tau_2) = (-)^w \sum_{\ell=1}^u \frac{\binom{u+v-\ell-1}{u-\ell}}{\Gamma(\ell)} N^{\ell-1} \left[\sum_{\alpha=0}^{\lfloor \frac{2w-u-v}{2} \rfloor} \frac{4(-)^\alpha \zeta(2\alpha) \binom{2w-2\alpha-\ell-1}{u+v-\ell-1}}{(2\pi)^{2\alpha} (4\pi\tau_2)^{w-\ell-2\alpha}} \sigma_{1+2\alpha-2w}(N) + \frac{\binom{2w-\ell-2}{2w-u-v-1}}{(4\pi\tau_2)^{w-\ell-1}} \sigma_{2-2w}(N) \right] \quad (\text{D.21})$$

The contributions from $\mathcal{C}_{u,v;w}^{(4)}$ come from $\mathcal{R}_{u,v;w,k}^{(i,1)}$ for $i = 2, 3, 4$, as well as from $\mathcal{R}_{u,v;w,k}^{(4,0)}$. They can be written collectively as

$$F_{u,v;w}^{(N)(4)}(\tau_2) = \sum_{k=k_-}^{k_+} \sum_{\ell=1}^{\ell_+} \frac{M_{u,v;w}^{k,\ell}(N)}{(4\pi\tau_2)^{w-\ell-1}} + \sum_{k=k_-}^{w+v} \sum_{\ell=1}^{k-u-v} \sum_{\beta=1}^u \frac{H_{u,v;w}^{k,\ell,\beta}(N)}{(4\pi\tau_2)^{w-\ell-\beta}} \quad (\text{D.22})$$

where k_- , k_+ , and ℓ_+ are as defined in (D.16) and

$$\begin{aligned}
 M_{u,v;w}^{k,\ell}(N) &= \frac{(-)^v \binom{2w-k-1}{w+v-k} \binom{k-\ell-2}{u-1,v-1,k-u-v-\ell}}{\Gamma(\ell)} N^{\ell-1} \mu_{u,v;w}^{(1)k,\ell}(N) \\
 &+ \frac{(-)^v \binom{2w-k-1}{w+v-k} \binom{k-\ell-2}{u-\ell,v-1,k-u-v-1}}{\Gamma(\ell)} N^{\ell-1} \mu_{u,v;w}^{(2)k,\ell}(N) \\
 &+ \frac{(-)^u \binom{2w-k-1}{w+u-k} \binom{k-\ell-2}{u-\ell,v-1,k-u-v-1}}{\Gamma(\ell)} N^{\ell-1} \mu_{u,v;w}^{(3)k,\ell}(N) \quad (\text{D.23})
 \end{aligned}$$

Note that we are utilizing the convention put forth in (D.17). The $\mu_{u,v;w}^{(i)k,\ell}(N)$ for $i = 1, 2, 3$ are defined by,

$$\begin{aligned}
 \mu_{u,v;w}^{(1)k,\ell}(N) &= \zeta_{sv}(k-\ell-1) \sigma_{1-2w+k-\ell}(N) - \sigma_{2-2w}(N) + \sum_{0 < m|N} \frac{S_{0,k-\ell-1}(m)}{m^{2w-k+\ell-1}} \\
 \mu_{u,v;w}^{(2)k,\ell}(N) &= \sum_{0 < m|N} \frac{S_{2w-k,k-\ell-1}(m)}{m^{\ell-1}} + (-)^\ell \sum_{0 < m|N} \frac{S_{k-\ell-1,2w-k}(m)}{m^{\ell-1}} \\
 \mu_{u,v;w}^{(3)k,\ell}(N) &= \zeta_{sv}(2w-k) \sigma_{2-k}(N) - \sigma_{2-2w}(N) - \sum_{0 < m|N} \frac{S_{0,2w-k}(m)}{m^{k-2}} \quad (\text{D.24})
 \end{aligned}$$

We have also defined

$$\begin{aligned}
 H_{u,v;w}^{k,\ell,\beta}(N) &= \theta(N-2) \frac{(-)^v \binom{2w-k-1}{w+v-k} \binom{k-\ell-\beta-1}{u-\beta,v-1,k-u-v-\ell}}{\Gamma(\ell)\Gamma(\beta)} \\
 &\times \sum_{N_1=1}^{N-1} N_1^{\beta-1} (N-N_1)^{\ell-1} V_{\beta,2w-k+\ell,k-\ell-\beta}(N_1, N-N_1) \quad (\text{D.25})
 \end{aligned}$$

where again we are using the convention of (D.17).

The coefficients $M_{u,v;w}^{k,\ell}(N)$ evaluated on integer-valued indices and arguments are linear combinations of rational numbers and rational multiples of odd zeta values. Odd zeta values naively appear in all $\mu_{u,v;w}^{(i)k,\ell}(N)$ for $i = 1, 2, 3$. However, there are actually no odd zeta values arising from $\mu_{u,v;w}^{(3)k,\ell}(N)$, since the factor of $\zeta_{sv}(2w-k)$ appearing in (D.24) cancels against the zeta value arising from the definition of $S_{0,2w-k}(m)$, see (C.17). Hence we obtain contributions from only the first two lines of (D.24), which are given by

$$\begin{aligned}
 \mathcal{M}_{u,v;w}^{k,\ell}(N) &= \frac{2(-)^v \binom{2w-k-1}{w+v-k} \Gamma(k-\ell-1)}{\Gamma(v)\Gamma(\ell)\Gamma(k-v-\ell)} N^{\ell-1} \quad (\text{D.26}) \\
 &\times \left[\binom{k-v-\ell-1}{k-u-v-\ell} \sigma_{1-2w+k-\ell}(N) \zeta_{sv}(k-\ell-1) \right. \\
 &\quad \left. + (-)^k \binom{k-v-\ell-1}{u-\ell} \left\{ \sum_{j=3}^{k-\ell-1} \binom{2w-\ell-j-2}{2w-k-1} \zeta_{sv}(j) \sigma_{2+j-2w}(N) \right. \right. \\
 &\quad \quad \left. \left. - \sum_{j=3}^{2w-k} \binom{2w-\ell-j-2}{k-\ell-2} \zeta_{sv}(j) \sigma_{2+j-2w}(N) \right\} \right]
 \end{aligned}$$

Once again, we are working with the convention of (D.17).

Finally, we find,

$$F_{u,v;w}^{(N)}(\tau_2) = \sum_{k=k_-}^{k_+} \sum_{\ell=1}^{\ell_+} \left[\frac{\mathcal{M}_{u,v;w}^{k,\ell}(N)}{(4\pi\tau_2)^{w-\ell-1}} + \sum_{\gamma=0}^{\gamma_+} \frac{\mathcal{H}_{u,v;w}^{k,\ell,\beta}(N)}{(4\pi\tau_2)^{w-\ell-\gamma}} \right] \quad (\text{D.27})$$

where

$$\gamma_+ = \max(u + v, 2w - u - v - \epsilon) \quad (\text{D.28})$$

$\epsilon = u + v \pmod{2}$ and the function $\mathcal{H}_{u,v;w}^{k,\ell,\gamma}(N)$ is obtained by combining $H_{u,v;w}^{k,\ell,\beta}(N)$ with the rational portions of $M_{u,v;w}^{k,\ell}(N)$, i.e. $M_{u,v;w}^{k,\ell}(N) - \mathcal{M}_{u,v;w}^{k,\ell}(N)$, as well as with the contributions from (D.20) and (D.21), such that

$$\begin{aligned} \sum_{k=k_-}^{k_+} \sum_{\ell=1}^{\ell_+} \sum_{\gamma=0}^{\gamma_+} \frac{\mathcal{H}_{u,v;w}^{k,\ell,\beta}(N)}{(4\pi\tau_2)^{w-\ell-\gamma}} &= F_{u,v;w}^{(N)(12)}(\tau_2) + F_{u,v;w}^{(N)(3)}(\tau_2) \\ &+ \sum_{k=k_-}^{w+v} \sum_{\ell=1}^{k-u-v} \sum_{\beta=1}^u \frac{H_{u,v;w}^{k,\ell,\beta}(N)}{(4\pi\tau_2)^{w-\ell-\beta}} + \sum_{k=k_-}^{k_+} \sum_{\ell=1}^{\ell_+} \frac{M_{u,v;w}^{k,\ell}(N) - \mathcal{M}_{u,v;w}^{k,\ell}(N)}{(4\pi\tau_2)^{w-\ell-1}} \end{aligned} \quad (\text{D.29})$$

For all integer-valued indices and arguments $\mathcal{H}_{u,v;w}^{k,\ell,\beta}(N)$ is a rational number.

E Proof of theorem 6.3

In this appendix we prove theorem 6.3. To do so we proceed in two parts. We first prove the linear independence of the spaces $\mathfrak{A}_w^{(1)}$ and $\mathfrak{A}_w^{(2)}$, and then move on to the more complicated case of $\mathfrak{A}_w^{(3)}$. Both parts are proven by means of holomorphic subgraph reduction and the sieve algorithm.

E.1 Independence of $\mathfrak{A}_w^{(1)}$ and $\mathfrak{A}_w^{(2)}$

As reviewed in section 6.3, the sieve algorithm involves determining the order in ∇ at which the first holomorphic Eisenstein series appears. It is easy to see that for $\mathcal{P}_k(w_1, w_2) \in \mathfrak{A}_w^{(1)}$, the first holomorphic Eisenstein series appears at order ∇^{w_2-k} , so that $\mathcal{P}_k(w_1, w_2) \in \mathcal{V}_{(w,w)}^{(w_2-k)}$.

On the other hand, elements of $\mathfrak{A}_w^{(2)}$ have $u + 1 < w - u - 1$, and hence the lowest entry in the exponent matrix of $\mathcal{A}_{u,u+1;w} \in \mathfrak{A}_w^{(2)}$ is u . As a result, we have,

$$\mathcal{A}_{u,u+1;w} \in \mathcal{V}_{(w,w)}^{(u)} \quad \text{for all} \quad \mathcal{A}_{u,u+1;w} \in \mathfrak{A}_w^{(2)} \quad (\text{E.1})$$

That is, upon application of the Cauchy-Riemann operator to elements of $\mathfrak{A}_w^{(2)}$, the first possible appearance of a holomorphic Eisenstein series is at order ∇^u . The holomorphic Eisenstein series in question appears through algebraic reduction identities (2.27), and one finds by explicit computation that,

$$\nabla^u \mathcal{A}_{u,u+1;w} = -(-1)^u \frac{\Gamma(2u+1)}{\Gamma(u+1)} \mathcal{G}_{2u+1} \mathcal{C}^+ \begin{bmatrix} w-u-1 & 0 \\ w-u & 0 \end{bmatrix} + \dots \quad (\text{E.2})$$

where the ellipsis represents elements of $\mathcal{V}_{(w+u,w-u)}$. However, since $2u + 1$ is odd, this holomorphic Eisenstein series vanishes. So we in fact have the stricter statement that,

$$\mathcal{A}_{u,u+1;w} \in \mathcal{V}_{(w,w)}^{(u+1)} \subset \mathcal{V}_{(w,w)}^{(u)} \quad \text{for all} \quad \mathcal{A}_{u,u+1;w} \in \mathfrak{A}_w^{(2)} \quad (\text{E.3})$$

This means that we may proceed to ∇^{u+1} , where one obtains the following holomorphic Eisenstein series via algebraic reduction,

$$\nabla^{u+1} \mathcal{A}_{u,u+1;w} = (-1)^u \frac{\Gamma(2u+2)}{\Gamma(u)} \mathcal{G}_{2(u+1)} E_{w-u-1} + \dots \quad (\text{E.4})$$

The ellipsis represents elements of $\mathcal{V}_{(w+u+1,w-u-1)}$. We are now in a position to prove the first part of the theorem. We begin by assuming a linear relation of the form

$$\sum_{w_2=2}^{\lfloor \frac{w-1}{2} \rfloor} \sum_{k=1}^{w_2-1} \alpha(w_2, k) \mathcal{P}_k(w-w_2, w_2) + \sum_{u=1}^{\lfloor \frac{w-3}{2} \rfloor} \beta(u) \mathcal{A}_{u,u+1;w} = 0 \quad (\text{E.5})$$

and then apply ∇ to it. Since $\mathfrak{A}_w \subset \mathcal{V}_{(w,w)}$, we have

$$\nabla : \mathfrak{A}_w \rightarrow \mathcal{V}_{(w+1,w-1)} \oplus \mathfrak{C}_{(w+1,w-1)} \quad (\text{E.6})$$

Applying ∇ to (E.5) produces only elements of $\mathcal{V}_{(w+1,w-1)}$, except for when it acts on $\mathcal{P}_{w_2-1}(w-w_2, w_2)$, in which case it produces

$$\sum_{w_2=2}^{\lfloor \frac{w-1}{2} \rfloor} \alpha(w_2, w_2-1) \tau_2^{2-2w_2} \nabla^{w_2} E_{w_2} \bar{\nabla}^{w_2-1} E_{w-w_2} \in \mathfrak{C}_{(w+1,w-1)} \quad (\text{E.7})$$

By the sieve algorithm, all terms not in $\mathcal{V}_{(w+1,w-1)}$ must cancel, so (E.5) requires the above to vanish. The form $\nabla^{w_2} E_{w_2}$ is proportional to G_{2w_2} by (2.22) so that all the terms for different values of w_2 must be linearly independent of one another, and we must have $\alpha(w_2, w_2-1) = 0$ for all $2 \leq w_2 \leq \lfloor \frac{w-1}{2} \rfloor$. Given these cancellations, the range of the sum over k in (E.5) now effectively has upper limit w_2-2 . By construction, for these values of k and w_2 , the image of ∇ on each term in (E.5) belongs to $\mathcal{V}_{(w+1,w-1)}$, and we may now proceed to ∇^2 ,

$$\nabla^2 : \mathfrak{A}_w \rightarrow \mathcal{V}_{(w+2,w-2)} \oplus \mathfrak{C}_{(w+2,w-2)} \quad (\text{E.8})$$

In addition to the contributions coming from $\mathcal{P}_{w_2-2}(w-w_2, w_2)$, there will now be a contribution towards $\mathfrak{C}_{(w+2,w-2)}$ coming from an element of $\mathfrak{A}_w^{(2)}$ as well. In particular, the image of ∇^2 on each term of the abridged (E.5) is in $\mathcal{V}_{(w+2,w-2)}$, except for the images of $\mathcal{P}_{w_2-2}(w-w_2, w_2)$ and $\mathcal{A}_{1,2;w}$, which have,

$$\sum_{w_2=3}^{\lfloor \frac{w-1}{2} \rfloor} \alpha(w_2, w_2-2) \mathcal{G}_{2w_2} \bar{\nabla}^{w_2-2} E_{w-w_2} + \beta(1) \mathcal{G}_4 E_{w-2} \in \mathfrak{C}_{(w+2,w-2)} \quad (\text{E.9})$$

For simplicity, we have absorbed unimportant factors of Gamma functions and τ_2 into $\alpha(w_2, w_2-2)$ and $\beta(1)$. For this expression to vanish, we require $\alpha(w_2, w_2-2) = \beta(1) = 0$. Having eliminated the elements of $\mathfrak{C}_{(w+2,w-2)}$, one may then move on to order ∇^3 . Iterating this argument, one inductively shows that all coefficients must vanish, and thus that all elements of $\mathfrak{A}_w^{(1)}$ and $\mathfrak{A}_w^{(2)}$ are independent.

E.2 Independence of $\mathfrak{A}_w^{(1)}$, $\mathfrak{A}_w^{(2)}$, and $\mathfrak{A}_w^{(3)}$

We shall now prove the linear independence of $\mathfrak{A}_w^{(3)}$ analogously to the case of $\mathfrak{A}_w^{(2)}$. The additional complication is that the holomorphic Eisenstein series which arise do so via holomorphic subgraph reduction in addition to algebraic reduction. In particular, note that for any $\mathcal{A}_{u,u+1;w} \in \mathfrak{A}_w^{(3)}$, by definition $w - u - 1 \leq u + 1$. Restricting temporarily to the case $u \neq \lfloor \frac{w-1}{2} \rfloor$, it follows that $w - u - 1$ is the lowest element in the exponent matrix, and hence,

$$\mathcal{A}_{u,u+1;w} \in \mathcal{V}_{(w,w)}^{(w-u-1)} \quad \text{for all} \quad \mathcal{A}_{u,u+1;w} \in \mathfrak{A}_w^{(3)} \quad (\text{E.10})$$

or equivalently

$$\nabla^{w-u-1} \mathcal{A}_{u,u+1;w} \in \mathcal{V}_{(2w-u-1,u+1)} \oplus \mathfrak{C}_{(2w-u-1,u+1)} \quad (\text{E.11})$$

The elements of $\mathfrak{C}_{(2w-u-1,u+1)}$ arise via holomorphic subgraph reduction, and are computed in closed form in lemma F.1 of appendix F, which yields

$$\nabla^{w-u-1} \mathcal{A}_{u,u+1;w} = \sum_{\ell=w-u}^{w-1} H_1(\ell) \mathcal{G}_\ell \mathcal{C}_\ell^+ + \sum_{\ell=w-u}^{2(w-u)-1} H_2(\ell) \mathcal{G}_\ell \mathcal{C}_\ell^+ + \dots \quad (\text{E.12})$$

when $v = u + 1$. \mathcal{C}_ℓ^+ is defined by,

$$\mathcal{C}_\ell^+ = \mathcal{C}^+ \begin{bmatrix} 2w - u - \ell - 1 & 0 \\ u + 1 & 0 \end{bmatrix} \quad (\text{E.13})$$

The ellipsis in (E.12) represent elements of $\mathcal{V}_{(2w-u-1,u+1)}$, while the functions $H_1(\ell)$, $H_2(\ell)$, and \mathcal{C}_ℓ^+ are obtained from (F.12) and (F.3) by setting $v = u + 1$,

$$\begin{aligned} H_1(\ell) &= \frac{(-)^w}{\Gamma(w-u)} \prod_{j=1}^{w-u-1} (\ell - j) \prod_{k=1}^{w-u-1} (w + k - \ell - 1) \\ H_2(\ell) &= \frac{(-)^{u+1}}{\Gamma(u)} \prod_{j=1}^{w-u-1} (\ell - j) \prod_{k=1}^{u-1} (2w - 2u + k - \ell - 1) \end{aligned} \quad (\text{E.14})$$

Importantly, we have noted that $u \leq w - 5$ in the definition of $\mathfrak{A}_w^{(3)}$ implies that $w - u - 1 \geq 4$, and then we have used (E.14) to obtain the lower bounds on the sums in (E.12). Each individual term in the remaining sums has non-vanishing coefficient.

We reemphasize that these are only the contribution arising from holomorphic subgraph reduction. As long as $u \neq \lfloor \frac{w-1}{2} \rfloor$, this is in fact all of the contributions. However, for $u = \lfloor \frac{w-1}{2} \rfloor$ one would expect an additional holomorphic Eisenstein series \mathcal{G}_w produced via algebraic reduction. For w odd this term is vanishing and the distinction is unimportant, whereas for w even we must take it into account. For $w \in 4\mathbb{N}$, the case of $u = \frac{w}{2}$ is also exceptional, since (E.12) vanishes. For the moment, we take $u > \lfloor \frac{w}{2} \rfloor$ to avoid these complications, returning to them at the end of the proof.

We now focus on the terms in (E.12) with the holomorphic Eisenstein series of lowest weight. We may begin by assuming that $w - u \in 2\mathbb{N} + 1$. If this is the case, then (E.12) has a term containing a holomorphic Eisenstein series \mathcal{G}_{w-u+1} with coefficient

$$H_1(w - u + 1) + H_2(w - u + 1) = (-)^{u+1}(w - u) \frac{\Gamma(w - 1)}{\Gamma(u)} \tag{E.15}$$

which is non-vanishing. Hence the lowest weight holomorphic Eisenstein series is \mathcal{G}_{w-u+1} .

In the case of $w - u \in 2\mathbb{N}$, one begins by considering the case $\ell = w - u$, to which both sums contribute. However, in this case $H_1(w - u) + H_2(w - u)$ vanishes. Thus one moves on to $\ell = w - u + 2$. There is always a contribution towards this term from the second sum in (E.12), since $u \leq w - 5$ implies that $2(w - u) - 1 \geq w - u + 4$. If the first sum does not contribute to this term, then the coefficient is automatically non-vanishing. If the first sum does contribute, one finds

$$H_1(w - u + 2) + H_2(w - u + 2) = \frac{1}{2}(-1)^{u+1}(w - 2u) \frac{\Gamma(w - 2)\Gamma(w - u + 2)}{\Gamma(u)\Gamma(w - u)} \tag{E.16}$$

which is non-vanishing for $u > \lceil \frac{w}{2} \rceil$. Thus the lowest weight holomorphic Eisenstein series produced is \mathcal{G}_{w-u+2} .

With this information, we may now begin to prove linear independence of $\mathfrak{A}_w^{(1)}$, $\mathfrak{A}_w^{(2)}$, and $\mathfrak{A}_w^{(3)}$. This is done in the same manner as before: we begin by writing a tentative linear combination, now including the additional contributions due to elements of $\mathfrak{A}_w^{(3)}$,

$$\sum_{w_2=2}^{\lceil \frac{w-1}{2} \rceil} \sum_{k=1}^{w_2-1} \alpha(w_2, k) \mathcal{P}_k(w - w_2, w_2) + \sum_{u=1}^{w-5} \beta(u) \mathcal{A}_{u, u+1; w} = 0 \tag{E.17}$$

At any order $n < 4$ in ∇ , the elements of $\mathfrak{A}_w^{(3)}$ do not give rise to elements of $\mathfrak{C}_{(w+n, w-n)}$, and one may proceed exactly as in the first part of the proof. On the other hand, at each order $4 \leq n < \lceil \frac{w-1}{2} \rceil$ in ∇ there is a single element of $\mathfrak{A}_w^{(3)}$ which is in $\mathcal{V}_{(w, w)}^{(n)}$, namely $\mathcal{A}_{w-n-1, w-n; w}$.⁴ By the reasoning of the previous paragraphs, this function produces elements of $\mathfrak{C}_{(w+n, w-n)}$ which include terms proportional to \mathcal{G}_{n+2} (n even) or \mathcal{G}_{n+3} (n odd). At the same order ∇^n , only $\mathcal{P}_{w_2-n}(w - w_2, w_2) \in \mathfrak{A}_w^{(1)}$ and $\mathcal{A}_{n-1, n; w} \in \mathfrak{A}_w^{(2)}$ contribute elements of $\mathfrak{C}_{(w+n, w-n)}$. Since the former requires $w_2 \geq n + 1$, the lowest weight holomorphic Eisenstein series which it can produce is $\mathcal{G}_{2(n+1)}$, while the latter contributes only a term containing \mathcal{G}_{2n} . Because $n \geq 4$, these are necessarily of higher weight than \mathcal{G}_{n+2} or \mathcal{G}_{n+3} , thus proving linear independence for all functions in $\mathcal{V}_{(w, w)}^{(n)}$ for $n < \lceil \frac{w-1}{2} \rceil$.

We now turn to the remaining cases of $n = \lceil \frac{w-1}{2} \rceil$ and, if w is even, $n = \frac{w}{2}$. In fact, as mentioned before it is only when w is even that exceptional phenomena occur, and hence we focus on the case of w even for the remainder of the proof. We consider separately the cases of $w \notin 4\mathbb{N}$ and $w \in 4\mathbb{N}$. If $w \notin 4\mathbb{N}$, the result (E.12) for $n = \lceil \frac{w-1}{2} \rceil = \frac{w}{2} - 1$ is unchanged, but the case of $n = \frac{w}{2}$ must be modified slightly: upon application of $\nabla^{\frac{w}{2}}$ to $\mathcal{A}_{\frac{w}{2}-1, \frac{w}{2}; w}$, one not only produces elements of $\mathfrak{C}_{(3w/2, w/2)}$ via holomorphic subgraph

⁴The upper bound on n is equivalent to the earlier bound $u > \lceil \frac{w}{2} \rceil$.

reduction as per (E.12), but also a term via algebraic reduction. In particular, a term proportional to \mathcal{G}_w is produced by applying algebraic reduction to the image of $\nabla^{\frac{w}{2}}$ on the $\mathcal{C}_{\frac{w}{2}, \frac{w}{2}-1; w}$ contained in $\mathcal{A}_{\frac{w}{2}-1, \frac{w}{2}; w}$. This new contribution cancels the term proportional to \mathcal{G}_w in the second sum of (E.12), and we are left with

$$\nabla^{\frac{w}{2}} \mathcal{A}_{\frac{w}{2}-1, \frac{w}{2}; w} = \sum_{\ell=w/2+1}^{w-2} (H_1(\ell) + H_2(\ell)) \mathcal{G}_\ell \mathcal{C}_\ell^+ + \dots \tag{E.18}$$

When $w \in 4\mathbb{N}$, one must make the same modification (E.18) to the case $n = \frac{w}{2}$. But there is also a more subtle modification in the case of $n = \frac{w}{2} - 1$. Naively, we would assume that $\nabla^{\frac{w}{2}-1} \mathcal{A}_{\frac{w}{2}, \frac{w}{2}+1; w} \in \mathcal{V}_{(3w/2-1, w/2+1)} \oplus \mathfrak{C}_{(3w/2-1, w/2+1)}$. However, from (F.13) we see that for these choices of w and u all elements of $\mathfrak{C}_{(3w/2-1, w/2+1)}$ in (E.12) cancel, and we must proceed to the next order in ∇ to obtain the first holomorphic Eisenstein series. That is, we actually have

$$\mathcal{A}_{\frac{w}{2}, \frac{w}{2}+1; w} \in \mathcal{V}_{(w, w)}^{(w/2)} \quad \text{for all} \quad \mathcal{A}_{\frac{w}{2}, \frac{w}{2}+1; w} \in \mathfrak{A}_w^{(3)} \quad \text{and} \quad w \in 4\mathbb{N} \tag{E.19}$$

and hence $\mathcal{A}_{\frac{w}{2}, \frac{w}{2}+1; w}$ contributes non-holomorphic Eisenstein series at the same order in ∇ as $\mathcal{A}_{\frac{w}{2}-1, \frac{w}{2}; w}$. The elements of $\mathfrak{C}_{(3w/2, w/2)}$ appearing upon application of $\nabla^{w/2}$ to $\mathcal{A}_{\frac{w}{2}, \frac{w}{2}+1; w}$ are obtained in appendix G, with the final results given by (G.12).

To complete the proof of independence, we return to our tentative linear combination (E.17) and show that all coefficients must vanish at orders $\nabla^{\frac{w}{2}-1}$ and $\nabla^{\frac{w}{2}}$ for $w \in 2\mathbb{Z}$. If $w \notin 4\mathbb{Z}$, the proof proceeds as before for $\nabla^{\frac{w}{2}-1}$, and we need special consideration only for $\nabla^{\frac{w}{2}}$. Note that there is no contribution from $\mathfrak{A}_w^{(1)}$ or $\mathfrak{A}_w^{(2)}$ at this order (since these by definition have vanishing intersection with $\mathcal{V}_{(w, w)}^{(w/2)}$), but there is a non-vanishing contribution (E.18) from $\mathfrak{A}_w^{(3)}$. The coefficient $\beta(\frac{w}{2} - 1)$ in the linear combination must then vanish, completing the proof for $w \notin 4\mathbb{Z}$.

For $w \in 4\mathbb{Z}$, there are no contributions from elements of $\mathfrak{A}_w^{(3)}$ at order $\nabla^{\frac{w}{2}-1}$. Instead, there are two contributions at order $\nabla^{\frac{w}{2}}$, namely from $\mathcal{A}_{\frac{w}{2}-1, \frac{w}{2}; w}$ and $\mathcal{A}_{\frac{w}{2}, \frac{w}{2}+1; w}$. As before, there are no contributions from elements of $\mathfrak{A}_w^{(1)}$ or $\mathfrak{A}_w^{(2)}$ at this order. Note that $\mathcal{A}_{\frac{w}{2}-1, \frac{w}{2}; w}$ produces elements of $\mathfrak{C}_{(3w/2, w/2)}$ as dictated by (E.18), while $\mathcal{A}_{\frac{w}{2}, \frac{w}{2}+1; w}$ produces elements of $\mathfrak{C}_{(3w/2, w/2)}$ as dictated by (G.12). The contributions from (E.18) can be seen to be proportional to the first term of the first line of (G.12). The proof is then completed by noting that (G.12) has remaining non-zero terms.

F Holomorphic subgraph reduction

We begin with the following lemma.

Lemma F.1. *For $1 \leq u < v \leq w-1$ and $w-v < u$, the lowest order ∇ -derivative on $\mathcal{A}_{u, v; w}$ which yields a holomorphic subgraph is ∇^{w-v} , with the contribution from holomorphic subgraph reduction given by,*

$$\nabla^{w-v} \mathcal{A}_{u, v; w} = \sum_{\ell=4}^{w+u-v} H_1(\ell) \mathcal{G}_\ell \mathcal{C}_\ell^+ + \sum_{\ell=4}^{2w-u-v} H_2(\ell) \mathcal{G}_\ell \mathcal{C}_\ell^+ + \dots \tag{F.1}$$

The ellipsis represents terms in $\mathcal{V}_{(2w-v,v)}$ and the functions $H_i(\ell)$ are given by,

$$\begin{aligned} H_1(\ell) &= \frac{(-)^w \Gamma(\ell) \Gamma(2w - v - \ell)}{\Gamma(w - u) \Gamma(\ell + v - w) \Gamma(w + u - v - \ell + 1)} \\ H_2(\ell) &= \frac{(-)^v \Gamma(\ell) \Gamma(2w - v - \ell)}{\Gamma(u) \Gamma(\ell + v - w) \Gamma(2w - u - v - \ell + 1)} \end{aligned} \tag{F.2}$$

We have used the following abbreviation,

$$\mathcal{C}_\ell^+ = \mathcal{C}^+ \begin{bmatrix} 2w - v - \ell & 0 \\ v & 0 \end{bmatrix} \tag{F.3}$$

To prove this, we begin by noting that the conditions $1 \leq u < v \leq w - 1$ and $w - v < u$ imply $w - v < w - u$ and $w - v < v$. Hence $w - v$ is the smallest non-zero exponent in the modular graph function $\mathcal{A}_{u,v;w}$ and as such $\nabla^n \mathcal{A}_{u,v;w} \in \mathcal{V}_{(w+n,w-n)}$ for all $n < w - v$. The first possible appearance of a holomorphic subgraph is at $n = w - v$.

The holomorphic subgraph reduction contribution to the derivative $\nabla^{w-v} \mathcal{A}_{u,v;w}$ arises solely from the first term in (6.1). Focusing on this term, repeated use of (6.9) gives

$$\begin{aligned} \nabla^{w-v} \mathcal{A}_{u,v;w} &= \sum_{m=0}^{w-v} \binom{w-v}{m} \frac{\Gamma(w + u - v - m) \Gamma(w - u + m)}{\Gamma(u) \Gamma(w - u)} \\ &\quad \times \mathcal{C}^+ \begin{bmatrix} u + w - v - m & 0 & w - u + m \\ -w + v + m & v & w - v - m \end{bmatrix} + \dots \end{aligned} \tag{F.4}$$

where the ellipsis represents terms in $\mathcal{V}_{(2w-v,v)}$. The only holomorphic subgraph contribution arises from the following rearrangement using the momentum conservation identities (2.4),

$$\mathcal{C}^+ \begin{bmatrix} u + w - v - m & 0 & w - u + m \\ -w + v + m & v & w - v - m \end{bmatrix} = (-)^{w+v+m} \mathcal{C}^+ \begin{bmatrix} u + w - v - m & 0 & w - u + m \\ 0 & v & 0 \end{bmatrix} + \dots \tag{F.5}$$

which in turn may be evaluated using the holomorphic subgraph reduction formula of (6.10). The second line of (6.10) does not contribute, since the first term does not yield a holomorphic subgraph and the part in brackets cancels. Putting the pieces together, we find,

$$\nabla^{w-v} \mathcal{A}_{u,v;w} = \sum_{m=0}^{w-v} \left(\sum_{\ell=4}^{w+u-v-m} h_1(m, \ell) \mathcal{G}_\ell \mathcal{C}_\ell^+ + \sum_{\ell=4}^{w-u+m} h_2(m, \ell) \mathcal{G}_\ell \mathcal{C}_\ell^+ \right) + \dots \tag{F.6}$$

where the ellipsis represents terms in $\mathcal{V}_{(2w-v,v)}$ and the functions $h_i(m, \ell)$ are given by,

$$\begin{aligned} h_1(m, \ell) &= (-1)^{w+m} \binom{w-v}{m} \frac{\Gamma(w + u - v - m) \Gamma(2w - v - \ell)}{\Gamma(u) \Gamma(w - u) \Gamma(w + u - v - m - \ell + 1)} \\ h_2(m, \ell) &= (-1)^{w+m} \binom{w-v}{m} \frac{\Gamma(w - u + m) \Gamma(2w - v - \ell)}{\Gamma(u) \Gamma(w - u) \Gamma(w - u + m - \ell + 1)} \end{aligned} \tag{F.7}$$

Next, we interchange the summation over m and ℓ in (F.6) to obtain

$$\begin{aligned} \nabla^{w-v} \mathcal{A}_{u,v;w} = & \sum_{\ell=4}^u \left(\sum_{m=0}^{w-v} h_1(m, \ell) \right) \mathcal{G}_\ell \mathcal{C}_\ell^+ + \sum_{\ell=u+1}^{w+u-v} \left(\sum_{m=0}^{w+u-v-\ell} h_1(m, \ell) \right) \mathcal{G}_\ell \mathcal{C}_\ell^+ \\ & + \sum_{\ell=4}^{w-u} \left(\sum_{m=0}^{w-v} h_2(m, \ell) \right) \mathcal{G}_\ell \mathcal{C}_\ell^+ + \sum_{\ell=w-u+1}^{2w-u-v} \left(\sum_{m=\ell-w+u}^{w-v} h_2(m, \ell) \right) \mathcal{G}_\ell \mathcal{C}_\ell^+ + \dots \end{aligned} \quad (\text{F.8})$$

The sums over m are proportional to hypergeometric functions evaluated at unit argument and may be evaluated using Gauss's formula,

$${}_2F_1(a, b; c; 1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} \quad (\text{F.9})$$

and the reflection product formula for Γ -functions,

$$\Gamma(1-z)\Gamma(z) = \frac{\pi}{\sin \pi z} \quad (\text{F.10})$$

with the final result being

$$\begin{aligned} \sum_{m=0}^{w-v} h_1(m, \ell) &= \sum_{m=0}^{w+u-v-\ell} h_1(m, \ell) = H_1(\ell) \\ \sum_{m=0}^{w-v} h_2(m, \ell) &= \sum_{m=\ell-w+u}^{w-v} h_2(m, \ell) = H_2(\ell) \end{aligned} \quad (\text{F.11})$$

Having proven lemma F.1, we have the following simple corollary,

Corollary F.2. *For the range of parameters u, v, w indicated in lemma F.1, the functions $H_i(\ell)$ are polynomials in ℓ of respective degrees $2w - u - v - 1$ and $w + u - v - 1$. Their only zeros in ℓ within their respective summation ranges in (F.1) are $w - v$ simple zeros at the integers $\{1, 2, \dots, w - v\}$.*

By inspection of (F.2), it is clear that for the ranges of u, v, w assumed in lemma F.1, the functions $H_1(\ell)$ and $H_2(\ell)$ factorize as follows,

$$\begin{aligned} H_1(\ell) &= \frac{(-)^w}{\Gamma(w-u)} \prod_{j=1}^{w-v} (\ell - j) \prod_{k=1}^{w-u-1} (w+u-v+k-\ell) \\ H_2(\ell) &= \frac{(-)^v}{\Gamma(u)} \prod_{j=1}^{w-v} (\ell - j) \prod_{k=1}^{u-1} (2w-u-v+k-\ell) \end{aligned} \quad (\text{F.12})$$

Within their respective summation ranges in (F.1), namely $4 \leq \ell \leq w+u-v$ for $H_1(\ell)$ and $4 \leq \ell \leq 2w-u-v$ for $H_2(\ell)$, the second products in both lines of (F.12) are non-vanishing. Thus the only zeros are $w - v$ simple zeros at the integers $\ell \in \{1, 2, \dots, w - v\}$, as claimed.

For the particular case of w even and $u = \frac{w}{2}$, the above expressions for $H_1(\ell)$ and $H_2(\ell)$ exhibit the following relation,

$$H_2(\ell) = (-)^v H_1(\ell) \quad \text{for } w = 2u \quad (\text{F.13})$$

In the case that $v = u + 1 \in 2\mathbb{N} + 1$, all elements of $\mathfrak{C}_{(2w-v,v)}$ cancel from the right-hand side of (F.1) and the sieve algorithm requires that we proceed to the next order in ∇ to identify the first holomorphic subgraph. This is more involved, and is discussed in appendix G.

G A special case

As discussed after corollary F.2, for $w \in 4\mathbb{N}$, $u = \frac{w}{2}$, and $v = u + 1$ all elements of $\mathfrak{C}_{(2w-v,v)}$ cancel from the right-hand side of (F.1). In this case the sieve algorithm demands that we proceed to the next order in ∇ , i.e. $\nabla^{w-v+1} = \nabla^{\frac{w}{2}}$, to obtain the first holomorphic Eisenstein series. In other words, $\mathcal{A}_{\frac{w}{2}, \frac{w}{2}+1; w} \in \mathcal{V}_{(w,w)}^{(w/2)}$ for $w \in 4\mathbb{N}$. Obtaining the elements of $\mathfrak{C}_{(3w/2, w/2)}$ explicitly in this case is more involved than in appendix F, but follows the same strategy.

We consider $\mathcal{A}_{u,v;w} = \mathcal{C}_{u,v;w} - \mathcal{C}_{v,u;w}$ and focus on the first term on the right-hand side. In order to identify all elements of $\mathfrak{C}_{(3w/2, w/2)}$, at each order in ∇ it no longer suffices to keep only the terms with the smallest lower right entry in the exponent matrix. Instead, we must also keep terms with next-to-smallest lower right entry, since these may still produce holomorphic Eisenstein series after the remaining ∇ are applied. The terms with next-to-smallest lower right entry at level ∇^s arise from terms with smallest lower right entry at order ∇^{s-1} . In particular, from (F.4) and (F.5) we see that the terms with smallest lower right entry at order ∇^{s-1} are

$$\begin{aligned} \nabla^{s-1} \mathcal{C}_{u,v;w} = & \sum_{m=0}^{s-1} (-1)^{m+s-1} \binom{s-1}{m} \frac{\Gamma(u+s-1-m)\Gamma(w-u+m)}{\Gamma(u)\Gamma(w-u)} \\ & \times \mathcal{C}^+ \begin{bmatrix} u+s-1-m & 0 & w-u+m \\ 0 & v & w-v-s+1 \end{bmatrix} + \dots \end{aligned} \quad (\text{G.1})$$

The terms of next-to-smallest lower right entry at order ∇^s are then obtained by applying ∇ to the above and keeping only the terms which, via momentum conservation identities, subtract 1 from the bottom center entry of the exponent matrix, producing the modular graph form,

$$-(u+s-1-m) \mathcal{C}^+ \begin{bmatrix} u+s-m & 0 & w-u+m \\ 0 & v-1 & w-v-s+1 \end{bmatrix} + \dots \quad (\text{G.2})$$

where we have neglected terms which do not have next-to-smallest lower right entry. Then in order to identify the elements of $\mathfrak{C}_{(w+n, w-n)}$ produced by these functions at order ∇^n , we may consider only the terms for which, upon application of ∇ , the value of the lower right entry is reduced (i.e. we may neglect any functions which have further subtractions on the bottom center entry, since such terms cannot produce any holomorphic Eisenstein series at order ∇^n). In particular, by the same reasoning as for (F.4), it follows that

$$\begin{aligned} \nabla^{n-s} \mathcal{C}^+ \begin{bmatrix} u+s-m & 0 & w-u+m \\ 0 & v-1 & w-v-s+1 \end{bmatrix} = \\ \sum_{r=0}^{n-s} (-1)^{r+n-s} \binom{n-s}{r} \frac{\Gamma(u-m+n-r)\Gamma(w-u+m+r)}{\Gamma(u+s-m)\Gamma(w-u+m)} \\ \times \mathcal{C}^+ \begin{bmatrix} u-m+n-r & 0 & w-u+m+r \\ 0 & v-1 & w-v-n+1 \end{bmatrix} + \dots \end{aligned} \quad (\text{G.3})$$

are the terms which must be kept. Hence the elements of $\mathfrak{C}_{(w+n,w-n)}$ coming from functions which experienced the single subtraction on their bottom center entry at order ∇^s can be obtained by considering the elements of $\mathfrak{C}_{(w+n,w-n)}$ produced by

$$\begin{aligned} \nabla^{n-s}\nabla^s\mathcal{C}_{u,v;w} &= \sum_{m=0}^{s-1} \sum_{r=0}^{n-s} (-1)^{r+n+m} \binom{n-s}{r} \binom{s-1}{m} \frac{\Gamma(u-m+n-r)\Gamma(w-u+m+r)}{\Gamma(u)\Gamma(w-u)} \\ &\quad \times \mathcal{C}^+ \begin{bmatrix} u-m+n-r & 0 & w-u+m+r \\ 0 & v-1 & w-v-n+1 \end{bmatrix} + \dots \end{aligned} \tag{G.4}$$

Finally, in order to capture all holomorphic Eisenstein series arising in this way, we must sum over all s in the range $1 \leq s \leq n-1$. Specifying that $n = w - v + 1$, $w \in 4\mathbb{Z}$, $u = w/2$ and $v = u + 1$, the complete set of elements of $\mathfrak{C}_{(3w/2,w/2)}$ are contained in

$$\nabla^{w/2}\mathcal{C}_{\frac{w}{2},\frac{w}{2}+1;w} = \sum_{s=1}^{w/2-1} \sum_{m=0}^{s-1} \sum_{r=0}^{w/2-s} \tilde{g}(s,m,r,\ell) \mathcal{C}^+ \begin{bmatrix} w-m-r & w/2+m+r & 0 \\ 0 & 0 & w/2 \end{bmatrix} + \dots \tag{G.5}$$

where we have defined

$$\tilde{g}(s,m,r,\ell) = (-1)^{m+r} \binom{w/2-s}{r} \binom{s-1}{m} \frac{\Gamma(w-m-r)\Gamma(w/2+m+r)}{\Gamma(w/2)^2} \tag{G.6}$$

We may then use holomorphic subgraph reduction (6.10) to obtain the final result,

$$\begin{aligned} \nabla^{w/2}\mathcal{C}_{\frac{w}{2},\frac{w}{2}+1;w} &= \sum_{s=1}^{w/2-1} \sum_{m=0}^{s-1} \sum_{r=0}^{w/2-s} \left\{ \sum_{\ell=4}^{w-m-r} g_1(s,m,r,\ell) \mathcal{G}_\ell \mathcal{C}^+ \begin{bmatrix} 3w/2-\ell & 0 \\ w/2 & 0 \end{bmatrix} \right. \\ &\quad \left. + \sum_{\ell=4}^{w/2+m+r} g_2(s,m,r,\ell) \mathcal{G}_\ell \mathcal{C}^+ \begin{bmatrix} 3w/2-\ell & 0 \\ w/2 & 0 \end{bmatrix} \right\} + \dots \end{aligned} \tag{G.7}$$

where we have defined

$$\begin{aligned} g_1(s,m,r,\ell) &= \binom{3w/2-\ell-1}{w-m-r-\ell} \tilde{g}(s,m,r,\ell) \\ g_2(s,m,r,\ell) &= \binom{3w/2-\ell-1}{w/2+m+r-\ell} \tilde{g}(s,m,r,\ell) \end{aligned} \tag{G.8}$$

This is the contribution towards $\mathfrak{C}_{(3w/2,w/2)}$ at order $\nabla^{w/2}$ coming from $\mathcal{C}_{\frac{w}{2},\frac{w}{2}+1;w}$ in,

$$\mathcal{A}_{\frac{w}{2},\frac{w}{2}+1;w} = \mathcal{C}_{\frac{w}{2},\frac{w}{2}+1;w} - \mathcal{C}_{\frac{w}{2}+1,\frac{w}{2};w} \tag{G.9}$$

When calculating the total contribution to $\mathfrak{C}_{(3w/2,w/2)}$ from the full odd modular graph function, we must also consider contributions coming from $\mathcal{C}_{\frac{w}{2}+1,\frac{w}{2};w}$. These include elements of $\mathfrak{C}_{(3w/2,w/2)}$ coming from algebraic subgraph reduction, as well as from holomorphic

subgraph reduction since $u = \frac{w}{2}$. The terms arising from algebraic subgraph reduction are found to be of the form

$$\nabla^{w/2} \mathcal{C}_{\frac{w}{2}+1, \frac{w}{2}; w} \Big|_{alg.red.} = \frac{\Gamma(w)}{\Gamma(w/2+1)} \mathcal{G}_{w+1} \mathcal{C}^+ \begin{bmatrix} w/2-1 & 0 \\ w/2 & 0 \end{bmatrix} + \dots \quad (G.10)$$

But since we are considering w even, the holomorphic Eisenstein series in this case vanishes. Thus we have only the contribution coming from holomorphic subgraph reduction, which follows directly from (F.1) and is

$$\nabla^{w/2} \mathcal{C}_{\frac{w}{2}+1, \frac{w}{2}; w} = \sum_{\ell=4}^{w+1} H'_1(\ell) \mathcal{G}_\ell \mathcal{C}_\ell^{+'} + \sum_{\ell=4}^{w-1} H'_2(\ell) \mathcal{G}_\ell \mathcal{C}_\ell^{+'} + \dots \quad (G.11)$$

where $H'_1(\ell)$, $H'_2(\ell)$, and $\mathcal{C}_\ell^{+'}$ are obtained from (F.2) and (F.3) by first interchanging $u \leftrightarrow v$, and then substituting the required values for u and v . Adding (G.7) and (G.11) then gives the total contribution to $\mathfrak{C}_{(3w/2, w/2)}$ for the special functions (E.19), which is

$$\begin{aligned} \nabla^{w/2} \mathcal{A}_{\frac{w}{2}, \frac{w}{2}+1; w} = & - \sum_{\ell=w/2+2}^{w-2} (H'_1(\ell) + H'_2(\ell)) \mathcal{G}_\ell \mathcal{C}_\ell^{+'} - H'_1(w) \mathcal{G}_w \mathcal{C}_w^{+'} \\ & + \sum_{s=1}^{w/2-1} \sum_{m=0}^{s-1} \sum_{r=0}^{w/2-s} \left\{ \sum_{\ell=4}^{w-m-r} g_1(s, m, r, \ell) \mathcal{G}_\ell \mathcal{C}^+ \begin{bmatrix} 3w/2-\ell & 0 \\ w/2 & 0 \end{bmatrix} \right. \\ & \left. + \sum_{\ell=4}^{w/2+m+r} g_2(s, m, r, \ell) \mathcal{G}_\ell \mathcal{C}^+ \begin{bmatrix} 3w/2-\ell & 0 \\ w/2 & 0 \end{bmatrix} \right\} + \dots \end{aligned} \quad (G.12)$$

for $w \in 4\mathbb{N}$. The dots represent elements of $\mathcal{V}_{(3w/2, w/2)}$. Note that we have used the fact that $H'_1(\frac{w}{2}) + H'_2(\frac{w}{2}) = 0$.

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