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Johannes Blümlein
Carsten Schneider
Peter Paule *Editors*

Elliptic Integrals, Elliptic Functions and Modular Forms in Quantum Field Theory

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Preface

Elliptic functions, elliptic integrals and modular forms play a central role in the theory of analytic calculations of Feynman parameter integrals at higher loop order. They occur at the next level of complexity after the iterative integrals over certain alphabets or the nested sums, which host a wide range of simpler structures and have been studied in detail and applied in many physics calculations during the last two decades.

The integration-by-part technique, which is widely applied in the solution of complex calculations, provides a natural way to obtain the associated set of systems of linear single-variate ordinary differential equations with rational coefficients in the differential variable x and the dimensional parameter $\varepsilon = D - 4$. These can be systematically decoupled, leading to one ordinary differential equation of high order. Whenever this equation factorizes into first-order factors, all solutions are given by iterative integrals. In massive three-loop problems, one observes that this decoupling cannot be achieved and one is also left with irreducible second-order systems, normally with more than three singularities. One seeks now ${}_2F_1$-solutions of these second-order equations, allowing for the main argument being a rational function in the variable x.

In a large series of cases, these solutions can be expressed by complete elliptic integrals in case of inclusive quantities. In more differential cases, also incomplete elliptic integrals may occur. In the former case, the connection to modular forms is obvious and one seeks solutions in terms of ratios of Dedekind's η-functions. These modular forms are either meromorphic or, in more special cases, holomorphic and are connected to the elliptic polylogarithms and can be expanded into associated q-series.

Due to this, the mathematics of modular forms is of central importance for the analytic solution of Feynman diagrams, which motivated the workshop *Elliptic Integrals, Elliptic Functions and Modular Forms in Quantum Field Theory*, held at Zeuthen, Germany, October 23–26, 2017. It has been organized and funded in part as one of the annual workshops of Kolleg Mathematik Physik Berlin. This workshop was meant to cover a larger part of related topics in this field bringing together mathematicians and theoretical physicists presenting survey talks on a variety of topics. They are published in this volume together with additional invited contributions. In most of the contributions, aspects of symbolic computation play an essential role.

A classical approach to elliptic solutions in Feynman diagram calculations relies on dispersion relations. Their cuts give the excess to the inner phase space structure of the corresponding graphs, remaining partly invisible by just studying the associated differential equations. This method has been reviewed by *E. Remiddi*. It also provides a very lucid way in studying even more involved topologies in the future, providing the corresponding integrand structures up to one or more additional Hilbert transforms.

In the contributions by *L. Adams, S. Weinzierl, C. Duhr et al.* and by *J. Blümlein*, a direct link between Feynman integrals evaluating to elliptic integrals and their representation in terms of modular forms has been given. They appear as iterated integrals of modular forms. Conversely, one may start with the modular forms and find the associated differential equations. In general, the solutions are given by iterated integrals over non-iterative integrals, the simplest of which is ${}_2F_1$-functions. This applies even to non-decoupling situations of order 3 and larger, with other non-iterative integrals appearing as iterated letters. In the elliptic case, the holomorphic modular forms have representations in terms of Lambert–Eisenstein series, while the meromorphic ones are weighted in addition by powers of Dedekind's η-function. *M. van Hoeij* discussed general analytic solutions of second- and third-order differential equations with more singularities. Numerical implementations are considered by *C. Bogner et al.* on fast converging q-series. Precise numerical implementations of elliptic functions, the Jacobi ϑ-functions, modular forms, elliptic integrals and the arithmetic–geometric mean have been discussed by *F. Johansson*.

Elliptic integrals appear in various massive higher-order calculations in quantum chromodynamics, as pointed out in the contributions by *S. Weinzierl, J. Blümlein, E. Remiddi and R. Bonciani et al.* Currently, very important calculations are those of the production cross section of top and anti-top quark pairs (*R. Bonciani et al.*) and also Higgs boson production at the Large Hadron Collider (LHC) at CERN. *D. Kreimer* studied the conceptual relation between scattering theory for Feynman amplitudes and the structure of suitable outer spaces, motivated by the work of Vogtmann and Culler. *P. Vanhove* discussed the relation of Feynman integrals, toric geometry and mirror symmetry, determining the minimal differential operator acting on the Feynman integrals considering the maximal cut. In this calculation, also Calabi–Yau structures are found.

Applications of iterated integrals on an elliptic curve in string perturbation theory have been reviewed by *J. Brödel and O. Schlotterer* pointing out the relation to elliptic multiple zeta values. Related work has been presented by *F. Zerbini* on modular and holomorphic graph functions from superstring amplitudes.

H. Cohen discussed the computation of Fourier expansions at all cusps of any modular form of integral or half-integral weight. Its implementation is available in the current release of the `Pari/GP` package. Far-reaching results on Bessel moments are presented in the contributions by *K. Acres, D. Broadhurst and Y. Zhou*, along with Rademacher sums and L-functions. The contribution by *M. L. Dawsey and K. Ono* deals with q-analogs of Euler's zeta function evaluations. In particular, they put interesting recent developments by Z.-W. Sun and A. Goswami into a general framework; to this end, they use state-of-art theory in modular forms and complex multiplication. *R. Hemmecke, C.-S. Radu and L. Ye* prove that the ideal of all polynomial relations among the classical Jacobi ϑ-functions are generated by only two polynomials. This result is accomplished by new ideal–theoretic insight of elliptic ϑ-quotients and sophisticated Gröbner basis considerations. *J. Frye and F. Garvan* present the two new `Maple` packages: `thetaids` and `ramarobinsids`. They allow to prove generalized η-product identities using the valence formula for modular functions, which is also applicable to ϑ_i-functions and for finding and proving identities for generalizations of Ramanujan's $G(q)$ and $H(q)$ and extensions by S. Robins. *A. Straub and R. Osburn* study interpolated sequences and critical L-values of modular forms.

P. Paule and C. Schneider established new algebraic connections between summation problems involving generic sequences and difference field/ring theory taking special care of concrete sequences arising in contexts like analysis, combinatorics, number theory and special functions. The elaborated symbolic summation theory for unspecified sequences can be considered as the first steps toward an algorithmic framework for the treatment of summation identities involving elliptic functions or modular forms.

Given the size of the topical area under discussion, the different contributions can of course only provide a start of further investigation and treatment and they are not meant to be complete. The field will develop on the physics side first by applying the different techniques to solve the elliptic cases. By exploring more and more involved structures beyond this level, one will be naturally lead to much deeper mathematical structures and even more advanced solution methods. As experienced in the past, one can be sure that the analytic calculation of complex Feynman diagrams will trigger quite a series of new developments in mathematics, and conversely, physics will profit significantly from results already being available in various branches of mathematics, in particular also, symbolic computation.

The transparencies of the talks presented are available at the page https://indico.desy.de/indico/event/18291/timetable/#all. Financial support of this conference by Kolleg Mathematik Physik Berlin is gratefully acknowledged.

Zeuthen, Germany — Johannes Blümlein
Linz, Austria — Peter Paule
Linz, Austria — Carsten Schneider
September 2018

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Eta Quotients and Rademacher Sums

Kevin Acres and David Broadhurst

Abstract Eta quotients on $\Gamma_0(6)$ yield evaluations of sunrise integrals at 2, 3, 4 and 6 loops. At 2 and 3 loops, they provide modular parametrizations of inhomogeneous differential equations whose solutions are readily obtained by expanding in the nome q. Atkin–Lehner transformations that permute cusps ensure fast convergence for all external momenta. At 4 and 6 loops, on-shell integrals are periods of modular forms of weights 4 and 6 given by Eichler integrals of eta quotients. Weakly holomorphic eta quotients determine quasi-periods. A Rademacher sum formula is given for Fourier coefficients of an eta quotient that is a Hauptmodul for $\Gamma_0(6)$ and its generalization is found for all levels with genus 0, namely for $N = 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 13, 16, 18, 25$. There are elliptic obstructions at $N = 11, 14, 15, 17, 19, 20, 21, 24, 27, 32, 36, 49$, with genus 1. We surmount these, finding explicit formulas for Fourier coefficients of eta quotients in thousands of cases. We show how to handle the levels $N = 22, 23, 26, 28, 29, 31, 37, 50$, with genus 2, and the levels $N = 30, 33, 34, 35, 39, 40, 41, 43, 45, 48, 64$, with genus 3. We also solve examples with genera 4, 5, 6, 7, 8, 13.

1 Introduction

Elliptic obstructions to the evaluation of massive Feynman diagrams were recognized and surmounted more than 50 years ago by Sabry [30]. They occur in two-loop two-point integrals when three massive particles appear in an intermediate state [11]. The simplest example is the two-loop sunrise diagram with unit masses in two space-time dimensions, whose study was revolutionized in 2013, when Bloch and Vanhove [4]

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showed how to parametrize and solve its second order differential equation using eta quotients on $\Gamma_0(6)$.

Their solution was particularly bold, since they expand in a nome q that is small near the physical threshold where the external energy w is close to 3. Thus they achieve fast convergence near the branchpoint that frustrates other methods. The price to pay is that convergence is slow near any of the other three cusps of $\Gamma_0(6)$, which occur at $w = 0, 1, \infty$. We shall show how to use Atkin–Lehner transformations of eta quotients to expand about those cusps, achieving optimal efficiency.

Bloch, Kerr and Vanhove [5] conquered the corresponding three-loop problem, also using eta quotients on $\Gamma_0(6)$, thanks to the remarkable circumstance, noted more than 40 years ago by Joyce [20], that a transformation of variables relates solutions of the relevant homogeneous third-order differential equation to products of solutions of the second-order equation at two loops. Joyce's observation was made in the context of the physics of condensed matter. The relevance of his work on the diamond lattice to Feynman integrals was decoded in [2]. We shall use an Atkin–Lehner transformation to achieve optimal efficiency at three loops.

The role of $\Gamma_0(6)$ does not end at three loops. It is of the essence for the on-shell problems at 4 and 6 loops, where the relevant Bessel moments turn out to be Eichler integrals of eta quotients that are cusp forms of level 6 with modular weights 4 and 6, respectively. We shall review key results, which were until recently only conjectures [7–10], tested to many thousands of digits. For an account of how they were proved [34–37], see the lucid review by Zhou [38].

It is notable that this connection between number theory and Feynman integrals persists in the real world of four-dimensional space-time. The four-loop radiative corrections to the magnetic moment of the electron in quantum electrodynamics, evaluated with breath-taking skill by Laporta [23], contain a pair of Bessel moments [37] that are Eichler integrals. We conclude Sect. 2 with results that indicate that one of these is a quasi-period, in the sense of Brown [13]. Moreover we conjecturally identify quasi-periods at 6 loops.

Section 3 concerns a searching question raised by Johannes Blümlein at a recent conference held at the Hausdorff Centre for Mathematics, in Bonn. Is there a closed formula for the Fourier coefficients of the Hauptmodul of $\Gamma_0(6)$, of the type that Petersson [26] and Rademacher [22, 27, 28] found for Klein's j-invariant? We conjecturally answer in the affirmative, by giving a formula that serves this purpose for all levels with genus 0. Moreover we are able to extend its use to higher genera.

2 Eta Quotients in Quantum Field Theory

Broadhurst, Fleischer and Tarasov [12] gave the differential equation for the two-loop unit-mass sunrise integral in an arbitrary number D of space-time dimensions. At $D = 2$, this integral is a Bessel moment [2]

$$I(w^2) = 4\int_0^\infty I_0(wx)K_0^3(x)x\mathrm{d}x, \tag{1}$$

where w is the external energy, which enters the Bessel function $I_0(wx)$ via Fourier transformation. The Bessel function $K_0(x)$ is cubed, since three particles of unit mass connect the two vertices. Bloch and Vanhove [4] found a very neat modular parametrization of the differential equation at $D = 2$, which we here write as

$$-\left(q\frac{\mathrm{d}}{\mathrm{d}q}\right)^2 \frac{I(w^2)}{6f} = g, \quad w = \frac{3\eta_2^2\eta_3^4}{\eta_1^4\eta_6^2}, \quad f = \frac{\eta_1^6\eta_6}{\eta_2^3\eta_3^2}, \tag{2}$$

$$g = \frac{\eta_2^5\eta_3^4\eta_6}{\eta_1^4} = \frac{\eta_3^9}{\eta_1^3} + \frac{\eta_6^9}{\eta_2^3} = \sum_{n>0} \frac{n^2(q^n - q^{5n})}{1 - q^{6n}}, \quad \eta_n = q^{n/24}\prod_{k>0}(1 - q^{nk}), \tag{3}$$

with eta quotients determining the energy w, the integrating factor f, which is an elliptic integral determining the discontinuity across the cut for $w > 3$, and the inhomogeneous term g. Two easy integrations of the Lambert series for g then yield

$$\frac{I(w^2)}{f} = \frac{\pi \log(-1/q)}{\sqrt{3}} - 3\sum_{n>0} \frac{\chi_6(n)}{n^2}\frac{1 + q^n}{1 - q^n} \tag{4}$$

with $\chi_6(n) = \pm 1$ for $n = \pm 1 \bmod 6$ and $\chi_6(n) = 0$, otherwise. This solution is determined by the discontinuity across the cut and the finiteness of $I(1) = \pi^2/4$ [2]. In summary: after dividing $I(w^2)$ by the modular form f, with weight 1 and level 6, we obtain solution (4) by two integrations of the weight 3 modular form g with respect to z, where $q = \exp(2\pi\mathrm{i}z)$. Such integrals of modular forms are referred to as Eichler integrals.

We remark that modular parametrizations of differential equations were used in [3], to elucidate proofs of rationality of zeta values, and in [21], for problems in statistical physics.

2.1 Atkin–Lehner Transformations of Eta Quotients

Now set $q = \exp(2\pi\mathrm{i}z)$ with $\Im z > 0$ and consider the transformations [15]

$$z \longmapsto z_2 = \frac{2z - 1}{6z - 2}, \quad z \longmapsto z_3 = \frac{3z - 2}{6z - 3}, \quad z \longmapsto z_6 = \frac{-1}{6z}, \tag{5}$$

which permute the cusps at $z = 0, \frac{1}{2}, \frac{1}{3}, \infty$. Then, with $q_k = \exp(2\pi\mathrm{i}z_k)$,

$$-\left(q_k\frac{\mathrm{d}}{\mathrm{d}q_k}\right)^2 \frac{I(w^2)}{6f_k(z_k)} = g_k(z_k), \tag{6}$$

$$f_2(z) = \frac{\eta_2^6\eta_3}{\eta_1^3\eta_6^2}, \quad f_3(z) = \frac{\eta_2\eta_3^6}{\eta_1^2\eta_6^3}, \quad f_6(z) = \frac{\eta_1\eta_6^6}{\eta_2^2\eta_3^3}, \tag{7}$$

$$g_2(z) = \frac{\eta_1^5\eta_3\eta_6^4}{\eta_2^4}, \quad g_3(z) = \frac{\eta_1^4\eta_2\eta_6^5}{\eta_3^4}, \quad g_6(z) = \frac{\eta_1\eta_2^4\eta_3^5}{\eta_6^4}. \tag{8}$$

From the alternative differential equations (6), we obtain alternative expansions:

$$\frac{I(w^2)}{f_2(z_2)} = \sum_{n=1}^{\infty} \frac{3\chi_3(n)}{n^2} \frac{(1-q_2^n)^2}{1+q_2^{2n}} = I(0) - \sum_{n=1}^{\infty} \frac{6\chi_3(n)}{n^2} \frac{q_2^n}{1+q_2^{2n}}, \tag{9}$$

$$\frac{I(w^2)}{f_3(z_3)} = \sum_{n=1}^{\infty} \frac{2\chi_2(n)}{n^2} \frac{(1-q_3^n)^3}{1-q_3^{3n}} = I(1) - \sum_{n=1}^{\infty} \frac{6\chi_2(n)}{n^2} \frac{q_3^n}{1+q_3^n+q_3^{2n}}, \tag{10}$$

$$\frac{I(w^2)}{f_6(z_6)} = -3\log^2(-q_6) + \sum_{n=1}^{\infty} \frac{6}{n^2} \frac{q_6^n}{1-q_6^n+q_6^{2n}}, \tag{11}$$

with $\chi_2(n) = 0, 1$, for $n = 0, 1 \bmod 2$, and $\chi_3(n) = -1, 0, 1$, for $n = -1, 0, 1 \bmod 3$.

Then for any real value of w^2 there is an optimal choice of nome in which to expand, which may be determined as follows. Let

$$w_1^2 = w^2, \quad w_2^2 = \frac{w^2-9}{w^2-1}, \quad w_3^2 = \frac{9}{w^2}, \quad w_6^2 = \frac{9}{w_2^2}. \tag{12}$$

For $w^2 \in [-3,\ 9-6\sqrt{2}]$ set $k=2$, else for $w^2 \in [9-6\sqrt{2},\ 3]$ set $k=3$, else for $w^2 \in [3,\ 9+6\sqrt{2}]$ set $k=1$, else set $k=6$. Then compute $w_k \in [\sqrt{3}, \sqrt{3}+\sqrt{6}]$ and obtain the optimal nome $q_k = Q(w_k)$ from

$$Q(x) = \exp\left(\frac{-\pi\ \mathrm{agm}(1,\sqrt{r})}{\mathrm{agm}(1,\sqrt{1-r})}\right), \quad r = \frac{16x}{(x+3)(x-1)^3}, \tag{13}$$

by the lightning-fast process of the arithmetic-geometric mean. This results in a small real nome $q_k \in [-\exp(-\pi/\sqrt{3}),\ \exp(-\pi\sqrt{2/3})]$ and hence $|q_k| < 0.16304$. If $k=2$, use (9); if $k=3$, use (10); if $k=6$, use (11); if $k=1$ use $q=q_1$ in (4) and extract a Clausen value from

$$\sum_{n>0} \frac{\chi_6(n)}{n^2} \frac{1+q^n}{1-q^n} = C_2 + \sum_{n>0} \frac{\chi_6(n)}{n^2} \frac{2q^n}{1-q^n}, \quad C_2 = \frac{5\,\mathrm{Cl}_2(\pi/3)}{\sqrt{27}} = \frac{5I(0)}{12}. \tag{14}$$

The authors of [6] expand in $q_M = -q_2$, thereby encountering η_4 and η_{12} in

$$f_M(z) = f_2\left(z+\frac{1}{2}\right) = \frac{\eta_1^3\eta_4^3\eta_6}{\eta_2^3\eta_3\eta_{12}}, \quad g_M(z) = g_2\left(z+\frac{1}{2}\right) = -\frac{\eta_2^{11}\eta_6^7}{\eta_1^5\eta_3\eta_4^5\eta_{12}}. \tag{15}$$

Since they expand about the cusp at $w=0$, they inevitably face issues of slow convergence near the cusps at $w = 1, 3, \infty$. Moreover they had to address delicate questions of analytic continuation at the on-shell point $w = 1$. Our procedure of invariably expanding about the *nearest* cusp avoids all such problems.

Such use of Atkin–Lehner transformations to achieve efficient expansions in small nomes is well known to mathematicians who compute with modular forms [16]. We recommend exploitation of the transformations (5) to physicists who encounter problems that involve the congruence subgroup $\Gamma_0(6)$. For example, the authors of [1] encountered, at 3 loops, a second-order equation with complicated coefficients and powers of $\log(x)$ in the inhomogeneous term. Their homogeneous equation has a hypergeometric solution

$$H(x) = \frac{(x^2-1)^2}{9(x^2+3)} \sum_{n=0}^{\infty} \frac{(4/3)_n (5/3)_n}{n!(n+1)!} \left(\frac{x^2(x^2-9)^2}{(x^2+3)^3} \right)^{n+1} \tag{16}$$

where $(a)_n = \Gamma(a+n)/\Gamma(a)$ is the Pochhammer symbol. We obtained

$$H\left(3\frac{\eta_1^2\eta_6^4}{\eta_2^4\eta_3^2}\right) = \frac{1}{2}\left(\frac{\eta_1^{14}\eta_6^{10}}{\eta_2^{22}\eta_3^2} + \frac{\eta_1^6\eta_6^4}{\eta_2^{12}\eta_3^2}\left(\frac{\eta_1^4\eta_6^8}{\eta_2^8\eta_3^4} + \frac{1}{3}\right) q\frac{\mathrm{d}}{\mathrm{d}q}\right) \frac{\eta_2^6\eta_3}{\eta_1^3\eta_6^2} \tag{17}$$

as a modular parametrization of the homogeneous solution, where the derivative with respect to q results from a complete integral of the second kind. It would be interesting to investigate whether an Atkin–Lehner transformation may be used to avoid a singularity that was encountered at $x = \frac{1}{3}$ at intermediate stages of the work in [1].

For our next advertisement of the virtue of Atkin–Lehner transformation, we turn to the three-loop equal-mass sunrise integral. Bailey, Borwein, Broadhurst and Glasser [2] developed the expansion in t of

$$J(t) = 8\int_0^\infty I_0(\sqrt{t}x)K_0^4(x)x\mathrm{d}x = 7\zeta(3) + O(t). \tag{18}$$

A neat and novel q-expansion comes from exploiting a transformation [2, 20] from w^2, at two loops, to $t = 10 - w^2 - 9/w^2$, at three loops. Then we obtain the modular parametrization

$$t = 10 - w^2 - \frac{9}{w^2} = -64\left(\frac{\eta_2\eta_6}{\eta_1\eta_3}\right)^6, \tag{19}$$

$$\left(q\frac{\mathrm{d}}{\mathrm{d}q}\right)^3 \frac{J(t)}{(wf/3)^2} = 24h, \quad h = \frac{\eta_2^{16}}{\eta_1^8} - 9\frac{\eta_6^{16}}{\eta_3^8} = \sum_{n>0} \frac{n^3(q^n - 8q^{3n} + q^{5n})}{1-q^{6n}}, \tag{20}$$

$$\frac{J(t)}{(wf/3)^2} = J(0) + 24\sum_{n>0} \frac{\phi(n)}{n^3}\frac{q^n}{1-q^n}, \tag{21}$$

with $\phi(n) = 0, 1, 0, -8, 0, 1$, for $n = 0, 1, 2, 3, 4, 5 \bmod 6$. The `Pari-GP` procedure

```
z(t)={local(x=2/(sqrt(4-t)+sqrt(16-t)),
a=sqrt((1-x)^3*(1+3*x)));
I/2*agm(a,4*x*sqrt(x))/agm(a,sqrt((1+x)^3*(1-3*x)));}
```

returns the correct value of z for the nome $q = \exp(2\pi\mathrm{i}z)$, for all real t. Expansion (21) is highly efficient for $t \in [-8, 8]$, where $|q| \le \exp(-\sqrt{2}\pi/3) < 0.22742$. For the rest of the real t-axis, we exploit the involution $z \longmapsto z_6 = -1/(6z)$, which gives $t \longmapsto t_6 = 64/t$, with fixed points at $t = \pm 8$. For $t_6 \in [-8, 8]$ we use

$$\left(q_6\frac{\mathrm{d}}{\mathrm{d}q_6}\right)^3 \frac{J(t)}{(wf_6(z_6))^2} = -24h_6(z_6), \tag{22}$$

$$h_6(z) = -\, t_6 h = 1 + 2h - 30\sum_{n>0}\frac{n^3(q^{2n} + q^{4n} - 8q^{6n})}{1 - q^{6n}}, \tag{23}$$

$$\frac{J(t)}{(wf_6(z_6))^2} = -4\log^3(q_6) + 24\sum_{n>0}\frac{15\phi(n+3) - \phi(n)}{n^3}\frac{1 + q_6^n}{1 - q_6^n}, \tag{24}$$

in agreement with the result proved by Bloch, Kerr and Vanhove [5]. Extracting

$$C_3 = \sum_{n>0}\frac{15\phi(n+3) - \phi(n)}{n^3} = \frac{2\zeta(3)}{3} \tag{25}$$

we achieve a highly efficient expansion in $q_6 = \exp(-\pi\mathrm{i}/(3z))$ for $64/t \in [-8, 8]$, with a strong check of consistency with (21) in the neighbourhoods of $t = \pm 8$, where both expansions work well.

2.2 *Eichler Integrals of Eta Quotients for On-Shell Sunrise Integrals*

On-shell sunrise integrals lead us to consider Bessel moments of the form

$$M(a, b, c) = \int_0^\infty I_0^a(x)K_0^b(x)x^c\mathrm{d}x. \tag{26}$$

For $L > 3$, the off-shell L-loop integral

$$S_L(t) = \int_0^\infty \frac{\mathrm{d}x_1}{x_1}\cdots\int_0^\infty \frac{\mathrm{d}x_L}{x_L}\,\frac{1}{(1 + \sum_{j=1}^L x_j)(1 + \sum_{k=1}^L 1/x_k) - t} \tag{27}$$

has not yielded to the methods given above for $L = 2, 3$. By contrast, the on-shell values $S_L(1) = 2^L M(1, L+1, 1)$ with $L+2$ Bessel functions yield Eichler integrals of cusp forms of weights 4 and 6 on $\Gamma_0(6)$ at $L = 4$ and $L = 6$ loops, namely integrals of the form $\int_0^\infty f(\mathrm{i}y) y^{s-1} \mathrm{d}y$, where $f(z)$ is a cusp form with weight L and s is a integer with $L > s > 0$. First we consider the situation at $L = 3$ loops, where a modular form of weight 3 occurs.

At 3 loops, with 5 Bessel functions, the on-shell problem is solved by the weight 3 level 15 cusp form

$$f_{3,15}(z) = (\eta_3\eta_5)^3 + (\eta_1\eta_{15})^3 = \sum_{n>0} A_5(n) q^n = -\frac{f_{3,15}(-1/(15z))}{(-15)^{3/2} z^3} \tag{28}$$

with complex multiplication in $\mathbf{Q}(\sqrt{-15})$. If the Kronecker symbol $\left(\frac{p}{15}\right) = \left(\frac{p}{3}\right)\left(\frac{p}{5}\right)$ is negative, for prime p, then $A_5(p) = 0$. For $\Re s > 2$, there is a convergent L-series

$$L_5(s) = \sum_{n>0} \frac{A_5(n)}{n^s} = \prod_p \frac{1}{1 - A_5(p)p^{-s} + \left(\frac{p}{15}\right) p^{2-2s}} \tag{29}$$

whose analytic continuation is provided by the Eichler integral

$$L_5(s) = \frac{(2\pi)^s}{\Gamma(s)} \int_0^\infty f_{3,15}(\mathrm{i}y) y^{s-1} \mathrm{d}y \tag{30}$$

with critical values

$$L_5(1) = \frac{5}{\pi^2} M(1, 4, 1), \quad L_5(2) = \frac{4}{3} M(2, 3, 1). \tag{31}$$

At 4 loops, with 6 Bessel functions, the on-shell problem is solved by the weight 4 level 6 cusp form

$$f_{4,6}(z) = (\eta_1\eta_2\eta_3\eta_6)^2 = \sum_{n>0} A_6(n) q^n = \frac{f_{4,6}(-1/(6z))}{6^2 z^4}. \tag{32}$$

For $\Re s > 5/2$, there is a convergent L-series

$$L_6(s) = \sum_{n>0} \frac{A_6(n)}{n^s} = \frac{1}{1 + 2^{1-s}} \frac{1}{1 + 3^{1-s}} \prod_{p>3} \frac{1}{1 - A_6(p)p^{-s} + p^{3-2s}} \tag{33}$$

whose analytic continuation is provided by the Eichler integral

$$L_6(s) = \frac{(2\pi)^s}{\Gamma(s)} \int_0^\infty f_{4,6}(\mathrm{i}y) y^{s-1} \mathrm{d}y \tag{34}$$

with critical values

$$L_6(2) = \frac{2}{\pi^2} M(1,5,1) = \frac{2}{3} M(3,3,1), \tag{35}$$

$$L_6(1) = \frac{2}{\pi^2} M(2,4,1) = \frac{3}{\pi^2} L_6(3). \tag{36}$$

At 6 loops, with 8 Bessel functions, the on-shell problem is solved by the weight 6 level 6 cusp form

$$f_{6,6}(z) = \frac{\eta_2^9 \eta_3^9}{\eta_1^3 \eta_6^3} + \frac{\eta_1^9 \eta_6^9}{\eta_2^3 \eta_3^3} = \sum_{n>0} A_8(n) q^n = -\frac{f_{6,6}(-1/(6z))}{6^3 z^6}. \tag{37}$$

For $\Re s > 7/2$, there is a convergent L-series

$$L_8(s) = \sum_{n>0} \frac{A_8(n)}{n^s} = \frac{1}{1-2^{2-s}} \frac{1}{1+3^{2-s}} \prod_{p>3} \frac{1}{1 - A_8(p) p^{-s} + p^{5-2s}} \tag{38}$$

whose analytic continuation is provided by the Eichler integral

$$L_8(s) = \frac{(2\pi)^s}{\Gamma(s)} \int_0^\infty f_{6,6}(\mathrm{i}y) y^{s-1} \mathrm{d}y \tag{39}$$

with critical values

$$L_8(4) = \frac{4}{9\pi^2} M(1,7,1) = \frac{4}{9} M(3,5,1) = \frac{\pi^2}{9} L_8(2), \tag{40}$$

$$L_8(5) = \frac{4}{27} M(2,6,1) = \frac{2\pi^2}{21} M(4,4,1) = \frac{2\pi^2}{21} L_8(3) = \frac{\pi^4}{54} L_8(1). \tag{41}$$

2.3 *Eichler Integrals for Quasi-periods at Level 6*

In [13] Francis Brown associated a pair of periods and a pair of quasi-periods to the weight 12 level 1 modular form $\Delta(z) = \eta_1^{24}$. The periods are a pair of Eichler integrals that determine critical values of the L-series at odd and even integers. No concrete integrals were given for the quasi-periods. Rather it was asserted that numerical values may be obtained by an undeclared regularization of integrals of a weakly holomorphic modular form $\Delta'(z) = 1/q + O(q^2)$.

In the case of the level 6 modular forms that yield 4-loop and 6-loop Feynman integrals the situation is cleaner, since the periods are Eichler integrals of eta quotients, $f_{4,6}$ and $f_{6,6}$, with 4 cusps. Thus we may hope to find weakly holomorphic modular forms, $g_{4,6}$ and $g_{6,6}$, that yield quasi-periods as well defined Eichler integrals with a base-point at a cusp free of singularities. A test is provided by the condition that a 2×2 determinant formed from a pair of periods and a pair of quasi-periods should be an algebraic multiple of a power of π, as is trivially ensured for modular forms of weight 2 by Legendre's relation between pairs of complete elliptic integrals of first and second kind.

At 4 loops, we achieved this with Eichler integrals

$$\frac{D_2}{2} = \frac{M(1,5,1)}{\pi^4} = \frac{4M(1,5,3)}{\pi^4} + \frac{5E_2}{18} \tag{42}$$

$$\frac{3D_1}{5} = \frac{M(2,4,1)}{\pi^3} = \frac{4M(2,4,3)}{\pi^3} + \frac{E_1}{3} \tag{43}$$

$$\begin{bmatrix} D_s \\ E_s \end{bmatrix} = -\int_{1/\sqrt{3}}^{\infty} \begin{bmatrix} f_{4,6}\left(\frac{1+\mathrm{i}y}{2}\right) \\ g_{4,6}\left(\frac{1+\mathrm{i}y}{2}\right) \end{bmatrix} y^{s-1}\mathrm{d}y, \tag{44}$$

$$g_{4,6}(z) = \frac{(w^2-3)^2(w^4+9)}{8w^4} f_{4,6}(z) = 5q + 102q^2 + 945q^3 + O(q^4), \tag{45}$$

$$D_1E_2 - D_2E_1 = \frac{1}{24\pi^3}. \tag{46}$$

At 6 loops, it is conjecturally achieved by

$$\det \begin{bmatrix} M(1,7,1) & 32M(1,7,3) - 64M(1,7,5) \\ M(2,6,1) & 32M(2,6,3) - 64M(2,6,5) \end{bmatrix} = \frac{5\pi^6}{192}, \tag{47}$$

$$\frac{F_2}{4} = \frac{M(1,7,1)}{\pi^6} \stackrel{?}{=} \frac{32M(1,7,3) - 64M(1,7,5)}{\pi^6} + \frac{35G_2}{108}, \tag{48}$$

$$\frac{9F_1}{28} = \frac{M(2,6,1)}{\pi^5} \stackrel{?}{=} \frac{32M(2,6,3) - 64M(2,6,5)}{\pi^5} + \frac{5G_1}{12}, \tag{49}$$

$$\begin{bmatrix} F_s \\ G_s \end{bmatrix} = -\int_{1/\sqrt{3}}^{\infty} \begin{bmatrix} f_{6,6}\left(\frac{1+\mathrm{i}y}{2}\right) \\ g_{6,6}\left(\frac{1+\mathrm{i}y}{2}\right) \end{bmatrix} (3y^2-1)y^{s-1}\mathrm{d}y, \tag{50}$$

$$g_{6,6}(z) = \frac{(w^2-3)^4}{16w^4} f_{6,6}(z) = q + 36q^2 + 567q^3 + 5264q^4 + O(q^5), \tag{51}$$

$$F_1G_2 - F_2G_1 \stackrel{?}{=} \frac{1}{4\pi^5}, \tag{52}$$

where the question marks indicate unproven discoveries, checked to thousands of digits of numerical precision.

3 Rademacher Sums for Fourier Coefficients of Eta Quotients

For positive integers N, M and n, we define the Rademacher sums

$$R_{N,M}(n) = \sum_{c>0,\ \gcd(c,N)=1} \frac{2\pi I_1(4\pi\sqrt{nM/N}/c)}{\sqrt{nN/M}\,c} K(c,N,M,n) \tag{53}$$

Table 1 Eta quotients T_N/B_N of genus 0 with Fourier coefficients $R_{N,1}(n)/R_{N,1}(1)$

N	$R_{N,1}(1)$	T_N	B_N	OEIS
2	4096	η_2^{24}	η_1^{24}	A014103
3	729	η_3^{12}	η_1^{12}	A121590
4	256	η_4^{8}	η_1^{8}	A092877
5	125	η_5^{6}	η_1^{6}	A121591
6	72	$\eta_2\eta_6^{5}$	$\eta_1^{5}\eta_3$	A128638
7	49	η_7^{4}	η_1^{4}	A121593
8	32	$\eta_2^2\eta_8^{4}$	$\eta_1^{4}\eta_4^2$	A107035
9	27	η_9^{3}	η_1^{3}	A121589
10	20	$\eta_2\eta_{10}^{3}$	$\eta_1^{3}\eta_5$	A095846
12	12	$\eta_2^2\eta_3\eta_{12}^{3}$	$\eta_1^{3}\eta_4\eta_6^2$	A187100
13	13	η_{13}^{2}	η_1^{2}	A121597
16	8	$\eta_2\eta_{16}^{2}$	$\eta_1^{2}\eta_8$	A123655
18	6	$\eta_2\eta_3\eta_{18}^{2}$	$\eta_1^{2}\eta_6\eta_9$	A128129
25	5	η_{25}	η_1	A092885

as sums of Bessel functions multiplied by Kloosterman sums

$$K(c,N,M,n) = \sum_{r\in[1,c],\ \gcd(r,c)=1} \exp\left(\frac{2\pi\mathrm{i}(Mr-ns)}{c}\right)\Bigg|_{Nrs\,=\,1\ \mathrm{mod}\ c}. \tag{54}$$

In (53) the sum is over all positive integers c coprime to N. In (54) the sum is over the integers $r\in[1,c]$ coprime to c and $s\in[1,c]$ is the inverse of Nr modulo c. It follows from these definitions that $R_{N,M}(n)/M = R_{N,n}(M)/n$ and that $R_{N,M}(n) = R_{dN,dM}(n)$ for every positive integer d that divides N.

3.1 Genus 0

We found that $R_{N,1}(n)/R_{N,1}(1)$ is the coefficient of q^n in an eta quotient T_N/B_N defining an OEIS sequence in the genus 0 cases of Table 1, where the eta quotients agree with the canonical Hauptmoduln in [24, Table 8].

For $n>0$, Rademacher [27] obtained $R_{1,1}(n)$ as the coefficient of q^n of

$$j(z) = \frac{1}{\eta_1^{24}}\left(1+240\sum_{n>0}\frac{n^3q^n}{1-q^n}\right)^3 = \frac{1}{q}+744+196884q+O(q^2) \tag{55}$$

which is invariant under $z\mapsto(az+b)/(cz+d)$ with integers satisfying $ad-bc=1$.

We remark that analytic continuation of (53) to $n = 0$ gives $R_{1,1}(0) = 24$, which differs from the constant term 744 in (55). Our work concerns only the values of $R_{N,M}(n)$ for integers $n > 0$.

The congruence subgroup $\Gamma_0(N)$ is the group of Möbius transformations with $N|c$. The Hauptmodul

$$\frac{\eta_2\eta_6^5}{\eta_1^5\eta_3} = q + 5q^2 + 19q^3 + 61q^4 + 174q^5 + 455q^6 + 1112q^7 + \cdots \tag{56}$$

of $\Gamma_0(6)$ has a Fourier coefficient $R_{6,1}(n)/72 = \mathrm{A128638}(n)$, which we are now able to evaluate at large n. We found that this Fourier coefficient is odd if and only if the core (i.e. the square-free part) of n is a divisor of 6. We determined the probably prime values of $\mathrm{A128638}(n)$ for $n \in [1, 900000000]$ and found these occur at surprisingly few values of n, namely these: 2, 3, 4, 9, 32, 48, 324, 578, 864, 121032, 940896, 11723776, 88360000, 180848704, 198443569.

We remark that A128638(900000000), with 66832 decimal digits, would be rather hard to compute in the absence of a Rademacher-sum formula.

3.2 Further Examples of Integer Sequences

We found several integer sequences of the form $R_{N,M}(n)/D$, with $\gcd(N, M) = 1$, $N > M > 1$ and integer D, as for example in Table 2.

We identified some of the generating functions, as follows

$$\sum_{n>0} R_{3,2}(n)q^n = \frac{3^7\eta_3^{12}}{\eta_1^{12}}\left(8 + \frac{3^5\eta_3^{12}}{\eta_1^{12}}\right) \tag{57}$$

$$\sum_{n>0} R_{5,2}(n)q^n = \frac{5^3\eta_5^{6}}{\eta_1^{6}}\left(12 + \frac{5^3\eta_5^{6}}{\eta_1^{6}}\right) \tag{58}$$

$$\sum_{n>0} R_{7,2}(n)q^n = \frac{7^2\eta_7^{4}}{\eta_1^{4}}\left(8 + \frac{7^2\eta_7^{4}}{\eta_1^{4}}\right) \tag{59}$$

$$\sum_{n>0} R_{9,2}(n)q^n = \frac{3^4\eta_9^{3}}{\eta_1^{3}}\left(2 + \frac{3^2\eta_9^{3}}{\eta_1^{3}}\right) \tag{60}$$

$$\sum_{n>0} R_{13,2}(n)q^n = \frac{13\eta_{13}^{2}}{\eta_1^{2}}\left(4 + \frac{13\eta_{13}^{2}}{\eta_1^{2}}\right) \tag{61}$$

$$\sum_{n>0} R_{16,3}(n)q^n = 8\left(\frac{\eta_2^{18}}{\eta_1^{12}\eta_4^{6}} - 1\right). \tag{62}$$

Table 2 Examples of integer sequences $R_{N,M}(n)/D$

N	M	D	Sequence
3	2	3^7	8, 339, 6552, 82796, 790896, 6171606, 41232064, 243306300,…
4	3	2^{10}	33, 1800, 42412, 633024, 7003278, 62405984, 471069624, 3114275328,…
5	2	5^3	12, 197, 1824, 12426, 68780, 327819, 1391472, 5383270, 19289244,…
6	5	432	145, 10085, 286435, 5004925, 63619086, 642751655, 5445694040,…
7	2	7^2	8, 81, 504, 2476, 10248, 37590, 125328, 387384, 1123992, 3092369,…
8	3	2^7	9, 132, 1132, 7200, 37566, 169648, 685368, 2532096, 8688909,…
9	2	3^4	2, 15, 72, 287, 984, 3051, 8704, 23286, 58968, 142677, 331728,…
10	3	80	6, 63, 418, 2139, 9216, 35004, 120594, 384147, 1146842, 3241083,…
11	8	11^2	234, 11950, 266994, 3812019, 40551362, 348772038, 2548265460,…
12	5	72	25, 435, 4255, 30255, 174126, 859305, 3766760, 15014775, 55334545,…
13	2	13	4, 21, 72, 222, 600, 1509, 3536, 7902, 16860, 34740, 69264, 134412, …
14	5	56	17, 229, 1852, 11213, 55998, 243084, 946991, 3382221, 11242933,…
15	7	45	67, 1398, 15919, 128386, 826187, 4509396, 21688133, 94244610,…
16	3	2^5	3, 18, 76, 264, 810, 2264, 5880, 14400, 33583, 75132, 162180, 339296,…
17	3	17	5, 26, 107, 352, 1045, 2814, 7091, 16842, 38225, 83260, 175329,…
18	5	36	10, 95, 580, 2770, 11226, 40340, 132080, 401255, 1145740, 3104412,…
19	2	19	1, 4, 10, 25, 55, 116, 229, 440, 809, 1455, 2541, 4354, 7300, 12050,…

Moreover,

$$\sum_{n>0} R_{18,2}(n)q^n = 4\left(\frac{\eta_2^6\eta_3^2}{\eta_1^6\eta_6^2} - 1\right) \tag{63}$$

$$\sum_{n>0} R_{27,2}(n)q^n = 3\left(\frac{\eta_3^4}{\eta_1^3\eta_9} - 1\right) \tag{64}$$

$$\sum_{n>0} R_{32,3}(n)q^n = 4\left(\frac{\eta_2^2\eta_4^4}{\eta_1^4\eta_8^2} - 1\right) \tag{65}$$

$$\sum_{n>0} R_{36,5}(n)q^n = 6\left(\frac{\eta_2^5\eta_3^5}{\eta_1^7\eta_6^3} - 1\right) \tag{66}$$

$$\sum_{n>0} R_{48,7}(n)q^n = 6\left(\frac{\eta_2^8\eta_3^4}{\eta_1^8\eta_4^2\eta_6^2} - 1\right) \tag{67}$$

$$\sum_{n>0} R_{64,3}(n)q^n = 2\left(\frac{\eta_2\eta_4^2}{\eta_1^2\eta_8} - 1\right) \tag{68}$$

$$\sum_{n>0} R_{64,7}(n)q^n = 4\left(\frac{\eta_2^7}{\eta_1^6\eta_8} - 1\right). \tag{69}$$

When $N > 1$ has genus 0, $R_{N,M}(n)$ is an integer sequence generated by a polynomial of degree M in the eta quotient that generates $R_{N,1}(n)$. Thus, for example, we may compute the coefficient of q^n in $(\eta_{25}/\eta_1)^P$ from a linear combination of Rademacher-type formulas for $R_{25,M}(n)$ with $M \in [1, P]$, using polynomials in $g = \sum_{n>0} R_{25,1}(n)q^n = 5\eta_{25}/\eta_1$ as follows:

$$\sum_{n>0} R_{25,2}(n)q^n = 2g + g^2 \tag{70}$$

$$\sum_{n>0} R_{25,3}(n)q^n = 6g + 3g^2 + g^3 \tag{71}$$

$$\sum_{n>0} R_{25,4}(n)q^n = 12g + 10g^2 + 4g^3 + g^4 \tag{72}$$

$$\sum_{n>0} R_{25,5}(n)q^n = 25g + 25g^2 + 15g^3 + 5g^4 + g^5 = \frac{5^3\eta_5^6}{\eta_1^6} \tag{73}$$

$$\sum_{n>0} R_{25,6}(n)q^n = 42g + 60g^2 + 44g^3 + 21g^4 + 6g^5 + g^6 \tag{74}$$

$$\sum_{n>0} R_{25,7}(n)q^n = 77g + 126g^2 + 119g^3 + 70g^4 + 28g^5 + 7g^6 + g^7 \tag{75}$$

$$\sum_{n>0} R_{25,8}(n)q^n = 120g + 260g^2 + 288g^3 + 210g^4 + 104g^5 + 36g^6 + 8g^7 + g^8. \tag{76}$$

3.3 Genus 1

The genus $g_0(N)$ of $\Gamma_0(N)$ is computed in `Pari-GP` by a procedure

```
g0(N)={local(f=factor(N),t=vector(4,k,1),p,r,n);
for(k=1,matsize(f)[1],p=f[k,1];r=f[k,2];n=p^r;
t[1]*=n*(1+1/p);t[2]*=if(n==2,1,if(p%4==1,2));
t[3]*=if(n==3,1,if(p%3==1,2));
t[4]*=if(r%2,2*p^((r-1)/2),(p+1)*p^(r/2-1)));
1+t[1]/12-t[2]/4-t[3]/3-t[4]/2;}
```

that combines 4 multiplicative functions [18, 25, 31].

We conjecture that only when N has genus 0 is $R_{N,1}(n)$ an integer sequence. To deal with genus 1, we introduced the additional parameter M into $R_{N,M}(n)$. For each level N with genus 1, we specify in Table 3 the prime values of $M < 1000$, coprime to N, for which $R_{N,M}(n)$ is an integer sequence.

Table 3 Primes M such that $R_{N,M}(n)$ is an integer sequence for N with genus 1

N	primes $M < 1000$
11	19, 29, 199, 569, 809
14	5, 11, 23, 71, 101, 263, 503
15	7, 23, 31, 79, 167, 431, 479, 983
17	3, 11, 47, 359, 967
19	2, 23, 257, 449, 509, 521, 641
20	11, 131, 251, 491, 599
21	23, 31, 47, 71, 127, 367, 383, 743
24	7, 47, 191, 383, 439
27	$M = 2 \bmod 3$
32	$M = 3 \bmod 4$
36	$M = 5 \bmod 6$
49	$M = 3, 5, 6 \bmod 7$

At genus 1, the criterion for whether $R_{N,M}(n)$ forms an integer sequence is provided by the Fourier expansion of the unique weight 2 cusp form of level N, which we denote by $f_N = \sum_{M>0} C_{N,M} q^M$. Specifically,

$$f_{11} = (\eta_1\eta_{11})^2 \tag{77}$$
$$f_{14} = \eta_1\eta_2\eta_7\eta_{14} \tag{78}$$
$$f_{15} = \eta_1\eta_3\eta_5\eta_{15} \tag{79}$$
$$f_{17} = q - q^2 - q^4 - 2q^5 + 4q^7 + 3q^8 - 3q^9 + 2q^{10} - 2q^{13} + \cdots \tag{80}$$
$$f_{19} = q - 2q^3 - 2q^4 + 3q^5 - q^7 + q^9 + 3q^{11} + 4q^{12} - 4q^{13} \ldots \tag{81}$$
$$f_{20} = (\eta_2\eta_{10})^2 \tag{82}$$
$$f_{21} = q - q^2 + q^3 - q^4 - 2q^5 - q^6 - q^7 + 3q^8 + q^9 + 2q^{10} + 4q^{11} - q^{12} + \cdots \tag{83}$$
$$f_{24} = \eta_2\eta_4\eta_6\eta_{12} \tag{84}$$
$$f_{27} = (\eta_3\eta_9)^2 \tag{85}$$
$$f_{32} = (\eta_4\eta_8)^2 \tag{86}$$
$$f_{36} = \eta_6^4 \tag{87}$$
$$f_{49} = q + q^2 - q^4 - 3q^8 - 3q^9 + 4q^{11} - q^{16} - 3q^{18} + 4q^{22} \ldots \tag{88}$$

with explicit formulas for $N = 17, 19, 21, 49$ given below in (97)–(99).

For N with genus 1, we found that $R_{N,M}(n)$ is an integer sequence if and only if $C_{N,M} = 0$. Moreover

$$\overline{R}_{N,M}(n) = R_{N,M}(n) - C_{N,M}R_{N,1}(n) \tag{89}$$

is always an integer sequence, with $\overline{R}_{N,1}(n) = 0$, by construction.

Table 4 Elliptic curves E_N for N with genus 1

N	$C_{N,2}$	$C_{N,3}$	E_N
11	-2	-1	$Y^2+6XY+121Y=X^3+38X^2+363X$
14	-1	-2	$Y^2+3XY+56Y=X^3+25X^2+168X$
15	-1	-1	$Y^2+3XY+45Y=X^3+23X^2+135X$
17	-1	0	$Y^2+3XY+34Y=X^3+18X^2+85X$
19	0	-2	$Y^2+19Y=X^3+16X^2+76X$
20	0	-2	$Y^2+20Y=X^3+13X^2+60X$
21	-1	1	$Y^2+3XY+21Y=X^3+13X^2+42X$
24	0	-1	$Y^2+12Y=X^3+11X^2+36X$
27	0	0	$Y^2+9Y=X^3+9X^2+27X$
32	0	0	$Y^2+8Y=X^3+6X^2+16X$
36	0	0	$Y^2+6Y=X^3+6X^2+12X$
49	1	0	$Y^2-3XY=X^3+3X^2+7X$

With $G_{N,M}=\sum_{n>0}\overline{R}_{N,M}(n)q^n$, we found at $N=21$ that

$$7\left(\frac{\eta_3\eta_7^3}{\eta_1^3\eta_{21}}-1\right)=G_{21,2}, \tag{90}$$

$$3^3\left(\frac{\eta_3^7\eta_7}{\eta_1^7\eta_{21}}-1\right)=G_{21,4}+G_{21,3}+2G_{21,2}, \tag{91}$$

$$7^2\left(\frac{\eta_3^2\eta_7^6}{\eta_1^6\eta_{21}^2}-1\right)=G_{21,4}+2G_{21,3}+5G_{21,2}, \tag{92}$$

$$\frac{3^3 7\eta_3^4\eta_{21}^2}{\eta_1^6}=G_{21,4}-2G_{21,3}-G_{21,2}, \tag{93}$$

$$\frac{3^3 7^2\eta_3\eta_{21}^5}{\eta_1^5\eta_7}=G_{21,4}-5G_{21,3}+5G_{21,2}, \tag{94}$$

$$\frac{3^3 7\eta_3^6\eta_7^2}{\eta_1^8}=G_{21,5}-2G_{21,2}, \tag{95}$$

$$\frac{3^3 7^2\eta_3^3\eta_7\eta_{21}^3}{\eta_1^7}=G_{21,5}-3G_{21,4}+4G_{21,2}. \tag{96}$$

For each level N with genus 1, we found that $(X, Y)=(G_{N,2}, G_{N,3})$ is a point on an elliptic curve E_N specified in Table 4 and verified up to $O(q^{20000})$. Moreover $G_{N,M}=P_0(X)+P_1(X)Y$ where P_0 and P_1 are polynomials with degrees not exceeding $M/2$ and $(M-3)/2$, respectively.

With $N=21$, relations (90)–(92) show that $X=G_{21,2}$ is determined by an eta quotient and that $Y=G_{21,3}$ is determined by 3 eta quotients. The transformation $(X, Y)=(x-5, y-x-3)$ yields a minimal model $y^2+xy=x^3-4x-1$, whose small coefficients were noted in [19].

Applying the `ellak` procedure of `Pari-GP` to E_N, we reproduce the Fourier coefficients of $f_N = \sum_{M>0} C_{N,M}\, q^M$. Thanks to work recorded at OEIS, we are able to provide formulas for f_N in the 4 cases where a single eta quotient does not suffice, namely for $N = 17, 19, 21, 49$:

$$f_{17} = \eta_1\eta_{17}\,(\psi_2\phi_{17} - \psi_{34}\phi_1)\,, \quad f_{19} = (\psi_4\phi_{38} - \psi_1\psi_{19} + \psi_{76}\phi_2)^2\,, \tag{97}$$

$$f_{21} = \frac{3(\eta_7^3\eta_9^3 + \eta_1\eta_7^2\eta_9^2\eta_{63} + \eta_1^2\eta_7\eta_9\eta_{63}^2)}{2\eta_3\eta_{21}} - \frac{\eta_3^4\eta_7^2}{2\eta_1^2} + \frac{7\eta_3\eta_7\eta_{21}^3}{2\eta_1} - \frac{3\eta_3^4\eta_7\eta_{63}}{2\eta_1\eta_9}, \tag{98}$$

$$f_{49} = \theta_{7,14}^3\left(q\theta_{21,28} + q^2\theta_{14,35} - q^4\theta_{7,42}\right), \tag{99}$$

$$\psi_n = \frac{\eta_{2n}^2}{\eta_n}, \quad \phi_n = \frac{\eta_{2n}^5}{\eta_n^2\eta_{4n}^2}, \quad \theta_{a,b} = \sum_{n=-\infty}^{\infty}\left(-q^a\right)^{(n^2+n)/2}\left(-q^b\right)^{(n^2-n)/2}, \tag{100}$$

with (99) recorded in [14]. At $N = 49$, we have complex multiplication, with $C_{49,p} = 0$ for prime $p = 3, 5, 6 \bmod 7$. Moreover we have a pair of eta quotients,

$$x = \frac{\eta_{49}}{\eta_1} = \frac{G_{49,2}}{7}, \quad y = \frac{\eta_7^4}{\eta_1^4} = \frac{G_{49,7}}{7^2}, \tag{101}$$

with Fourier coefficients given by Rademacher sums. The latter is determined by $G_{49,2}$ and $G_{49,3}$. Hence the elliptic curve E_{49} provides an algebraic relation between these eta quotients, namely

$$(2y - 7x - 35x^2 - 49x^3)^2 = (4x + 21x^2 + 28x^3)(1 + 7x + 7x^2)^2. \tag{102}$$

At $N = 21$, we found 2937 eta quotients whose Fourier coefficients are linear combinations of $R_{21,M}(n)$ with $M \le 50$. Including the unit quotient, the tally of 2938 is the coefficient of x^{50} in the generating function

$$T_{21}(x) = \frac{1 - x + x^2 - x^3 + 2x^4}{(1-x)^2(1-x^4)^2} \tag{103}$$

which predicts a total of 22126 eta quotients with Fourier coefficients determined by $R_{21,M}(n)$ for $M \le 100$. We have identified all of these.

At $N = 36$, with 9 divisors, the corresponding tallies of eta quotients are spectacularly large. Using Padé approximants, the generating function was found to be

$$T_{36}(x) = \frac{H(x) + x^{18}H(1/x)}{(1-x)^4(1-x^3)^2(1-x^4)^2(1-x^{12})}, \tag{104}$$

$$H(x) = 1 - 3x + 6x^2 - 3x^3 + 6x^4 + x^5 + x^6 + 4x^7 + 4x^8 + x^9, \tag{105}$$

giving 49307076 eta quotients with Fourier coefficients determined by $R_{36,M}(n)$ for $M \le 50$ and 8204657877 for $M \le 100$. We were able to identify all of these, by taking products of 78 eta quotients found at $M \le 12$ and eliminating redundancies.

Using more refined methods, we also validated the monstrous tally of 180919436828 for $M \leq 150$.

From the denominator of $T_{36}(x) = \sum_{n\geq 0}(c(M)+1)x^M$ it is clear that the number $c(M)$ of non-trivial eta quotients determined by our procedures may be found by polynomial interpolation at integers with the same residue modulo 12. We denote the result by $c(M) = p(M) + q_r(M)/12$ for $M = r \bmod 12$, with a leading polynomial

$$p(n) = \frac{(n+1)(n+3)(n+5)(n+7)(n+9)(n+11)((n+6)^2-7)}{1935360} - 1 \quad (106)$$

of degree 8 and sub-dominant terms that are at most quadratic:

$$q_0(n) = q_3(n) + q_4(n) + 5, \quad (107)$$

$$q_1(n) = q_5(n) = q_7(n) = q_{11}(n) = 0, \quad (108)$$

$$q_2(n) = q_{10}(n) = \frac{2(n+6)^2-5}{512}, \quad (109)$$

$$q_3(n) = q_9(n) = \frac{(n+3)(n+9)}{9}, \quad (110)$$

$$q_4(n) = q_8(n) = q_2(n) + \frac{(n+4)(n+8)}{16}, \quad (111)$$

$$q_6(n) = q_2(n) + q_3(n) + 1. \quad (112)$$

The situation at the prime levels $N = 11, 17, 19$ is rather different. Here we have a wealth of Rademacher sums but only one eta quotient. Consider the case $N = 19$. Since $f_{19} = q + O(q^3)$, we have $C_{19,2} = 0$ and hence $R_{19,2}(n)$ yields integers. As noted, the sequence $R_{19,2}(n)/19$ begins with

$$1, 4, 10, 25, 55, 116, 229, 440, 809, 1455, 2541, 4354, 7300, 12050, \ldots$$

This sequence may be developed using η_{19}^4/η_1^4, which is determined by $G_{19,2}$ and $G_{19,3}$. The elliptic curve relating the latter pair gives an algebraic relation between $G_{19,2}$ and the eta quotient, namely

$$s^3/e_{19} = 1 + 8s + 19e_{19}, \quad s = G_{19,2}/19, \quad e_{19} = \eta_{19}^4/\eta_1^4, \quad (113)$$

from which the expansion of $s = q + O(q^2)$ is easy developed, iteratively.

Similarly, at $N = 11$ and $N = 17$ we obtain the algebraic relations

$$t^5/e_{11} = 1 + 13t + 34t^2 + 11^2 e_{11}, \quad t = G_{11,2}/11^2, \quad e_{11} = \eta_{11}^{12}/\eta_1^{12}, \quad (114)$$

$$u^4/e_{17} = 16 + 64u + 34u^2 - 17^2 e_{17}, \quad u = G_{17,2}/17, \quad e_{17} = \eta_{17}^6/\eta_1^6, \quad (115)$$

and hence develop the expansions of $t = q + O(q^2)$ and $u = 2q + O(q^2)$.

Intermediate between the plethora of eta quotients at $N = 36$, with 9 divisors, and their relative scarcity at $N = 11, 17, 19, 49$, with less than 4 divisors, sit the remaining genus 1 levels, $N = 14, 15, 20, 21, 24, 27, 32$. Proceeding as for $N = 21$, we found the generating functions

$$T_{14}(x) = \frac{1 + x^3 + 2x^4 + x^6 + x^7}{(1-x)(1-x^2)(1-x^3)(1-x^6)}, \tag{116}$$

$$T_{15}(x) = T_{21}(x) = \frac{1 - x + x^2 - x^3 + 2x^4}{(1-x)^2(1-x^4)^2}, \tag{117}$$

$$T_{20}(x) = \frac{1 - x + x^2 + 4x^3 + 2x^4 + 3x^6 + x^7 + x^8}{(1-x)^2(1-x^2)^2(1-x^3)(1-x^6)}, \tag{118}$$

$$T_{24}(x) = \frac{(1+x^3)\left(h(x) + x^6 h(1/x)\right)}{(1-x)^3(1-x^2)^3(1-x^4)^2}, \quad h(x) = 1 - 2x + 3x^2 + 2x^3, \tag{119}$$

$$T_{27}(x) = \frac{1 - x^{11}}{(1-x)(1-x^2)(1-x^3)(1-x^5)(1-x^6)}, \tag{120}$$

$$T_{32}(x) = \frac{1 - x + x^2 + 2x^3 + x^4 - x^5 + x^6}{(1-x)^2(1-x^2)^2(1-x^4)^2}, \tag{121}$$

with the coefficient of x^m in $T_N(x)$ giving the number of eta quotients whose Fourier coefficients are determined by linear combinations of the Rademacher sums $R_{N,M}(n)$ with $M \leq m$.

3.4 Rational Rademacher Sums

There are 5 levels with genus greater than 0 for which it appears that the Rademacher sums $R_{N,M}(n)$ are rational for all positive integers M and n, namely $N = 27, 32, 36, 49$ with genus 1 and $N = 64$ with genus 3. At genus 1, we convert these rationals to the integers

$$\overline{R}_{N,M}(n) = R_{N,M}(n) - C_{N,M} R_{N,1}(n), \tag{122}$$

which vanish at $M = 1$. The rationals $R_{64,M}(n)$ do not form integer sequences for $M = 1, 2, 5 \bmod 8$. To remedy this, we define

$$g_{8k+r} = \sum_{n>0} \left(R_{64,8k+r}(n) - c_{k,r} R_{64,r}(n)\right) q^n, \tag{123}$$

$$c_{k,1} = C_{32,8k+1}, \quad c_{k,2} = C_{32,4k+1}, \quad c_{k,5} = -C_{32,8k+5}/2, \tag{124}$$

with $k \geq 0$, $r \in [1, 8]$ and $c_{k,r} = 0$ for $r = 3, 4, 6, 7, 8$. Then g_M has integer Fourier coefficients, which vanish for $M = 1, 2, 5$. Eta quotients appear in

$$\frac{g_3}{2} = \frac{\eta_2 \eta_4^2}{\eta_1^2 \eta_8} - 1, \quad \frac{g_4}{8} = \frac{\eta_2 \eta_{16}^2}{\eta_1^2 \eta_8}, \quad \frac{g_6}{4} = \frac{\eta_2^2 \eta_4^4}{\eta_1^4 \eta_8^2} - 1, \quad \frac{g_7}{4} = \frac{\eta_2^7}{\eta_1^6 \eta_8} - 1, \quad \frac{g_8}{32} = \frac{\eta_2^2 \eta_8^4}{\eta_1^4 \eta_4^2}. \tag{125}$$

Moreover, $g_6 = (4 + g_3)g_3$, $g_7 = 2g_3 + (2 + g_3)g_4$, $g_8 = (4 + g_4)g_4$.

We found that $(X, Y) = (g_3 + 2, g_4 + 2)$ is a point on the genus 3 curve

$$Y(Y^2 + 4) = X^4 \tag{126}$$

and that $g_M = P_0(X) + P_1(X)Y + P_2(X)Y^2$, with P_n a polynomial of degree at most $\lfloor (M - 4n)/3 \rfloor$. Every eta quotient of that form has Fourier coefficients that are linear combinations of Rademacher sums at $N = 64$.

3.5 Genus 2

It is instructive to compare the genus 3 case $N = 64$ with the genus 2 case $N = 50$. For the latter we construct integer sequences as follows:

$$\overline{R}_{50,M}(n) = \begin{cases} R_{50,M}(n) - d(M)R_{50,1}(n), & \text{for } M = 1, 4 \bmod 5, \\ R_{50,M}(n) + d(M)R_{50,2}(n), & \text{for } M = 2, 3 \bmod 5, \\ R_{50,M}(n), & \text{for } M = 0 \bmod 5, \end{cases} \tag{127}$$

$$\sum_{M>0} d(M)q^M = f_{50} = q - q^2 + q^3 + q^4 - q^6 + 2q^7 - q^8 - 2q^9 + O(q^{11}), \tag{128}$$

where f_{50} is the weight 2 level 50 Hecke eigenform whose Fourier coefficients $d(M)$ are obtained from the L-series of the elliptic curve $y(y + x + 1) = x^3 - x - 2$. Then $G_{50,M} = \sum_{n>0} \overline{R}_{50,M}(n)q^n$ vanishes by construction at $M = 1, 2$ and yields eta quotients at $M = 3, 5$, with

$$\frac{G_{50,3}}{5} = \frac{\eta_2\eta_{25}^2}{\eta_1^2\eta_{50}} - 1, \quad \frac{G_{50,5}}{20} = \frac{\eta_2\eta_{10}^3}{\eta_1^3\eta_5}. \tag{129}$$

The Fourier coefficients of $G_{50,4}$ are also identified by an eta quotient: $\overline{R}_{50,4}(n)/10$ is the coefficient of q^{2n} in the Fourier expansion of η_{25}/η_1.

We found that $(X, Y) = (G_{50,3}, G_{50,4})$ is a point on the curve

$$Y^3 + 4(X + 5)Y^2 + 2(X + 5)(X + 10)Y = X(X + 5)(X^2 + 8X + 20) \tag{130}$$

which `Sage` confirmed as having genus 2.

Proceeding similarly for $(X, Y) = (G_{N,3}, G_{N,4})$ we found the curves

$$Y^3 + 55Y^2 - 2(X^2 + 11X - 484)Y = X(X^3 + 34X^2 + 473X + 2904) \tag{131}$$

$$Y^3 + 2(4X + 69)Y^2 + (9X^2 + 460X + 4761)Y = X(X^3 + 55X^2 + 1035X + 6348) \tag{132}$$

$$Y^3 + 8(X + 13)Y^2 + 4(X + 13)(3X + 52)Y = X(X + 13)(X^2 + 28X + 208) \tag{133}$$

$$Y^3 + 21Y^2 + (5X^2 + 70X + 392)Y = X(X + 14)(X^2 + 14X + 56) \tag{134}$$

$$Y^3+2(2X+29)Y^2-(4X^2-58X-841)Y=X(X^3+31X^2+406X+1682) \quad (135)$$
$$Y^3+2(4X+31)Y^2+(11X^2+217X+961)Y=X(X^3+31X^2+310X+961) \quad (136)$$
$$Y^3-8XY^2-X(2X+259)Y=X(X^3-10X^2+148X+1369) \quad (137)$$

at $N = 22, 23, 26, 28, 29, 31, 37$, respectively. All have genus 2.

3.6 Genus 3

We found these genus 3 curves for $N = 30, 33, 34, 35, 39, 40, 41, 43, 45, 48, 64$:

$$\begin{aligned}&Y^2(Y-2X)(Y-3X)+X(7X^2-30X+75)Y\\&=X^5+25X(4X-5),\ \text{with } (X,Y)=(G_{30,4}+5, G_{30,5}+10),\end{aligned} \quad (138)$$
$$\begin{aligned}&Y^4+X(5X-11)Y^2-X^2(4X-11)Y\\&=X^3(X^2-11X+22),\ \text{with } (X,Y)=(G_{33,4}+11, G_{33,5}+11),\end{aligned} \quad (139)$$
$$\begin{aligned}&Y^4+10XY^3+X(21X-221)Y^2+2X(3X^2-119X+867)Y\\&=X(X^4-2X^3+51X^2-578X+4913),\ \text{with } (X,Y)=(G_{34,4}+17, G_{34,5}+17),\end{aligned} \quad (140)$$
$$\begin{aligned}&Y^4+10(X-3)Y^3+(31X^2-210X+800)Y^2+(12X^3+25X^2+200X-2000)Y\\&=X(X^4-5X^3-15X^2-200X-2000),\ \text{with } (X,Y)=(G_{35,4}+20, G_{35,5}+10),\end{aligned} \quad (141)$$
$$\begin{aligned}&Y^4+5XY^3+3X(X+13)Y^2-X(19X^2-234X+507)Y\\&=X(X^4-14X^3+234X^2-1690X+2197),\ \text{with } (X,Y)=(G_{39,4}+13, G_{39,5}+13),\end{aligned} \quad (142)$$
$$Y^4=X(X+5)(X^2(X+4)-4Y^2),\ \text{with } (X,Y)=(G_{40,4}, G_{40,5}), \quad (143)$$
$$\begin{aligned}&Y^4+(10X-41)Y^3+X(30X-451)Y^2+X^2(11X-1681)Y\\&=X^3(X^2+70X+2214),\ \text{with } (X,Y)=(G_{41,4}, G_{41,5}+41),\end{aligned} \quad (144)$$
$$\begin{aligned}&32Y^4+(40X+43)Y^3+(94X^2+1591X+9245)Y^2+X(49X^2+946X+5547)Y\\&=X^3(X^2+21X+129),\ \text{with } (X,Y)=(G_{43,3}, G_{43,5}-2G_{43,3}),\end{aligned} \quad (145)$$
$$(Y^2+5X)^2=X^3(X^2-Y),\ \text{with } (X,Y)=(G_{45,4}+5, G_{45,5}+5), \quad (146)$$
$$Y^4=X^3(X-3)(X-4),\ \text{with } (X,Y)=(G_{48,4}+6, G_{48,5}+6), \quad (147)$$
$$Y(Y^2+4)=X^4,\ \text{with } (X,Y)=(G_{64,3}+2, G_{64,4}+2), \quad (148)$$

where the final curve at $N = 64$ was already given in (126) and was obtained by subtractions that make $G_{64,M}$ vanish at $M = 1, 2, 5$. At $N = 43$, the subtractions make $G_{43,M}$ vanish at $M = 1, 2, 4$. In all other cases with genus 3, $G_{N,M}$ vanishes for $M = 1, 2, 3$.

3.7 Genus 4

At $N = 81$, we found that $(X, Y) = (G_{81,5}, G_{81,6})$ lies on the genus 4 curve

$$Y^3(Y+3)^2 + 3(X+3)^3(Y+3)(2Y+3) = (X+3)^6, \quad \frac{Y}{3} = \frac{\eta_3^4}{\eta_1^3\eta_9} - 1. \tag{149}$$

The Fourier coefficients of $X/9$ form an integer sequence beginning with

$$1, 2, 4, 7, 13, 21, 35, 55, 87, 132, 200, 295, 434, 625, 897, 1267, 1782, 2475, \ldots$$

for $n = 1$ to 18. The general term is given by Rademacher sums as

$$\frac{R_{81,5}(n) + R_{81,2}(n)}{9} = \frac{\exp(4\pi\sqrt{5n}/9)}{27(4n^3/5)^{1/4}}\left(1 - \frac{27}{32\pi\sqrt{5n}} + O(1/n)\right). \tag{150}$$

The Fourier coefficients of $Y/9$ form an integer sequence beginning with

$$1, 3, 6, 13, 24, 45, 77, 132, 216, 351, 552, 861, 1313, 1986, 2952, 4354, 6336, \ldots$$

for $n = 1$ to 17. The general term is given by a Rademacher sum

$$\frac{R_{81,6}(n)}{9} = \frac{\exp(4\pi\sqrt{6n}/9)}{27(2n^3/3)^{1/4}}\left(1 - \frac{27}{32\pi\sqrt{6n}} + O(1/n)\right). \tag{151}$$

3.8 Genus 5

At $N = 72$, with genus 5, we obtain integer Fourier coefficients in

$$G_{72,M} = \sum_{n>0} \overline{R}_{72,M}(n)q^n, \quad \overline{R}_{72,M}(n) = R_{72,M}(n) - \sum_{r=1,2,3,5,7} p_r(M)R_{72,r}(n), \tag{152}$$

$$\eta_{12}^2\eta_{18}^4/\eta_{36}^2 = \sum_{n>0} p_1(n)q^n, \quad \eta_{12}^4 = \sum_{n>0} p_2(n)q^n, \quad \eta_6\eta_{12}\eta_{18}\eta_{36} = \sum_{n>0} p_3(n)q^n, \tag{153}$$

$$\eta_6^2\eta_{36}^4/\eta_{18}^2 = \sum_{n>0} p_5(n)q^n, \quad \eta_6^4 = \sum_{n>0} \left(p_1(n) - 4p_7(n)\right)q^n. \tag{154}$$

Then $G_{72,M}$ vanishes for $M = 1, 2, 3, 5, 7$. Moreover $(G_{72,4},\ G_{72,6})$ is a point on the elliptic curve E_{36}, while $(G_{72,6},\ G_{72,9})$ lies on E_{24}. Eliminating $G_{72,6}$, we obtain a genus 5 curve from the resultant:

$$\left(Y^2+12Y+34-2(X+2)^3\right)^2=\left((X+2)^3+1\right)\left((X+2)^3-2\right)^2, \quad (155)$$

$$X=G_{72,4}=\frac{6\eta_2\eta_3\eta_{18}^2}{\eta_1^2\eta_6\eta_9}, \quad Y=G_{72,9}=\frac{6\eta_2^5\eta_3^2\eta_6}{\eta_1^6\eta_4\eta_{12}}-6. \quad (156)$$

The Fourier coefficients of $X/6$ are the integers $R_{18,1}(n)/6 = \mathrm{A}128129(n)$. The Fourier coefficients of $Y/12$ form an integer sequence beginning with

3, 11, 33, 87, 210, 473, 1008, 2055, 4035, 7674, 14196, 25629, 45282, 78472, ...

for $n=1$ to 14. The general term is given by Rademacher sums as

$$\frac{R_{24,3}(n)+R_{24,1}(n)}{12}=\frac{\exp(\pi\sqrt{2n})}{24(2n^3)^{1/4}}\left(1-\frac{3}{8\pi\sqrt{2n}}+O(1/n)\right). \quad (157)$$

3.9 Genus 6

Moving on to the genus 6 case $N=121$, we determined that subtractions of $R_{121,r}(n)$ are needed for the 6 values $r=1,2,3,4,6,11$. The coefficients of these subtractions are determined by four new forms and two old forms of weight 2 and level 121. The new forms are the L-series of the elliptic curves $y^2+xy+y=x^3+x^2-30x-76$, $y^2+y=x^3-x^2-7x+10$, $y^2+xy=x^3+x^2-2x-7$ and $y^2+y=x^3-x^2-40x-221$. The old forms are $(\eta_1\eta_{11})^2$ and $(\eta_{11}\eta_{121})^2$. The first two non-zero integer series are

$$\overline{R}_{121,5}(n)=R_{121,5}(n)-R_{121,4}(n)-R_{121,3}(n), \quad \overline{R}_{121,7}(n)=R_{121,7}(n)+R_{121,6}(n). \quad (158)$$

We expect their generators, $G_{121,5}$ and $G_{121,7}$, to define a curve of genus 6 with degree 7 in $G_{121,5}$ and degree 5 in $G_{121,7}$. This is indeed the case. We found that $(X,Y)=(G_{121,5}/11, G_{121,7}/11)$ is a point on the curve

$$\begin{aligned}Y^5-20XY^4+5X(10X-9)Y^3 &= X(132X^3-64X^2-33X+31)Y^2\\ &+X(33X^4+95X^3-48X^2-5X+9)Y\\ &+X(121X^6-66X^5+23X^4+18X^3-9X^2+1)\end{aligned} \quad (159)$$

which `Sage` confirmed as having genus 6. Since integer combinations of Rademacher sums are computable with ease, we are able to validate this curve up to $O(q^{1000})$ in a matter of seconds.

3.10 Genus 7

In the genus 7 case $N = 100$, we determined that subtractions of $R_{100,r}(n)$ are required for the 7 values $r = 1, 2, 3, 4, 5, 7, 9$, with coefficients determined by 6 old forms of weight 2 and level 100 and a new form

$$f_{100} = q + 2q^3 - 2q^7 + q^9 - 2q^{13} + 6q^{17} - 4q^{19} - 4q^{21} - 6q^{23} - 4q^{27} + 6q^{29} + O(q^{31}) \tag{160}$$

which is the L-series of the elliptic curve $y^2 = x^3 - x^2 - 33x + 62$.

We found that $(X, Y) = (G_{100,6} + 5, G_{100,15} + 10)$ lies on the genus 7 curve

$$\begin{aligned} Y^6 &= X(3X^4 - 90X^3 + 415X^2 - 560X + 200)Y^4 \\ &- X(3X^9 + 20X^8 - 350X^7 + 1795X^6 - 4790X^5 \\ &+ 7805X^4 - 8350X^3 + 7325X^2 - 4625X + 1375)Y^2 \\ &+X(X^2 + 2X+5)(X^4 - 6X^3 + 14X^2 - 10X + 5)^2(X^4 - 5X^3 + 15X^2 - 25X + 25), \end{aligned} \tag{161}$$

with $X/5 = \eta_2\eta_{25}^2/(\eta_1^2\eta_{50})$ and the Fourier coefficients of $Y/10$ given by

$$1, 6, 26, 88, 258, 686, 1688, 3904, 8594, 18142, 36946, 72952, 140184, 262948, \ldots$$

for $n = 0$ to 13, and in general by $(R_{100,15}(n) + 2R_{100,5}(n))/10$ for $n > 0$.

3.11 Genus 8

When $N = p^2$ with prime $p = 12k + 1$, the genus of $\Gamma_0(N)$ is given by $g_0(N) = 3k(4k - 1) - 1$. Setting $k = 1$, we obtain $g_0(169) = 8$. Moreover $N = 169$ is the largest level with genus 8. We devised a procedure of 8 subtractions that gives integer sequences $\overline{R}_{169,M}(n)$ by subtracting multiples of $R_{169,r}(n)$, with $r = 1, 2, 3, 4, 5, 6, 8, 9$. The subtraction coefficients are determined by 8 modular forms of level 169 and weight 2, of which two have Fourier coefficients in $\mathbf{Q}(\sqrt{3})$. The rest have coefficients in the cubic number fields $x(x^2 - 1) = \pm(1 - 2x^2)$.

Our first non-zero integer sequence occurs at $M = 7$, where

$$\overline{R}_{169,7}(n) = R_{169,7}(n) - R_{169,6}(n) - R_{169,5}(n) + R_{169,2}(n) \tag{162}$$

is the coefficient of q^n in $G_{169,7} = 13\eta_{169}/\eta_1$. There is no subtraction at $M = 13$, where $G_{169,13} = G_{13,1} = 13\eta_{13}^2/\eta_1^2$.

We found that $(X, Y) = (G_{169,7}/13, G_{169,13}/13)$ is point on a genus 8 curve with degree 13 in X and degree 7 in Y, namely

$$Y^7 = 143XY^6 + 156X(39X^2 - 17X + 3)Y^5 + X\sum_{k=2}^{6} P_k(X)Y^{6-k}, \tag{163}$$

$$P_2(X) = 26(3211X^4 - 2249X^3 + 819X^2 - 173X + 19), \tag{164}$$

$$P_3(X) = 26(21970X^6 - 18759X^5 + 8619X^4 - 2743X^3 + 663X^2 - 111X + 10), \tag{165}$$

$$P_4(X) = 26(169X^4 - 104X^3 + 39X^2 - 8X + 1)(507X^4 - 169X^3 + 26X^2 - 13X + 3), \tag{166}$$

$$\begin{aligned} P_5(X) = 13(&371293X^{10} - 371293X^9 + 199927X^8 - 81289X^7 \\ &+ 28561X^6 - 8619X^5 + 2197X^4 - 481X^3 + 91X^2 - 13X + 1), \end{aligned} \tag{167}$$

$$\begin{aligned} P_6(X) = &4826809X^{12} - 4826809X^{11} + 2599051X^{10} - 1113879X^9 + 428415X^8 \\ &- 142805X^7 + 41743X^6 - 10985X^5 + 2535X^4 - 507X^3 + 91X^2 - 13X + 1. \end{aligned} \tag{168}$$

3.12 Genus 13

Finally, we studied $N = 144$, with genus 13. Integer sequences are obtained after subtractions at $r = 1, 2, 3, 4, 5, 6, 7, 9, 10, 11, 13, 14, 19$, with coefficients determined by 11 old forms and two new forms. The old forms were already encountered as eta quotients at $N = 48$ and $N = 72$. They determine the subtractions for $R_{144,M}(n)$ when M is divisible by 3 or 2. The new forms relate to the subtractions that are needed when M is coprime to 6. One of these new forms is the eta quotient

$$f_{144a} = \frac{\eta_{12}^{12}}{\eta_4^6\eta_{24}^4} = q + 4q^7 + 2q^{13} - 8q^{19} - 5q^{25} + 4q^{31} + \cdots \tag{169}$$

The other has Fourier coefficients determined by the L-series of the elliptic curve $y^2 = x^3 + 6x + 7$, which gives

$$f_{144b} = q + 2q^5 + 4q^{11} - 2q^{13} - 2q^{17} + 4q^{19} - 8q^{23} - q^{25} - 6q^{29} - 8q^{31} + \ldots \tag{170}$$

We reduced this to a telling combination of 5 eta quotients with weight 2:

$$f_{144b} = \frac{\eta_{24}^3\eta_{36}^2\eta_{72}}{\eta_{48}\eta_{144}} + \frac{2\eta_{12}\eta_{24}^2\eta_{72}^4}{\eta_{36}\eta_{48}\eta_{144}} + \frac{4\eta_{12}^2\eta_{48}\eta_{72}\eta_{144}}{\eta_{24}} - \frac{2\eta_{12}\eta_{24}^3\eta_{72}\eta_{144}^2}{\eta_{36}\eta_{48}^2} + \frac{4\eta_{12}^2\eta_{144}^4}{\eta_{72}^2} \tag{171}$$

with $C_1(M) + 2C_5(M) + 4C_{11}(M) - 2C_{13}(M) + 4C_{19}(M)$ giving the coefficient of q^M in (171), where $C_r(M)R_{144,r}(n)$ is subtracted from $R_{144,M}(n)$ to make $\overline{R}_{144,M}(n)$ an integer sequence. The subtraction at $r = 7$ is determined by the eta quotient in (169) where the coefficient of q^M is $C_1(M) + 4C_7(M) + 2C_{13}(M) - 8C_{19}(M)$. Hence we determine all the subtractions by eta quotients.

We are left with 6 values of $M < 20$ for which $G_{144,M} = \sum_{n>0} \overline{R}_{144,M}(n)q^n$ is non-zero, namely $M = 8, 12, 15, 16, 17, 18$. To produce a genus 13 curve we should choose a coprime pair of M values. The simplest choice is the pair (8, 15). We know that $(G_{144,8}, G_{144,18}) = (G_{72,4}, G_{72,9})$ gives a point on the genus 5 curve (155) found at $N = 72$. Moreover $(G_{144,15}, G_{144,18}) = (G_{48,5}, G_{48,6})$ gives a point on a genus 3 curve that is not hard to determine. Then, by taking a resultant to eliminate $G_{144,18}$, we determined that $(X, Y) = (G_{144,8} + 2, G_{144,15} + 6)$ lies on the genus 13 curve

$$(Y^4 - 8(X^3 + 1)^2)^2 = (X^3 + 1)(X^6 + 20X^3 - 8)^2 \tag{172}$$

neatly parametrized by eta quotients as follows

$$\frac{X}{2} = \frac{\eta_2^3\eta_3}{\eta_1^3\eta_6}, \quad \frac{Y}{6} = \frac{\eta_2^2\eta_6^4}{\eta_1^4\eta_{12}^2}. \tag{173}$$

3.13 Remarks

Remark 1. After we completed this work, Yajun Zhou kindly called our attention to [17, Theorem 8.12]. The methods used there may be capable of furnishing proofs of some of our empirical findings in Sect. 3, following the approach that Knopp [22] attributes to Rademacher [28] as an "entirely fresh viewpoint", namely by adopting formulas (53), (54) as definitions of Fourier coefficients of objects $G_{N,M}$ and demonstrating that the latter have the required modular properties. At genus 0, with a unique Hauptmodul, that could furnish a proof of Table 1. At higher genera, more work might be needed.

Remark 2. We conclude this section with a note on the approach in [32, 33] to modular curves. In [33, Section 4.1], Yifan Yang gives modular curves, up to level $N = 50$, that are parametrized by quotients of "generalized" Dedekind eta functions [32], in the many cases where the eta function itself is insufficient to solve the problem. Moreover his q-expansions are highly singular as $q \to 0$. Our approach was quite different. We began with an explicit formula (53) that reproduces, at $M = 1$, the Fourier coefficients of the genus 0 eta quotients taken as "canonical" Hauptmoduln in [24, Table 8], which vanish as $q \to 0$. At genus 1, after subtraction of the non-integer sequence $R_{N,1}(n)$, we obtained $G_{N,M} = \sum_{n>0} \overline{R}_{N,M}(n)q^n$ as Fourier series with integer coefficients, vanishing at $q = 0$. Then $G_{N,2}$ and $G_{N,3}$ parametrize our modular curve. We were able to extend this to higher genera. It may be that our explicit Fourier coefficients are capable of reproducing those of Yang's "generalized" Dedekind eta quotients, after performing a Fricke involution $z \longmapsto -1/(Nz)$ on his Ansätze. We have not investigated this, since it lay outside the remit of our title.

4 Conclusions

1. Eta quotients on $\Gamma_0(6)$, with 4 cusps, neatly solve the equal-mass two and three loop sunrise problems, whose differential equations with respect to the external energy have 4 singular points. This cannot continue, since at higher loops there is more than one pseudo-threshold.
2. Atkin–Lehner transformations on $\Gamma_0(6)$ yield optimal nomes.

3. For the on-shell problem, Eichler integrals of eta quotients on $\Gamma_0(6)$ yield Bessel moments at 4 and 6 loops that are periods or quasi-periods.
4. Rademacher sums yield the Fourier coefficients of a Hauptmodul for $\Gamma_0(6)$ and for all other levels of genus 0.
5. After subtractions determined by weight 2 cusp forms, they yield the Fourier coefficients of vast numbers of eta quotients.
6. They yield the Fourier coefficients of parametrizations of modular curves, irrespective of whether the Fourier series are eta quotients.

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On a Class of Feynman Integrals Evaluating to Iterated Integrals of Modular Forms

Luise Adams and Stefan Weinzierl

Abstract In this talk we discuss a class of Feynman integrals, which can be expressed to all orders in the dimensional regularisation parameter as iterated integrals of modular forms. We review the mathematical prerequisites related to elliptic curves and modular forms. Feynman integrals, which evaluate to iterated integrals of modular forms go beyond the class of multiple polylogarithms. Nevertheless, we may bring for all examples considered the associated system of differential equations by a non-algebraic transformation to an ε-form, which makes a solution in terms of iterated integrals immediate.

1 Introduction

It is an open and interesting question to which class of transcendental functions Feynman integrals evaluate. At present, we do not have a general answer. However, there are sub-classes of Feynman integrals for which the class of functions is known. First of all, there is the class of Feynman integrals evaluating to multiple polylogarithms. This covers in particular all one-loop integrals. Starting from two-loops, there are Feynman integrals which cannot be expressed in terms of multiple polylogarithms. The simplest example is given by the two-loop equal-mass sunrise integral [1–20]. Integrals, which do not evaluate to multiple polylogarithms are now an active field of research in particle physics [21–42] and string theory [43–48]. In this talk we focus on a class of Feynman integrals which evaluate to iterated integrals of modular forms. Feynman integrals of this class are associated to one elliptic curve and depend on one scale $x = p^2/m^2$. They can be seen as generalisations of single-scale Feynman integrals evaluating to harmonic polylogarithms [49, 50]. We expect that all our

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examples are equally well expressible in terms of elliptic polylogarithms [14–17, 21, 23, 37–40, 51–56]. The representation in terms of iterated integrals of modular forms has certain advantages:

1. It combines nicely with the technique of differential equations, which by now is the main tool for solving Feynman integrals [57–67]. In fact, for all examples considered we are able to bring the system of differential equations into an ε-form.
2. It only involves a finite number of integration kernels. The integration kernels are modular forms.
3. It allows for an efficient numerical evaluation through the q-expansion around the cusps [25].

Let us also mention, that albeit an important sub-class, this class is not the end of the story. Multi-scale integrals beyond the class of multiple polylogarithms may involve more than one elliptic curve, as seen for example in the double box integral relevant to top-pair production with a closed top loop [27, 28].

2 Periodic Functions and Periods

Let us consider a non-constant meromorphic function f of a complex variable z. A period ω of the function f is a constant such that

$$f(z+\omega) = f(z) \tag{1}$$

for all z. The set of all periods of f forms a lattice Λ, which is either

1. trivial: $\Lambda = \{0\}$,
2. a simple lattice, generated by one period $\omega : \Lambda = \{n\omega \mid n \in \mathbb{Z}\}$,
3. a double lattice, generated by two periods ω_1, ω_2 with $\mathrm{Im}(\omega_2/\omega_1) \neq 0$:

$$\Lambda = \{n_1\omega_1 + n_2\omega_2 \mid n_1, n_2 \in \mathbb{Z}\}. \tag{2}$$

It is common practice to order these two periods such that $\mathrm{Im}(\omega_2/\omega_1) > 0$.

An example for a singly periodic function is given by

$$\exp(z)\,. \tag{3}$$

In this case the simple lattice is generated by $\omega = 2\pi i$. An example for a doubly periodic function is given by Weierstrass's $\wp$-function. Let Λ be the lattice generated by ω_1 and ω_2 Then

$$\wp(z) = \frac{1}{z^2} + \sum_{\omega\in\Lambda\backslash\{0\}} \left(\frac{1}{(z+\omega)^2} - \frac{1}{\omega^2} \right). \tag{4}$$

$\wp(z)$ is periodic with periods ω_1 and ω_2. Of particular interest are also the corresponding inverse functions. These are in general multivalued functions. In the case of the exponential function $x = \exp(z)$, the inverse function is given by

$$z = \ln(x). \tag{5}$$

The inverse function to Weierstrass's elliptic function $x = \wp(z)$ is an elliptic integral given by

$$z = \int_x^\infty \frac{dt}{\sqrt{4t^3 - g_2 t - g_3}} \tag{6}$$

with

$$g_2 = 60 \sum_{\omega \in \Lambda \backslash \{0\}} \frac{1}{\omega^4}, \qquad g_3 = 140 \sum_{\omega \in \Lambda \backslash \{0\}} \frac{1}{\omega^6}. \tag{7}$$

In both examples the periods can be expressed as integrals involving only algebraic functions. For the first example we may express the period of the exponential function as

$$2\pi i = 4i \int_0^1 \frac{dt}{\sqrt{1-t^2}}. \tag{8}$$

For the second example of Weierstrass's $\wp$-function let us assume that g_2 and g_3 are two given algebraic numbers. The periods are expressed as

$$\omega_1 = 2 \int_{t_1}^{t_2} \frac{dt}{\sqrt{4t^3 - g_2 t - g_3}}, \qquad \omega_2 = 2 \int_{t_3}^{t_2} \frac{dt}{\sqrt{4t^3 - g_2 t - g_3}}, \tag{9}$$

where t_1, t_2 and t_3 are the roots of the cubic equation $4t^3 - g_2 t - g_3 = 0$.

The representation of the periods of $\exp(z)$ and $\wp(z)$ in the form of Eqs. (8) and (9) is the motivation for the following generalisation, due to Kontsevich and Zagier [68]:

A numerical period is a complex number whose real and imaginary parts are values of absolutely convergent integrals of rational functions with rational coefficients, over domains in $\mathbb{R}^n$ given by polynomial inequalities with rational coefficients. Domains defined by polynomial inequalities with rational coefficients are called semi-algebraic sets.

We denote the set of numerical periods by $\mathbb{P}$. The numerical periods $\mathbb{P}$ are a countable set of numbers. We may replace in the above definition every occurrence of "rational function" with "algebraic function" and every occurrence of "rational number" with "algebraic number" without changing the set of numbers $\mathbb{P}$. Then it is clear, that the integrals in Eqs. (8) and (9) are numerical periods in the sense of the above definition, and so is for example ln 2, since

$$\ln 2 = \int_1^2 \frac{dt}{t}. \tag{10}$$

3 Elliptic Curves

A double lattice Λ arises naturally from elliptic curves. Let us consider the elliptic curve

$$E : w^2 - (z - z_1)(z - z_2)(z - z_3)(z - z_4) = 0, \tag{11}$$

where the roots z_j may depend on variables $x = (x_1, \ldots, x_t)$:

$$z_j = z_j(x), \qquad j \in \{1, 2, 3, 4\}. \tag{12}$$

We set

$$Z_1 = (z_3 - z_2)(z_4 - z_1), \quad Z_2 = (z_2 - z_1)(z_4 - z_3), \quad Z_3 = (z_3 - z_1)(z_4 - z_2). \tag{13}$$

Note that we have $Z_1 + Z_2 = Z_3$. We define the modulus and the complementary modulus of the elliptic curve E by

$$k^2 = \frac{Z_1}{Z_3}, \qquad \bar{k}^2 = 1 - k^2 = \frac{Z_2}{Z_3}. \tag{14}$$

Note that there are six possibilities of defining k^2. Our standard choice for the periods ψ_1, ψ_2 is

$$\psi_1 = \frac{4K(k)}{Z_3^{\frac{1}{2}}}, \quad \psi_2 = \frac{4iK\left(\bar{k}\right)}{Z_3^{\frac{1}{2}}}, \tag{15}$$

where $K(x)$ denotes the complete elliptic integral of the first kind. These two periods generate a lattice $\Lambda = \{n_1\psi_1 + n_2\psi_2 \mid n_1, n_2 \in \mathbb{Z}\}$. We denote the ratio of the two periods and the nome squared by

$$\tau = \frac{\psi_2}{\psi_1}, \qquad q = e^{2i\pi\tau}. \tag{16}$$

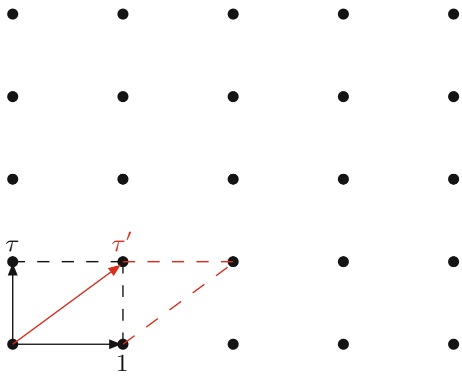

Fig. 1 The periods $(1, \tau)$ and $(1, \tau')$ generate the same lattice

Let us note that our choice of periods is not unique. Any other choice related to the original one by

$$\begin{pmatrix} \psi_2' \\ \psi_1' \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \psi_2 \\ \psi_1 \end{pmatrix}, \qquad \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}(2, \mathbb{Z}) \tag{17}$$

generates the same lattice Λ. This is shown in Fig. 1. In terms of τ and $\tau' = \psi_2'/\psi_1'$ the transformation in Eq. (17) reads

$$\tau' = \frac{a\tau + b}{c\tau + d} \tag{18}$$

and equals a Möbius transformation. In this talk we are in particular interested in the situation, where the roots z_j in Eq. (12) depend only on a single variable x. In this case we may exchange the variable x for the variable τ and study our problem as a function of τ.

4 Modular Forms

Let us now consider functions of τ. We are interested in functions with "nice" properties under transformations of the form as in Eq. (18). We denote by $\mathbb{H} = \{ \tau \in \mathbb{C} \mid \mathrm{Im}(\tau) > 0 \}$ the complex upper half plane and by $\overline{\mathbb{H}}$ the extended upper half plane

$$\overline{\mathbb{H}} = \mathbb{H} \cup \{\infty\} \cup \mathbb{Q}. \tag{19}$$

A meromorphic function $f : \mathbb{H} \to \mathbb{C}$ is a modular form of modular weight k for $\mathrm{SL}(2, \mathbb{Z})$ if

(i) f transforms under Möbius transformations as

$$f\left(\frac{a\tau+b}{c\tau+d}\right) = (c\tau+d)^k \cdot f(\tau) \qquad \text{for} \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}\,(2,\mathbb{Z}) \tag{20}$$

(ii) f is holomorphic on $\mathbb{H}$,
(iii) f is holomorphic at ∞.

We may also look at subgroups of $\mathrm{SL}\,(2,\mathbb{Z})$. The standard congruence subgroups are defined by

$$\begin{aligned} \Gamma_0(N) &= \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}\,(2,\mathbb{Z}) : c \equiv 0 \bmod N \right\}, \\ \Gamma_1(N) &= \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}\,(2,\mathbb{Z}) : a, d \equiv 1 \bmod N, \;\; c \equiv 0 \bmod N \right\}, \\ \Gamma(N) &= \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}\,(2,\mathbb{Z}) : a, d \equiv 1 \bmod N, \;\; b, c \equiv 0 \bmod N \right\}. \end{aligned} \tag{21}$$

Let us also introduce the following notation: For an integer k and a matrix $\gamma \in \mathrm{SL}\,(2,\mathbb{Z})$ we define $f|_k\gamma$ by

$$(f|_k\gamma)(\tau) = (c\tau+d)^{-k} \cdot f(\gamma(\tau)). \tag{22}$$

With this definition we may re-write the condition (i) in Eq. (20) as

$$f|_k\gamma = f \qquad \text{for all} \;\; \gamma \in \mathrm{SL}\,(2,\mathbb{Z})\,. \tag{23}$$

We may now define modular forms for a congruence subgroup Γ of $\mathrm{SL}\,(2,\mathbb{Z})$. A meromorphic function $f : \mathbb{H} \to \mathbb{C}$ is a modular form of modular weight k for Γ if

(i) f transforms as

$$f|_k\gamma = f \qquad \text{for all} \;\; \gamma \in \Gamma. \tag{24}$$

(ii) f is holomorphic on $\mathbb{H}$,
(iii) $f|_k\alpha$ is holomorphic at ∞ for all $\alpha \in \mathrm{SL}\,(2,\mathbb{Z})$.

For each congruence subgroup Γ of $\mathrm{SL}\,(2,\mathbb{Z})$ there is a smallest positive integer N, such that $\Gamma(N) \subseteq \Gamma$. The integer N is called the level of Γ. A modular form f for the congruence subgroup Γ of level N has the Fourier expansion

$$f(\tau) = \sum_{n=0}^{\infty} a_n q_N^n \qquad \text{with} \qquad q_N = e^{2\pi i\tau/N}. \tag{25}$$

f is called a cusp form, if $a_0 = 0$ in the Fourier expansion of $f|_k\alpha$ for all $\alpha \in \mathrm{SL}\,(2,\mathbb{Z})$.

5 Iterated Integrals

We review Chen's definition of iterated integrals [69]: Let M be a t-dimensional manifold and

$$\gamma : [0, 1] \to M \tag{26}$$

a path with start point $x_i = \gamma(0)$ and end point $x_f = \gamma(1)$. Suppose further that $\omega_1, \dots, \omega_k$ are differential 1-forms on M. Let us write

$$f_j(\lambda)\, d\lambda = \gamma^* \omega_j \tag{27}$$

for the pull-backs to the interval [0, 1]. For $\lambda \in [0, 1]$ the k-fold iterated integral of $\omega_1, \dots, \omega_k$ along the path γ is defined by

$$I_\gamma(\omega_1, \dots, \omega_k; \lambda) = \int\limits_0^\lambda d\lambda_1 f_1(\lambda_1) \int\limits_0^{\lambda_1} d\lambda_2 f_2(\lambda_2) \dots \int\limits_0^{\lambda_{k-1}} d\lambda_k f_k(\lambda_k). \tag{28}$$

We define the 0-fold iterated integral to be

$$I_\gamma(; \lambda) = 1. \tag{29}$$

We have

$$\frac{d}{d\lambda} I_\gamma(\omega_1, \omega_2, \dots, \omega_k; \lambda) = f_1(\lambda)\; I_\gamma(\omega_2, \dots, \omega_k; \lambda). \tag{30}$$

Let us now discuss two special cases: Multiple polylogarithms and iterated integrals of modular forms. Multiple polylogarithms are iterated integrals, where all differential one-forms are of the form

$$\gamma^* \omega_j = \frac{d\lambda}{\lambda - z_j}. \tag{31}$$

For $z_w \neq 0$ they are defined by [70–74]

$$G(z_1, \dots, z_w; y) = \int\limits_0^y \frac{dy_1}{y_1 - z_1} \int\limits_0^{y_1} \frac{dy_2}{y_2 - z_2} \dots \int\limits_0^{y_{w-1}} \frac{dy_w}{y_w - z_w}. \tag{32}$$

The number w is referred to as the weight of the multiple polylogarithm or the depth of the integral representation. Let us introduce the short-hand notation

$$G_{m_1, \dots, m_k}(z_1, \dots, z_k; y) = G(\underbrace{0, \dots, 0}_{m_1 - 1}, z_1, \dots, z_{k-1}, \underbrace{0 \dots, 0}_{m_k - 1}, z_k; y), \tag{33}$$

where all z_j for $j = 1, \dots, k$ are assumed to be non-zero. This allows us to relate the integral representation of the multiple polylogarithms to the sum representation of the multiple polylogarithms. The sum representation is defined by

$$\mathrm{Li}_{m_1,\dots,m_k}(x_1, \dots, x_k) = \sum_{n_1>n_2>\dots>n_k>0}^{\infty} \frac{x_1^{n_1}}{{n_1}^{m_1}} \dots \frac{x_k^{n_k}}{{n_k}^{m_k}}. \tag{34}$$

The number k is referred to as the depth of the sum representation of the multiple polylogarithm, the weight is now given by $m_1 + m_2 + \cdots m_k$. The relations between the two representations are given by

$$\begin{aligned} \mathrm{Li}_{m_1,\dots,m_k}(x_1, \dots, x_k) &= (-1)^k G_{m_1,\dots,m_k}\left(\frac{1}{x_1}, \frac{1}{x_1 x_2}, \dots, \frac{1}{x_1 \dots x_k}; 1\right), \\ G_{m_1,\dots,m_k}(z_1, \dots, z_k; y) &= (-1)^k \mathrm{Li}_{m_1,\dots,m_k}\left(\frac{y}{z_1}, \frac{z_1}{z_2}, \dots, \frac{z_{k-1}}{z_k}\right). \end{aligned} \tag{35}$$

If one further sets $g(z; y) = 1/(y - z)$, then one has

$$\frac{d}{dy} G(z_1, \dots, z_w; y) = g(z_1; y) G(z_2, \dots, z_w; y) \tag{36}$$

and

$$G(z_1, z_2, \dots, z_w; y) = \int_0^y dy_1 \; g(z_1; y_1) G(z_2, \dots, z_w; y_1). \tag{37}$$

One can slightly enlarge the set of multiple polylogarithms and define $G(0, \dots, 0; y)$ with w zeros for z_1 to z_w to be

$$G(0, \dots, 0; y) = \frac{1}{w!} (\ln y)^w . \tag{38}$$

This permits us to allow trailing zeros in the sequence $(z_1, \dots, z_w)$ by defining the function G with trailing zeros via Eqs. (37) and (38).

Our second example are iterated integrals of modular forms. Let $f_1(\tau)$, $f_2(\tau), \dots, f_k(\tau)$ be modular forms of a congruence subgroup. Let us further assume that $f_k(\tau)$ vanishes at the cusp $\tau = i\infty$. For iterated integrals of modular forms we set

$$\omega_j = 2\pi i \;\; f_j(\tau) \;\, d\tau. \tag{39}$$

Thus the k-fold iterated integral of modular forms is given by

$$(2\pi i)^k \int_{i\infty}^{\tau} d\tau_1 \;\, f_1(\tau_1) \int_{i\infty}^{\tau_1} d\tau_2 \;\, f_2(\tau_2) \dots \int_{i\infty}^{\tau_{k-1}} d\tau_k \;\, f_k(\tau_k) \, . \tag{40}$$

The case where $f_k(\tau)$ does not vanishes at the cusp $\tau = i\infty$ is discussed in [24, 75] and is similar to trailing zeros in the case of multiple polylogarithms.

6 Precision Calculations

Due to the smallness of all coupling constants g, we may compute at high energies an infrared-safe observable (for example the cross section σ for a particular process) reliable in perturbation theory:

$$\sigma = \left(\frac{g}{4\pi}\right)^4 \sigma_{LO} + \left(\frac{g}{4\pi}\right)^6 \sigma_{NLO} + \left(\frac{g}{4\pi}\right)^8 \sigma_{NNLO} + \cdots \tag{41}$$

The cross section is related to the square of the scattering amplitude

$$\sigma \sim |\mathscr{A}|^2, \tag{42}$$

and the perturbative expansion of the cross section follows from the perturbative expansion of the amplitude

$$\mathscr{A} = g^2 \mathscr{A}^{(0)} + g^4 \mathscr{A}^{(1)} + g^6 \mathscr{A}^{(2)} + \ldots, \tag{43}$$

where $\mathscr{A}^{(l)}$ contains l loops. The computation of the tree amplitude $\mathscr{A}^{(0)}$ poses no conceptional problem. For loop amplitudes we have to calculate Feynman integrals. Let us write

$$\mathscr{A}^{(l)} = \sum_j c_j I_j, \tag{44}$$

where the I_j's are Feynman integrals and the c_j's are coefficients, whose computation is tree-like. Without loss of generality we may take the set of Feynman integrals $\{I_1, I_2, \ldots\}$ to consist of scalar integrals [76, 77]. Let us now look closer on the Feynman integrals. A Feynman graph G with n external lines, r internal lines and l loops corresponds (up to prefactors) in D space-time dimensions to the family of Feynman integrals, indexed by the powers of the propagators ν_j

$$I^G_{\nu_1 \nu_2 \ldots \nu_r} = \frac{\prod\limits_{j=1}^{r} \Gamma(\nu_j)}{\Gamma(\nu - lD/2)} \left(\mu^2\right)^{\nu - lD/2} \int \prod_{s=1}^{l} \frac{d^D k_s}{i\pi^{\frac{D}{2}}} \prod_{j=1}^{r} \frac{1}{(-q_j^2 + m_j^2)^{\nu_j}}, \tag{45}$$

with $\nu = \nu_1 + \cdots + \nu_r$. The momenta flowing through the internal lines can be expressed through the independent loop momenta $k_1, \ldots, k_l$ and the external momenta $p_1, \ldots, p_n$ as

$$q_i = \sum_{j=1}^{l} \lambda_{ij} k_j + \sum_{j=1}^{n} \sigma_{ij} p_j, \qquad \lambda_{ij}, \sigma_{ij} \in \{-1, 0, 1\}. \tag{46}$$

After Feynman parametrisation we obtain

$$I^G_{\nu_1 \nu_2 \ldots \nu_r} = \int_{\Delta} \Omega \left(\prod_{j=1}^{r} x_j^{\nu_j - 1} \right) \frac{\mathcal{U}^{\nu-(l+1)D/2}}{\mathcal{F}^{\nu - lD/2}}. \tag{47}$$

The prefactors in the definition of the Feynman integral in Eq. (45) are chosen such that after Feynman parametrisation we obtain an expression without prefactors, as can be seen from Eq. (47). In Eq. (47) the integration is over

$$\Delta = \left\{ [x_1 : x_2 : \ldots : x_r] \in \mathbb{P}^{r-1} | x_i \geq 0 \right\}. \tag{48}$$

Here, $\mathbb{P}^{r-1}$ denotes the real projective space with $r-1$ dimensions. Ω is a differential $(r-1)$-form given by

$$\Omega = \sum_{j=1}^{r} (-1)^{j-1} \, x_j \; dx_1 \wedge \ldots \wedge \widehat{dx_j} \wedge \ldots \wedge dx_r, \tag{49}$$

where the hat indicates that the corresponding term is omitted. The functions $\mathcal{U}$ and $\mathcal{F}$ are obtained from first writing

$$\sum_{j=1}^{r} x_j (-q_j^2 + m_j^2) = -\sum_{a=1}^{l} \sum_{b=1}^{l} k_a M_{ab} k_b + \sum_{a=1}^{l} 2k_a \cdot Q_a - J, \tag{50}$$

where M is a $l \times l$ matrix with scalar entries and Q is a l-vector with D-vectors as entries. We then have

$$\mathcal{U} = \det(M), \quad \mathcal{F} = \det(M) \left(-J + Q M^{-1} Q \right) / \mu^2. \tag{51}$$

$\mathcal{U}$ and $\mathcal{F}$ are the first and second graph polynomial of the Feynman graph G [78].

The Feynman integral defined in Eq. (47) has an expansion as a Laurent series in the parameter $\varepsilon = (4-D)/2$ of dimensional regularisation:

$$I^G_{\nu_1 \nu_2 \ldots \nu_r} = \sum_{j=j_{\min}}^{\infty} f_j \varepsilon^j. \tag{52}$$

The coefficients f_j are in general functions of the Lorentz invariants

$$s_J = \left(\sum_{j \in J} p_j \right)^2, \tag{53}$$

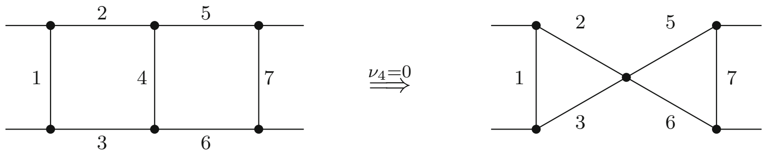

Fig. 2 If for some exponent we have $\nu_j = 0$, the corresponding propagator is absent and the topology simplifies

where the sum runs over a subset J of the external momenta, the internal masses m_i and the scale μ. We are interested in the question, to which class of functions the coefficients f_j belong. Let us first consider the situation, where we keep all Lorentz invariants, all masses and the scale fixed. Suppose that (i) all kinematical invariants s_J are negative or zero, (ii) all masses m_i and μ are positive or zero ($\mu \neq 0$) and (iii) all ratios of invariants and masses are rational, then it can be shown that all coefficients f_j in Eq. (52) are numerical periods [79].

Let us now return to the original problem and view the coefficients f_j as functions of the Lorentz invariants s_J, the internal masses m_i and the scale μ. Let us consider a family of Feynman integrals $I^G_{\nu_1\nu_2\dots\nu_r}$, including all its sub-topologies. A sub-topology G' is obtained by pinching in the graph G one or several internal lines. In the Feynman integral the corresponding propagators are then absent and the associated exponents ν_j are zero. This is shown in Fig. 2. Integration-by-parts identities [80, 81] allow us to express the Feynman integrals from the family $I^G_{\nu_1\nu_2\dots\nu_r}$ as a linear combination of a few master integrals, which we denote by $I = \{I_1, \dots, I_N\}$. Let us further denote by $x = (x_1, \dots, x_t)$ the vector of kinematic variables the master integrals depend on. The method of differential equations [57–65, 67] is a powerful tool to find the functions f_j in Eq. (52). Let x_k be a kinematic variable. Carrying out the derivative $\partial I_i / \partial x_k$ under the integral sign and using integration-by-parts identities allows us to express the derivative as a linear combination of the master integrals:

$$\frac{\partial}{\partial x_k} I_i + \sum_{j=1}^{N} a_{ij} I_j = 0. \tag{54}$$

Repeating the above procedure for every master integral and every kinematic variable we obtain a system of differential equations of Fuchsian type

$$(d + A)\, I = 0, \tag{55}$$

where A is a matrix-valued one-form

$$A = \sum_{i=1}^{t} A_i dx_i. \tag{56}$$

The matrix-valued one-form A satisfies the integrability condition $dA + A \wedge A = 0$.

Geometrically we have a vector bundle with a flat connection: The base space is parametrised by the coordinates $x = (x_1, \dots, x_t)$, the fibre is a N-dimensional vector space with basis $I = (I_1, \dots, I_N)$, the flat connection is given by A and called the Gauß–Manin connection.

Suppose A is of the form

$$A = \varepsilon \sum_j C_j \, d \ln p_j(x), \tag{57}$$

where all ε-dependence is in the prefactor, the C_j's are matrices with constant entries and the $p_j(x)$'s are polynomials in the external variables x, then the system of differential equations is easily solved in terms of multiple polylogarithms [63].

In this talk we consider the situation, where the master integrals depend only on a single variable τ and the connection one-form A is of the form

$$A = \varepsilon \sum_j F_j \; (2\pi i) \; d\tau, \tag{58}$$

where as before all ε-dependence is in the prefactor and the F_j's are matrices, whose entries are modular forms. In this case the system of differential equations is easily solved in terms of iterated integrals of modular forms.

A system of differential equations, where the only ε-dependence is in a prefactor like in Eq. (57) or Eq. (58) is said to be in ε-form. Clearly, it is advantageous to have the system in ε-form. There are two operations at our disposal to transform a system of differential equations, which follow from the geometric picture described above: We may change the variables in the base manifold and/or we may change the basis of the vectorspace in the fibre. A change of variables in the base manifold introduces a Jacobian: If $\tau' = \gamma(\tau)$ (for simplicity we consider the case where the base manifold is one-dimensional) we have

$$A' = A \, \frac{\partial \tau'}{\partial \tau}. \tag{59}$$

A change of the basis of the vectorspace in the fibre

$$I' = U I \tag{60}$$

transforms the connection into

$$A' = U A U^{-1} + U d U^{-1}. \tag{61}$$

7 Picard–Fuchs Operators

An extremely helpful tool for Feynman integral computations within the approach based on differential equations are the factorisation properties of Picard–Fuchs operators [66]. Let us consider an (unknown) function $f(\lambda)$ of a single variable λ, which obeys a (known) homogeneous differential equation of order r

$$\sum_{j=0}^{r} p_j(\lambda) \frac{d^j}{d\lambda^j} f(\lambda) = 0, \tag{62}$$

where the p_j's are polynomials in λ, such that the differential equation is of Fuchsian type. We call the differential operator

$$L = \sum_{j=0}^{r} p_j(\lambda) \frac{d^j}{d\lambda^j} \tag{63}$$

a Picard–Fuchs operator. Suppose that this operator factorises into linear factors:

$$L = \left(a_r(\lambda) \frac{d}{d\lambda} + b_r(\lambda) \right) \dots \left(a_2(\lambda) \frac{d}{d\lambda} + b_2(\lambda) \right) \left(a_1(\lambda) \frac{d}{d\lambda} + b_1(\lambda) \right). \tag{64}$$

Such a differential equation is easily solved. Let us denote the homogeneous solution of the jth factor by

$$\psi_j(\lambda) = \exp\left(- \int\limits_0^{\lambda} d\kappa \, \frac{b_j(\kappa)}{a_j(\kappa)} \right). \tag{65}$$

Then the full solution is given by iterated integrals as

$$\begin{aligned} f(\lambda) = & \; C_1 \psi_1(\lambda) + C_2 \psi_1(\lambda) \int\limits_0^{\lambda} d\lambda_1 \frac{\psi_2(\lambda_1)}{a_1(\lambda_1)\psi_1(\lambda_1)} \\ & + C_3 \psi_1(\lambda) \int\limits_0^{\lambda} d\lambda_1 \frac{\psi_2(\lambda_1)}{a_1(\lambda_1)\psi_1(\lambda_1)} \int\limits_0^{\lambda_1} d\lambda_2 \frac{\psi_3(\lambda_2)}{a_2(\lambda_2)\psi_2(\lambda_2)} + \cdots \end{aligned} \tag{66}$$

From Eq. (36) we see that multiple polylogarithms are of this form, i.e. have Picard–Fuchs operators, which factorise into linear factors.

The next more complicated situation is the case, where the Picard–Fuchs operator contains one irreducible second-order differential operator

$$a_j(\lambda) \frac{d^2}{d\lambda^2} + b_j(\lambda) \frac{d}{d\lambda} + c_j(\lambda). \tag{67}$$

As an example consider the differential equation

$$\left[\lambda \left(1 - \lambda^2\right) \frac{d^2}{d\lambda^2} + \left(1 - 3\lambda^2\right) \frac{d}{d\lambda} - \lambda \right] f(\lambda) = 0 \tag{68}$$

This second-order differential operator is irreducible. The solutions of the differential equation are $K(\lambda)$ and $K(\sqrt{1-\lambda^2})$, where $K(\lambda)$ is the complete elliptic integral of the first kind:

$$K(\lambda) = \int_0^1 \frac{dx}{\sqrt{\left(1-x^2\right)\left(1-\lambda^2 x^2\right)}}. \tag{69}$$

Let us now return to a system of differential equations as in Eq. (55). In general, such a system may depend on several kinematic variables $x = (x_1, \dots, x_t)$. We may reduce a multi-scale system to a single-scale system by setting $x_i(\lambda) = \alpha_i \lambda$ with $\alpha = [\alpha_1 : \dots : \alpha_t] \in \mathbb{CP}^{t-1}$ and by viewing the master integrals as functions of λ. For the derivative with respect to λ we have

$$\frac{d}{d\lambda} I = B I, \qquad B = \sum_{i=1}^{t} \alpha_i A_i. \tag{70}$$

In addition we may assume that the ε-dependence of the matrices A and B is polynomial, if this is not the case, a rescaling of the master integrals with ε-dependent prefactors will achieve this situation. Let us write

$$B = B^{(0)} + \sum_{j>0} \varepsilon^j B^{(j)}. \tag{71}$$

A system of ordinary first-order differential equations is easily converted to a higher-order differential equation for a single master integral. We may work modulo sub-topologies, therefore the order of the differential equation is given by the number N_s of master integrals in this sector. In order to find the required transformation we work in addition modulo ε-corrections, i.e. we focus on $B^{(0)}$. Let I be one of the master integrals $\{I_1, \dots, I_{N_s}\}$. We determine the largest number r, such that the matrix which expresses I, $(d/d\lambda)I, \dots, (d/d\lambda)^{r-1}I$ in terms of the original set $\{I_1, \dots, I_{N_s}\}$ has full rank. It follows that $(d/d\lambda)^r I$ can be written as a linear combination of $I, \dots, (d/d\lambda)^{r-1}I$. This defines the Picard–Fuchs operator L for the master integral I with respect to λ:

$$L I = 0, \qquad L = \sum_{k=0}^{r} p_k(\lambda) \frac{d^k}{d\lambda^k}. \tag{72}$$

L is easily found by transforming to a basis which contains $I, \dots, (d/d\lambda)^{r-1}I$. Although the Picard–Fuchs operator is a differential operator of order r, it is very often the case that this operator factorises. The factorisation can be obtained with standard algorithms [82]. Let us write for the factorisation into irreducible factors

$$L = L_1 L_2 \dots L_s, \tag{73}$$

where the differential operators L_i are irreducible. Since we started from the ε-independent matrix $B^{(0)}$, the differential operators L_i are ε-independent.

8 Feynman Integrals Evaluating to Iterated Integrals of Modular Forms

Let us now consider a few examples. We consider the Feynman integrals shown in Fig. 3. These are two-loop two-point or three-point integrals, depending on a single dimensionless variable

$$x = \frac{p^2}{m^2}. \tag{74}$$

All examples shown in Fig. 3 contain the equal-mass sunrise graph as a subtopology and are – as we will see – expressible in terms of iterated integrals of modular forms. In order to proceed we would like to

1. verify that the integrals depend only on a single elliptic curve,
2. identify the elliptic curve,
3. change the variable of the base manifold from x to the modular parameter τ,
4. change the basis of master integrals such that the transformed system of differential equations is in ε-form.

These steps can be done systematically. Let us start with the first step. In order to verify that the integrals depend only on a single elliptic curve we construct for all integrals (including all sub-topologies) the Picard–Fuchs operators as described in the previous section. We recall that for a specific integral we work modulo sub-topologies and modulo ε-corrections. We then look at the factorisations of the various Picard–Fuchs operators and verify, that there is only one second-order irreducible factor. All other factors are first order. The irreducible second-order differential operator is associated with the sunrise graph.

In the second step we identify the elliptic curve. For the sunrise graph this can be done either from the maximal cuts [83–89] or from the Feynman parameter representation. The former method generalises easily to more complicated Feynman integrals [27, 28] and we discuss it here. One finds for the sunrise integral in two space-time dimensions

$$\text{MaxCut}_{\mathscr{C}}\ I = \frac{u}{\pi^2} \int\limits_{\mathscr{C}} \frac{dz}{z^{\frac{1}{2}} \left(z+4\right)^{\frac{1}{2}} \left[z^2 + 2\left(1+x\right)z + \left(1-x\right)^2\right]^{\frac{1}{2}}}, \tag{75}$$

where u is an (irrelevant) phase and $\mathscr{C}$ an integration contour. The denominator of the integrand defines an elliptic curve, which we denote by E_x:

$$E_x : w^2 - z\left(z+4\right)\left[z^2 + 2\left(1+x\right)z + \left(1-x\right)^2\right] \;=\; 0. \tag{76}$$

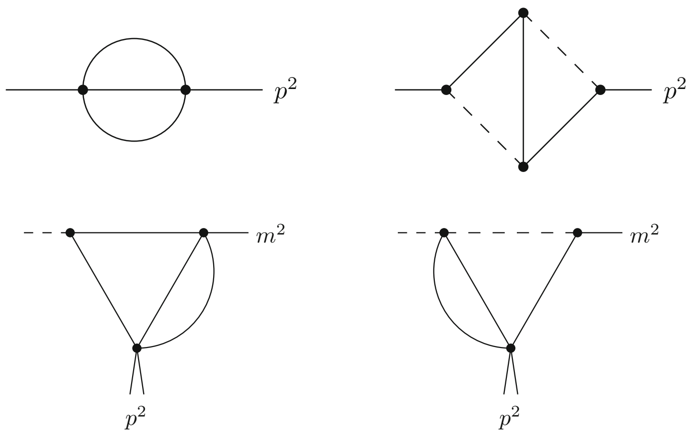

Fig. 3 Examples of Feynman integrals evaluating to iterated integrals of modular forms. Internal solid lines correspond to a propagator with mass m^2, internal dashed lines to a massless propagator. External dashed lines indicate a light-like external momentum

We denote the roots of the quartic polynomial in Eq. (76) by

$$z_1 = -4, \quad z_2 = -\left(1+\sqrt{x}\right)^2, \quad z_3 = -\left(1-\sqrt{x}\right)^2, \quad z_4 = 0. \tag{77}$$

We consider a neighbourhood of $x = 0$ without the branch cut of $\sqrt{x}$ along the negative real axis. The correct physical value is specified by Feynman's $i\delta$-prescription: $x \to x + i\delta$. The periods ψ_1, ψ_2 and the modular parameter τ are then defined by Eqs. (15) and (16), respectively.

In the third step we change the variable of the base manifold from x to the modular parameter τ. We recall that τ as a function of x is given by Eq. (16):

$$\tau = \frac{\psi_2}{\psi_1}. \tag{78}$$

In a neighbourhood of $x = 0$ we may invert Eq. (78). This gives

$$x = 9\frac{\eta\left(6\tau\right)^8 \eta\left(\tau\right)^4}{\eta\left(2\tau\right)^8 \eta\left(3\tau\right)^4}, \tag{79}$$

where η denotes Dedekind's eta-function. For the Jacobian we have

$$\frac{d\tau}{dx} = \frac{W}{\psi_1^2}, \tag{80}$$

where the Wronskian W is given by

$$W = \psi_1 \frac{d}{dx}\psi_2 - \psi_2 \frac{d}{dx}\psi_1 \quad = \quad -\frac{6\pi i}{x\,(x-1)\,(x-9)}. \tag{81}$$

In the fourth step we change the basis of master integrals such that the transformed system of differential equations is in ε-form. The essential new ingredient is the appropriate definition of the master integrals corresponding to the second-order irreducible differential operator. We need two master integrals for this case. The first master integral may be taken as the sunrise integral in $D = 2 - 2\varepsilon$ space-time dimensions divided by the ε^0-term of its maximal cut. This is familiar from the case of Feynman integrals, which evaluate to multiple polylogarithms. The difference lies in the fact, that for Feynman integrals, which evaluate to multiple polylogarithms, the maximal cut is an algebraic function, while in the case of the sunrise integral it is given by a complete elliptic integral. We thus set

$$I_1 = \varepsilon^2 \frac{\pi}{\psi_1} S_{111}\,(2-2\varepsilon, x)\,, \tag{82}$$

where $S_{111}(2-2\varepsilon, x)$ denotes the sunrise integral in $D = 2 - 2\varepsilon$ space-time dimensions with $\nu_1 = \nu_2 = \nu_3 = 1$. Let us turn to the second master integral: It is well-known in mathematics, that the first cohomology group for a family of elliptic curves E_x, parametrised by x, is generated by the holomorphic one form dz/w and its x-derivative. This motivates an ansatz, consisting of I_1 and its τ-derivative. One finds for the second master integral in the elliptic sector

$$I_2 = \frac{1}{\varepsilon}\frac{1}{2\pi i}\frac{d}{d\tau} I_1 + \frac{1}{24}\left(3x^2 - 10x - 9\right)\frac{\psi_1^2}{\pi^2} I_1. \tag{83}$$

The full set of master integrals is completed by transforming in addition the master integrals in the non-elliptic sectors. The entries on the diagonal of the transformation matrix for the non-elliptic sectors can be read off from the linear factors appearing in the factorisation of the Picard–Fuchs operators [66]. The non-diagonal entries are obtained from an ansatz along the lines of [90, 91].

Let us look at a specific example. We denote the two-loop tadpole integral by

$$I_0 = 4\varepsilon^2 S_{110}\,(2-2\varepsilon, x)\,. \tag{84}$$

Then we have for $I = (I_0, I_1, I_2)$

$$\frac{1}{2\pi i}\frac{d}{d\tau} I = \varepsilon\ A\ I, \tag{85}$$

where the matrix A is ε-independent and is given by

$$A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -f_2 & 1 \\ \frac{1}{4}f_3 & f_4 & -f_2 \end{pmatrix}. \tag{86}$$

The entries of A are given by

$$
\begin{aligned}
f_2 &= \frac{1}{2i\pi} \frac{\psi_1^2}{W} \frac{\left(3x^2 - 10x - 9\right)}{2x\,(x-1)\,(x-9)}, \\
f_3 &= \frac{\psi_1^3}{4\pi W^2}\ \frac{6}{x\,(x-1)\,(x-9)}, \\
f_4 &= \frac{1}{576} \frac{\psi_1^4}{\pi^4}\ (x+3)^4 .
\end{aligned} \tag{87}
$$

One checks that f_2, f_3 and f_4 are modular forms of $\Gamma_1(6)$ of modular weight 2, 3 and 4, respectively. We introduce a basis $\{e_1, e_2\}$ for the modular forms of modular weight 1 for the Eisenstein subspace $\mathcal{E}_1(\Gamma_1(6))$:

$$
e_1 \;=\; E_1\left(\tau; \chi_0, \chi_1\right), \;\; e_2 \;=\; E_1\left(2\tau; \chi_0, \chi_1\right), \tag{88}
$$

where $E_1(\tau, \chi_0, \chi_1)$ and $E_1(2\tau, \chi_0, \chi_1)$ are generalised Eisenstein series [92] and χ_0 and χ_1 denote primitive Dirichlet characters with conductors 1 and 3, respectively. The integration kernels may be expressed as polynomials in e_1 and e_2:

$$
\begin{aligned}
f_2 &= -6\left(e_1^2 + 6e_1e_2 - 4e_2^2\right), \\
f_3 &= 36\sqrt{3}\left(e_1^3 - e_1^2e_2 - 4e_1e_2^2 + 4e_2^3\right), \\
f_4 &= 324e_1^4.
\end{aligned} \tag{89}
$$

The solution for these Feynman integrals in terms of iterated integrals of modular forms follows now directly from the differential equation (85). The q-expansion of the iterated integrals provides an efficient method for the numerical evaluation [25, 93].

Let us close this paragraph with the observation that the integration kernels

$$
\omega_0 \;=\; \frac{dx}{x}, \qquad \omega_0 \;=\; \frac{dx}{x-1} \tag{90}
$$

may also be expressed as modular forms:

$$
\omega_0 \;=\; g_{2,0}\; 2\pi i\; d\tau, \qquad \omega_0 \;=\; g_{2,1}\; 2\pi i\; d\tau. \tag{91}
$$

The modular forms $g_{2,0}$ and $g_{2,1}$, both of modular weight 2, are given by

$$
\begin{aligned}
g_{2,0} &= \frac{1}{2i\pi} \frac{\psi_1^2}{W} \frac{1}{x} \;=\; -12\left(e_1^2 - 4e_2^2\right), \\
g_{2,1} &= \frac{1}{2i\pi} \frac{\psi_1^2}{W} \frac{1}{x-1} \;=\; -18\left(e_1^2 + e_1e_2 - 2e_2^2\right).
\end{aligned} \tag{92}
$$

This shows that the harmonic polylogarithms [49, 50] in the letters 0 and 1 are a subset of the iterated integrals of modular forms discussed in this talk.

9 Conclusions

In this talk we considered a class of Feynman integrals, which evaluate to iterated integrals of modular forms. These Feynman integrals are beyond the class of Feynman integrals, which evaluate to multiple polylogarithms. However, several important properties, known from the case of multiple polylogarithms, carry over: The system of differential equations can be brought into an ε-form, the iterated integrals satisfy a shuffle algebra and there is an efficient method for the numerical evaluation of the iterated integrals of modular forms based on the q-expansion. We considered single-scale integrals. We may view these Feynman integrals, which evaluate to iterated integrals of modular forms as generalisations of Feynman integrals, which may be expressed in terms of harmonic polylogarithms in the letters 0 and 1.

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Iterative Non-iterative Integrals in Quantum Field Theory

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Abstract Single scale Feynman integrals in quantum field theories obey difference or differential equations with respect to their discrete parameter N or continuous parameter x. The analysis of these equations reveals to which order they factorize, which can be different in both cases. The simplest systems decouple to linear differential equations which factorize to first-order. For them complete solution algorithms exist. The next interesting level is formed by those cases that decouple to linear differential equations in which also irreducible second-order factors emerge. We give a survey on the latter case. The solutions can be obtained as general $_2F_1$ solutions. The corresponding solutions of the associated inhomogeneous differential equations form so-called iterative non-iterative integrals. There are known conditions under which one may represent the solutions by complete elliptic integrals. In this case one may find representations in terms of meromorphic modular forms, out of which special cases allow representations in the framework of elliptic polylogarithms with generalized parameters. These are in general weighted by a power of $1/\eta(\tau)$, where $\eta(\tau)$ is Dedekind's η-function. Single scale elliptic solutions emerge in the ρ-parameter, which we use as an illustrative example. They also occur in the 3-loop QCD corrections to massive operator matrix elements and the massive 3-loop form factors.

1 Introduction

In this paper a survey is presented on the classes of special functions, represented by particular integrals, to which presently known single scale Feynman-integrals evaluate. Zero-scale integrals, also playing an important role in elementary particle physics, are given by special numbers, see e.g. [1–5]. To this class the expansion coefficients of the β-functions [6–8] and the renormalized masses, as well as $(g-2)$ [5], do belong. Single scale quantities depend on one additional parameter as e.g. the Mellin variable N, a momentum fraction or scale-ratio $x \in [0, 1]$ and

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similar quantities. To this class contribute e.g. the massless Wilson coefficients [9], the anomalous dimensions [10–12], and the massive Wilson coefficients at large virtualities Q^2 [13–17].

It is now interesting to see which function spaces span the analytic results of these quantities. Traditionally two representations are studied: (i) the Mellin space representation following directly from the light cone expansion [18] and (ii) its Mellin inversion, the x-space representation, with x the Bjorken variable or another ratio of invariants, which in particular has phenomenological importance.

In the first case the quantities considered obey difference equations, while in the second case the corresponding equations are differential equations which are related to the former ones [19]. In all the cases quoted above either the recurrences or the differential operators or both factorize at *first-order* after an appropriate application of decoupling formalisms [20–22]. Due to this all these cases can be solved algorithmically in any basis of representation, as has been shown in Ref. [23]. In N-space the solution is then possible using C. Schneider's packages `Sigma` [24, 25], `EvaluateMultiSum` and `SumProduction` [26]. Corresponding solutions in x-space can be obtained by using the method of differential equations [23, 27]. This applies both to the direct calculation of the Feynman diagrams as well as to the calculation of their master integrals which are obtained using the integration by parts relations [28].

The above class of problems is the first one in a row. In general, the difference and differential equation systems do not decouple at first-order, but will have higher order subsystems, i.e. of second-, third-, fourth-order etc., cf. [29]. Since the first-order case is solved completely [23], it is interesting to see which mathematical spaces represent the solution. In N-space next to pure rational function representations the nested harmonic sums emerge [30, 31]. They correspond to the harmonic polylogarithms in x-space [32]. At the next level generalized harmonic sums and iterated integrals of the Kummer-Poincaré type appear [3, 33, 34]. These are followed by iterated integrals over cyclotomic letters [2] and further by square-root valued letters, cf. [4], and their associated sums and special constants, cf. also [29, 35, 36]. This chain of functions is probably not complete yet, as one might think of more general Volterra-iterated integrals and their associated nested sums, which are also obeying first-order factorization. The main properties of these functions, such as their shuffling relations [37, 38] and certain general transformations are known. Most of the corresponding mathematical properties to effectively handle these special functions are implemented in the package `HarmonicSums` [2–4, 39, 40].

The next important problem is, how to deal with cases in which neither recurrences in N-space nor differential equations in x-space factorize at first-order. Here, the general solution can be given by so-called iterative non-iterative integrals,[1] implied by the representation of the solution through the variation of constant [42] for factoriza-

[1] Iterative non-iterative integrals have been introduced by the author in a talk on the 5th International Congress on Mathematical Software, held at FU Berlin, July 11–14, 2016, with a series of colleagues present, cf. [41].

tions to irreducible factors at *any order*. This, of course, is a quite general statement, calling for refinement w.r.t. the corresponding special functions at factorizations with irreducible factors at second-, third- etc. order. In this article we will deal with the 2nd order case, discussing results, which have been obtained in Refs. [43, 44] and by other authors recently. At present, in the single variate case, the highest order of irreducible factors being observed is second order, see e.g. Refs. [43–66].

2 Second-Order Differential Equations and ${}_2F_1$ Solutions

We consider the non-factorizable problem of order two in x-space. It is given by a corresponding differential equation of second-order, usually with more than three singularities. Below we will give illustrations for equations which emerge in the calculation of the ρ-parameter [44, 67]. These are Heun differential equations [68]. A second-order differential equation with three singularities can be mapped into a Gauß'differential equation [69]. In the case of more singularities, this is possible too, however, the argument in the ${}_2F_1$ function is a rational function through which the other singularities are described. It is of advantage to look for the latter type solutions, since the properties of the ${}_2F_1$ function are very well known [70–74].

We consider the non-factorizable linear differential equations of second-order

$$\left[\frac{d^2}{dx^2} + p(x)\frac{d}{dx} + q(x)\right]\psi(x) = N(x) , \tag{1}$$

with rational functions $r(x) = p(x), q(x)$, which may be decomposed into[2]

$$r(x) = \sum_{k=1}^{n_r} \frac{b_k^{(r)}}{x - a_k^{(r)}}, \qquad a_k^{(r)}, b_k^{(r)} \in \mathbb{Z} . \tag{2}$$

The homogeneous equation is solved by the functions $\psi_{1,2}^{(0)}(x)$, which are linearly independent, i.e. their Wronskian W obeys

$$W(x) = \psi_1^{(0)}(x)\frac{d}{dx}\psi_2^{(0)}(x) - \psi_2^{(0)}(x)\frac{d}{dx}\psi_1^{(0)}(x) \neq 0 . \tag{3}$$

The homogeneous Eq. (1) determines the well-known differential equation for $W(x)$

$$\frac{d}{dx}W(x) = -p(x)W(x) , \tag{4}$$

[2]In the present case only single poles appear; for Fuchsian differential equations $q(x)$ may have double poles.

which, by virtue of (2), has the solution

$$W(x) = \prod_{k=1}^{n_p} \left(\frac{1}{x - a_k^{(p)}} \right)^{b_k^{(p)}}, \tag{5}$$

normalizing the functions $\psi_{1,2}^{(0)}$ accordingly. A particular solution of the inhomogeneous equation (1) is then obtained by Euler–Lagrange variation of constants [42]

$$\psi(x) = \psi_1^{(0)}(x) \left[C_1 - \int dx\, \psi_2^{(0)}(x) n(x) \right] + \psi_2^{(0)}(x) \left[C_2 + \int dx\, \psi_1^{(0)}(x) n(x) \right], \tag{6}$$

with

$$n(x) = \frac{N(x)}{W(x)} \tag{7}$$

and two constants $C_{1,2}$ to be determined by special physical requirements. As examples we consider the systems of differential equations given in [67] for the $O(\varepsilon^0)$ terms in the dimensional parameter. These are master integrals determining the ρ-parameter at general fermion mass ratio at 3-loop order. The corresponding equations read

$$\begin{aligned} 0 = &\frac{d^2}{dx^2} f_{8a}(x) + \frac{9 - 30x^2 + 5x^4}{x(x^2-1)(9-x^2)} \frac{d}{dx} f_{8a}(x) - \frac{8(-3+x^2)}{(9-x^2)(x^2-1)} f_{8a}(x) \\ &- \frac{32x^2}{(9-x^2)(x^2-1)} \ln^3(x) + \frac{12(-9+13x^2+2x^4)}{(9-x^2)(x^2-1)} \ln^2(x) \\ &- \frac{6(-54+62x^2+x^4+x^6)}{(9-x^2)(x^2-1)} \ln(x) + \frac{-1161+251x^2+61x^4+9x^6}{2(9-x^2)(x^2-1)} \end{aligned} \tag{8}$$

$$\begin{aligned} f_{9a}(x) = &-\frac{5}{8}(-13 - 16x^2 + x^4) + \frac{x^2}{2}(-24 + x^2)\ln(x) + 3x^2 \ln^2(x) - \frac{2}{3} f_{8a}(x) \\ &+ \frac{x}{6} \frac{d}{dx} f_{8a}(x). \end{aligned} \tag{9}$$

Here, $\ln^k(x) = H_0^n(x) = n! H_{\underbrace{0,\ldots,0}_{n}}(x)$ is a harmonic polylogarithm.

There are more equations contributing to the problem, cf. [43], in which in the inhomogeneity more harmonic polylogarithms $H_{\mathbf{a}}(x)$ [32] contribute. Equation (8) is a Heun equation in x^2. Its homogeneous solutions, [43], are:

$$\psi_{1a}^{(0)}(x) = \sqrt{2\sqrt{3}\pi} \frac{x^2(x^2-1)^2(x^2-9)^2}{(x^2+3)^4} {}_2F_1\left[\begin{matrix} \frac{4}{3}, \frac{5}{3} \\ 2 \end{matrix}; z \right] \tag{10}$$

$$\psi_{2a}^{(0)}(x) = \sqrt{2\sqrt{3}\pi} \frac{x^2(x^2-1)^2(x^2-9)^2}{(x^2+3)^4} {}_2F_1\left[\begin{matrix} \frac{4}{3}, \frac{5}{3} \\ 2 \end{matrix}; 1 - z \right], \tag{11}$$

with

$$z = z(x) = \frac{x^2(x^2-9)^2}{(x^2+3)^3}\,. \tag{12}$$

The Wronskian for this system is

$$W(x) = x(9-x^2)(x^2-1). \tag{13}$$

These are single-${}_2F_1$ solutions, however, they are not given by single elliptic integrals. One first uses contiguous relations and then mappings according to the triangle group [75–77] and the algorithm described in Appendix A of [43] to obtain the solutions

$$\psi_{1b}^{(0)}(x) = \frac{\sqrt{\pi}}{4\sqrt{6}}\Biggl\{-(x-1)(x-3)(x+3)^2\sqrt{\frac{x+1}{9-3x}}\,{}_2F_1\left[\begin{matrix}\frac{1}{2},\frac{1}{2}\\1\end{matrix};z\right] + (x^2+3)(x-3)^2\sqrt{\frac{x+1}{9-3x}}\,{}_2F_1\left[\begin{matrix}\frac{1}{2},-\frac{1}{2}\\1\end{matrix};z\right]\Biggr\} \tag{14}$$

$$\psi_{2b}^{(0)}(x) = \frac{2\sqrt{\pi}}{\sqrt{6}}\Biggl\{x^2\sqrt{(x+1)(9-3x)}\,{}_2F_1\left[\begin{matrix}\frac{1}{2},\frac{1}{2}\\1\end{matrix};1-z\right] + \frac{1}{8}\sqrt{(x+1)(9-3x)}(x-3)(x^2+3)\,{}_2F_1\left[\begin{matrix}\frac{1}{2},-\frac{1}{2}\\1\end{matrix};1-z\right]\Biggr\}, \tag{15}$$

where

$$z(x) = -\frac{16x^3}{(x+1)(x-3)^3} \tag{16}$$

and

$${}_2F_1\left[\begin{matrix}\frac{1}{2},\frac{1}{2}\\1\end{matrix};z\right] = \frac{2}{\pi}\mathbf{K}(z) \tag{17}$$

$${}_2F_1\left[\begin{matrix}\frac{1}{2},-\frac{1}{2}\\1\end{matrix};z\right] = \frac{2}{\pi}\mathbf{E}(z)\,, \tag{18}$$

cf. [78]. Here **K** denotes the elliptic integral of the first and **E** the elliptic integral of the second kind.[3]

Analyzing the criteria given in [79, 80] one finds, that the solution (14,15) cannot be rewritten such, that the elliptic integral of the second kind, $\mathbf{E}(z)$, does not emerge in the solution. The corresponding inhomogeneous solution is now obtained by Eq. (6).

---

[3] Here we use the notation applied by `Mathematica`. In some part of the literature one defines: ${}_2F_1\left[\begin{matrix}\frac{1}{2},\frac{1}{2}\\1\end{matrix};k^2\right] = \frac{2}{\pi}\mathbf{K}(k)$, etc.

We would like to end this section by a remark on simple elliptic solutions, which are sometimes also obtained in x-space. They are given by complete elliptic integrals $\mathbf{K}$ and $\mathbf{E}$ of the argument $1-x$ or x. In Mellin space, they correspond to a *first-order* factorizable problem, cf. [64] for an example. The Mellin transform

$$\mathbf{M}[f(x)](N) = \int_0^1 dx x^{N-1} f(x) \tag{19}$$

yields

$$\mathbf{M}[\mathbf{K}(1-z)](N) = \frac{2^{4N+1}}{(1+2N)^2 \binom{2N}{N}^2} \tag{20}$$

$$\mathbf{M}[\mathbf{E}(1-z)](N) = \frac{2^{4N+2}}{(1+2N)^2(3+2N)\binom{2N}{N}^2}, \tag{21}$$

since

$$\mathbf{K}(1-z) = \frac{1}{2}\frac{1}{\sqrt{1-z}} \otimes \frac{1}{\sqrt{1-z}} \tag{22}$$

$$\mathbf{E}(1-z) = \frac{1}{2}\frac{z}{\sqrt{1-z}} \otimes \frac{1}{\sqrt{1-z}}\ . \tag{23}$$

The Mellin convolution is defined by

$$A(x) \otimes B(x) = \int_0^1 dz_1 \int_0^1 dz_2 \delta(x - z_1 z_2) A(z_1) B(z_2). \tag{24}$$

Equations (20) and (21) are hypergeometric terms in N, which has been shown already in Ref. [35] for $\mathbf{K}(1-x)$, see also [4]. As we outlined in Ref. [23] the solution of systems of differential equations or difference equations can always be obtained algorithmically in the case either of those factorizes to first-order. The transition to x-space is then straightforward.

3 Iterative Non-iterative Integrals

Differential operators factorizing at first-order, occurring in quantum-field theoretic calculations, have iterative integral solutions of the kind

$$F_{a_1,\ldots,a_k}(x) = \int_0^x dy_1 f_{a_1}(y_1) \int_0^{y_1} dy_2 f_{a_2}(y_2) \ldots \int_0^{y_{k-1}} dy_k f_{a_k}(y_k), \tag{25}$$

where $\mathfrak{A}$ is a certain alphabet and $\forall f_l(x) \in \mathfrak{A}$. The functions $f_l(x)$ are hyperexponential, i.e. $(1/f_l(x))df_l(x)/dx$ is a rational function. These solutions are d'Alembertian [81], and are covered by the Liouvillian solutions [82]. In particular, the spaces of iterative integrals discussed in Refs. [2, 4, 32, 34, 35] are examples for this.

As well-known, the integral representation of the ${}_2F_1$-function in the cases having been discussed above

$$ {}_2F_1\left[\begin{matrix} a, b \\ c \end{matrix}; z\right] = \frac{\Gamma(x)}{\Gamma(b)\Gamma(c-b)} \int_0^1 dt t^{b-1}(1-t)^{c-b-1}(1-zt)^{-a} \tag{26} $$

cannot be rewritten as an integral in which the z dependence is just given by its boundaries.[4] Therfore Eq. (6) contains *definite* integrals, over which one integrates *iteratively*. We have called these *iterative non-iterative integrals* in [41, 43]. They will also occur in the case that the degree of non-factorization is larger than one by virtue of the corresponding formula of the variation of the constant; the corresponding solutions of the homogeneous equations will have (multiple) integral representations with the same property like for Eq. (26).

The new iterative integrals are given by

$$ \begin{aligned} \mathbb{H}_{a_1,\ldots,a_{m-1};\{a_m;F_m(r(y_m))\},a_{m+1},\ldots,a_q}(x) = & \int_0^x dy_1 \hat{f}_{a_1}(y_1) \int_0^{y_1} dy_2 \ldots \int_0^{y_{m-1}} dy_m \hat{f}_{a_m}(y_m) \\ & \times F_m[r(y_m)] H_{a_{m+1},\ldots,a_q}(y_m), \end{aligned} \tag{27} $$

and cases in which more than one definite integral F_m appears. Here the $\hat{f}_{a_i}(y)$ are the usual letters of the different classes considered in [2–4, 32] multiplied by hyperexponential pre-factors

$$ r(y) y^{r_1}(1-y)^{r_2}, \quad r_i \in \mathbb{Q}, \; r(y) \in \mathbb{Q}[y] \tag{28} $$

and $F[r(y)]$ is given by

$$ F[r(y)] = F[r(y); g] \equiv \int_0^1 dz g(z, r(y)), \quad r(y) \in \mathbb{Q}[y], \tag{29} $$

such that the y-dependence cannot be transformed into one of the integration boundaries completely. We have chosen here $r(y)$ as a rational function because of concrete examples in this paper, which, however, is not necessary.

The further analytic representation of the functions $\mathbb{H}$ will be subject to the iterated functions $\hat{f}_l$ and F_m. We will turn to this in the case of the examples (6) for $\psi_{1(2)b}$ in Sect. 5.

---

[4] This will not apply to simpler cases like ${}_2F_1\left[\begin{matrix} 1,1 \\ 2 \end{matrix}; -z\right] = \ln(1+z)/z$ or ${}_2F_1\left[\begin{matrix} \frac{1}{2},1 \\ \frac{3}{2} \end{matrix}; z\right] = \arctan(z)/z$, however.

4 Numerical Representation

For physical applications numerical representations of the Feynman integrals have to be given. The use of integral-representations in `Mathematica` or `Maple` is possible, but usually too slow. One aims on efficient numerical implementations. In the case of multiple polylogarithms it is available in `Fortran` [83, 84], for cyclotomic polylogarithms in [84], where in the first case the method of Bernoulli-improvement is used [85]. For generalized polylogarithms a numerical implementation was given in [86]. All these representations are series representations. Furthermore, there exist numerical implementations for the efficient use of harmonic sums in complex contour integral calculations [87].

Also in the case of the solutions (6) analytic series representations can be given. This has been already the solution-strategy in [67], using power-series Ansätze, without further reference to the expected mathematical structure. It turns out, that series expansions around $x = 0, 1$ are not convergent in the whole interval $x \in [0, 1]$. However, they have a sufficient region of overlap. Some series expansions of the inhomogeneous solution even exhibit a singularity, cf. [43], although this singularity is an artefact of the series expansion only. Yet these solutions can be obtained analytically and they evaluate very fast numerically.

The first terms of the expansion of f_{8a} around $x = 0$ read

$$
\begin{aligned}
&f_{8a}(x) = \\
&-\sqrt{3}\Bigg[\pi^3\left(\frac{35x^2}{108} - \frac{35x^4}{486} - \frac{35x^6}{4374} - \frac{35x^8}{13122} - \frac{70x^{10}}{59049} - \frac{665x^{12}}{1062882}\right) + \Bigg(12x^2 - \frac{8x^4}{3} \\
&- \frac{8x^6}{27} - \frac{8x^8}{81} - \frac{32x^{10}}{729} - \frac{152x^{12}}{6561}\Bigg)\mathrm{Im}\left[\mathrm{Li}_3\left(\frac{e^{-\frac{i\pi}{6}}}{\sqrt{3}}\right)\right]\Bigg] - \pi^2\Bigg(1 + \frac{x^4}{9} - \frac{4x^6}{243} - \frac{46x^8}{6561} \\
&- \frac{214x^{10}}{59049} - \frac{5546x^{12}}{2657205}\Bigg) + \left(\frac{3}{2} + \frac{x^4}{6} - \frac{2x^6}{81} - \frac{23x^8}{2187} - \frac{107x^{10}}{19683} - \frac{2773x^{12}}{885735}\right)\psi^{(1)}\left(\frac{1}{3}\right) \\
&- \sqrt{3}\pi\left(\frac{x^2}{4} - \frac{x^4}{18} - \frac{x^6}{162} - \frac{x^8}{486} - \frac{2x^{10}}{2187} - \frac{19x^{12}}{39366}\right)\ln^2(3) - \Bigg[33x^2 - \frac{5x^4}{4} - \frac{11x^6}{54} \\
&- \frac{19x^8}{324} - \frac{751x^{10}}{29160} - \frac{2227x^{12}}{164025} + \pi^2\left(\frac{4x^2}{3} - \frac{8x^4}{27} - \frac{8x^6}{243} - \frac{8x^8}{729} - \frac{32x^{10}}{6561} - \frac{152x^{12}}{59049}\right) \\
&+ \left(-2x^2 + \frac{4x^4}{9} + \frac{4x^6}{81} + \frac{4x^8}{243} + \frac{16x^{10}}{2187} + \frac{76x^{12}}{19683}\right)\psi^{(1)}\left(\frac{1}{3}\right)\Bigg]\ln(x) + \frac{135}{16} + 19x^2 \\
&- \frac{43x^4}{48} - \frac{89x^6}{324} - \frac{1493x^8}{23328} - \frac{132503x^{10}}{5248800} - \frac{2924131x^{12}}{236196000} - \left(\frac{x^4}{2} - 12x^2\right)\ln^2(x) \\
&- 2x^2\ln^3(x) + O\left(x^{14}\ln(x)\right). \qquad (30)
\end{aligned}
$$

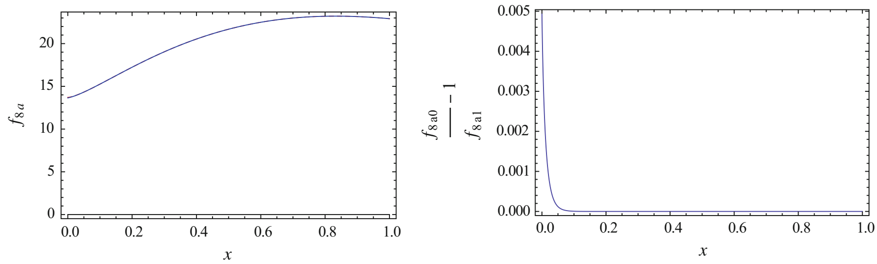

Fig. 1 The inhomogeneous solution of Eq. (8) as a function of x. Left panel: Red dashed line: expansion around $x = 0$; blue line: expansion around $x = 1$. Right panel: illustration of the relative accuracy and overlap of the two solutions $f_{8a}(x)$ around 0 and 1

Likewise, one may expand around $y = 1 - x = 0$ and obtains

$$\begin{aligned} f_{8a}(x) = & \frac{275}{12} + \frac{10}{3}y - 25y^2 + \frac{4}{3}y^3 + \frac{11}{12}y^4 + y^5 + \frac{47}{96}y^6 + \frac{307}{960}y^7 + \frac{19541}{80640}y^8 \\ & + \frac{22133}{120960}y^9 + \frac{1107443}{7741440}y^{10} + \frac{96653063}{851558400}y^{11} + \frac{3127748803}{34062336000}y^{12} \\ & + 7\Bigg(2y^2 - y^3 - \frac{1}{8}y^4 - \frac{1}{64}y^6 - \frac{1}{128}y^7 - \frac{3}{512}y^8 - \frac{1}{256}y^9 - \frac{47}{16384}y^{10} \\ & - \frac{69}{32768}y^{11} - \frac{421}{262144}y^{12}\Bigg)\zeta_3 + O(y^{13}) \,. \end{aligned} \tag{31}$$

In Fig. 1 a numerical illustration for the function $f_{8a}(x)$ is given together with the validity of the two expansions taking into account 50 terms. For many physics applications one would proceed in the above way and stop here. However, from the point of view of mathematics further interesting aspects arise to which we turn now.

5 Representation in Terms of Modular Forms

The iterative non-iterative integral (6) is non-iterative by virtue of the emergence of the two complete elliptic integrals $\mathbf{K}(z)$ and $\mathbf{E}(z)$, with the modulus squared

$$k^2 = z(x) \tag{32}$$

given by the rational function (16). Accordingly, the second solution depends on the functions $\mathbf{K}'(z) = \mathbf{K}(1 - z)$ and $\mathbf{E}'(z) = \mathbf{E}(1 - z)$. One may re-parameterize the problem referring to the nome

$$q = \exp(i\pi\tau), \tag{33}$$

as the new variable with

$$\tau = i\frac{\mathbf{K}(1-z(x))}{\mathbf{K}(z(x))} \quad \text{with} \quad \tau \in \mathbb{H} = \{z \in \mathbb{C}, \mathsf{Im}(z) > 0\}\,. \tag{34}$$

All functions contributing to the solutions (6, 14, 15) have now to be translated from x to q.

5.1 The Mathematical Framework

For the further discussion, a series of definitions is necessary, see also Refs. [88–110]. We will use Dedekind's η-function [111]

$$\eta(\tau) = \frac{q^{\frac{1}{12}}}{\phi(q^2)}, \quad \phi(q) = \prod_{k=1}^{\infty} \frac{1}{1-q^k}, \tag{35}$$

to express all quantities in the following. Here $\phi(q)$ denotes Euler's generating function of the partition function [112].

Definition 1 Let $r = (r_\delta)_{\delta|N}$ be a finite sequence of integers indexed by the divisors δ of $N \in \mathbb{N}\backslash\{0\}$. The function $f_r(\tau)$

$$f_r(\tau) := \prod_{\delta|N} \eta(\delta\tau)^{r_\delta}, \quad \delta, N \in \mathbb{N}\backslash\{0\}, \quad r_\delta \in \mathbb{Z}, \tag{36}$$

is called *η-ratio*. The η-ratios, up to differential operators in q, will represent all expressions in the following.

Let

$$\mathrm{SL}_2(\mathbb{Z}) = \left\{ M = \begin{pmatrix} a & b \\ c & d \end{pmatrix},\ a, b, c, d \in \mathbb{Z},\ \det(M) = 1 \right\}.$$

$\mathrm{SL}_2(\mathbb{Z})$ is the *modular group*.

For $g = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z})$ and $z \in \mathbb{C} \cup \{\infty\}$ one defines the Möbius transformation

$$gz \mapsto \frac{az+b}{cz+d}.$$

Let

$$S = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \text{and} \quad T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \quad S, T \in \mathrm{SL}_2(\mathbb{Z}).$$

The polynomials of S and T span $\mathrm{SL}_2(\mathbb{Z})$.

For $N \in \mathbb{N}\backslash\{0\}$ one considers the *congruence subgroups* of $\mathrm{SL}_2(\mathbb{Z})$, $\Gamma_0(N)$, $\Gamma_1(N)$ and $\Gamma(N)$, defined by

$$\Gamma_0(N) := \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z}), c \equiv 0 \pmod N \right\},$$
$$\Gamma_1(N) := \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z}), a \equiv d \equiv 1 \pmod N, \quad c \equiv 0 \,(\mathrm{mod}\, N) \right\},$$
$$\Gamma(N) := \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z}), a \equiv d \equiv 1 \pmod N, \quad b \equiv c \equiv 0 \pmod N \right\},$$

with $\mathrm{SL}_2(\mathbb{Z}) \supseteq \Gamma_0(N) \supseteq \Gamma_1(N) \supseteq \Gamma(N)$ and $\Gamma_0(N) \subseteq \Gamma_0(M), \; M|N$.
If $N \in \mathbb{N}\backslash\{0\}$, then the *index* of $\Gamma_0(N)$ in $\Gamma_0(1)$ is

$$\mu_0(N) = [\Gamma_0(1) : \Gamma_0(N)] = N \prod_{p|N} \left(1 + \frac{1}{p}\right).$$

The product is over the prime divisors p of N.

Definition 2 Let $x \in \mathbb{Z}\backslash\{0\}$. The analytic function $f : \mathbb{H} \to \mathbb{C}$ is a *holomorphic modular form* of *weight* $w = k$ for $\Gamma_0(N)$ and *character* $a \mapsto \left(\frac{x}{a}\right)$ if

1. $$f\left(\frac{az+b}{cz+d}\right) = \left(\frac{x}{a}\right)(cz+d)^k f(z), \quad \forall z \in \mathbb{H}, \; \forall \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \Gamma_0(N).$$
2. $f(z)$ is holomorphic in $\mathbb{H}$
3. $f(z)$ is holomorphic at the cusps of $\Gamma_0(N)$.

Here $\left(\frac{x}{a}\right)$ denotes the Jacobi symbol. A modular form is called a *cusp form* if it vanishes at the cusps.

For any congruence subgroup G of $\mathrm{SL}_2(\mathbb{Z})$ a *cusp* of G is an equivalence class in $\mathbb{Q} \cup \{\infty\}$ under the action of G.

Definition 3 A *meromorphic modular function* f for $\Gamma_0(N)$ and weight $w = k$ obeys

1. $f(\gamma z) = (cz+d)^k f(z), \quad \forall z \in \mathbb{H}$ and $\forall \gamma \in \Gamma_0(N)$
2. f is meromorphic in $\mathbb{H}$
3. f is meromorphic at the cusps of $\Gamma_0(N)$.

The q-expansion of a meromorphic modular form has the form

$$f^*(q) = \sum_{k=-N_0}^{\infty} a_k q^k, \quad \text{for some } \; N_0 \in \mathbb{N}.$$

Lemma 1 ([91, 94, 109]) *The set of functions $\mathscr{M}(k;N;x)$ for $\Gamma_0(N)$ and character x, defined above, forms a finite dimensional vector space over $\mathbb{C}$. In particular, for any non-zero function $f \in \mathscr{M}(k;N;x)$ we have*

$$\mathrm{ord}(f) \le b = \frac{k}{12}\mu_0(N). \tag{37}$$

The bound (37) on the dimension can be refined, see e.g. [105–108] for details.[5] The number of independent modular forms $f \in \mathscr{M}(k;N;x)$ is $\le b$, allowing for a basis representation in finite terms.

For any η-ratio f_r one can prove that there exists a minimal integer $l \in \mathbb{N}$, an integer $N \in \mathbb{N}$ and a character x such that

$$\bar{f}_r(\tau) = \eta^l(\tau) f_r(\tau) \in \mathscr{M}(k;N;x)$$

is a holomorphic modular form. All quantities which are expanded in q-series below will be first brought into the above form. In some cases one has $l = 0$. This form is of importance to obtain Lambert-Eisenstein series [114, 115], which can be rewritten in terms of elliptic polylogarithms [116].

A basis of the vector space of holomorphic modular forms is given by the associated Lambert-Eisenstein series with character and binary products thereof [89, 109].

The Lambert-Eisenstein series are given by

$$\sum_{k=1}^{\infty} \frac{k^\alpha q^k}{1-q^k} = \sum_{k=1}^{\infty} \sigma_\alpha(k) q^k, \quad \sigma_\alpha(k) = \sum_{d|k} d^\alpha, \quad \alpha \in \mathbb{N}. \tag{38}$$

They can be rewritten in terms of elliptic polylogarithms,

$$\mathrm{ELi}_{n;m}(x;y;q) := \sum_{k=1}^{\infty}\sum_{l=1}^{\infty} \frac{x^k}{k^n}\frac{y^l}{l^m} q^{kl} \tag{39}$$

by

$$\sum_{k=1}^{\infty} \frac{k^\alpha q^k}{1-q^k} = \sum_{k=1}^{\infty} k^\alpha \mathrm{Li}_0(q^k) = \sum_{k,l=1}^{\infty} k^\alpha q^{kl} = \mathrm{ELi}_{-\alpha;0}(1;1;q), \tag{40}$$

with $\mathrm{Li}_0(x) = x/(1-x)$. It also appears useful to define [61],

$$\overline{E}_{n;m}(x;y;q) = \begin{cases} \frac{1}{i}[\mathrm{ELi}_{n;m}(x;y;q) - \mathrm{ELi}_{n;m}(x^{-1};y^{-1};q)], & n+m \ \text{ even} \\ \mathrm{ELi}_{n;m}(x;y;q) + \mathrm{ELi}_{n;m}(x^{-1};y^{-1};q), & n+m \ \text{ odd.} \end{cases} \tag{41}$$

[5] The dimension of the corresponding vector space can be also calculated using the `Sage` program by W. Stein [113].

The multiplication relation of elliptic polylogarithms is given by [116]

$$\begin{aligned}&\mathrm{ELi}_{n_1,\dots,n_l;m_1,\dots,m_l;0,2o_2,\dots,2o_{l-1}}(x_1,\dots,x_l;y_1,\dots,y_l;q) = \\ &\mathrm{ELi}_{n_1;m_1}(x_1;y_1;q)\mathrm{ELi}_{n_2,\dots,n_l;m_2,\dots,m_l;2o_2,\dots,2o_{l-1}}(x_2,\dots,x_l;y_2,\dots,y_l;q),\end{aligned} \quad (42)$$

with

$$\begin{aligned}&\mathrm{ELi}_{n_,\dots,n_l;m_1,\dots,m_l;2o_1,\dots,2o_{l-1}}(x_1,\dots,x_l;y_1,\dots,y_l;q) \quad (43)\\ &= \sum_{j_1=1}^\infty \cdots \sum_{j_l=1}^\infty \sum_{k_1=1}^\infty \cdots \sum_{k_l=1}^\infty \frac{x_1^{j_1}}{j_1^{n_1}} \cdots \frac{x_l^{j_l}}{j_l^{n_l}} \frac{y_1^{k_1}}{k_1^{m_1}} \frac{y_l^{k_l}}{k_l^{m_l}} \frac{q^{j_1k_1+\dots+q_lk_l}}{\prod_{i=1}^{l-1}(j_ik_i+\dots+j_lk_l)^{o_i}}, l > 0.\end{aligned}$$

The logarithmic integral of an elliptic polylogarithm is given by

$$\begin{aligned}&\mathrm{ELi}_{n_1,\dots,n_l;m_1,\dots,m_l;2(o_1+1),2o_2,\dots,2o_{l-1}}(x_1,\dots,x_l;y_1,\dots,y_l;q) = \\ &\qquad \int_0^q \frac{dq'}{q'} \mathrm{ELi}_{n_1,\dots,n_l;m_1,\dots,m_l;2o_1,\dots,2o_{l-1}}(x_1,\dots,x_l;y_1,\dots,y_l;q').\end{aligned} \quad (44)$$

Similarly, cf. [61],

$$\begin{aligned}&\overline{E}_{n_1,\dots,n_l;m_1,\dots,m_l;0,2o_2,\dots,2o_{l-1}}(x_1,\dots,x_l;y_1,\dots,y_l;q) = \\ &\qquad \overline{E}_{n_1;m_1}(x_1;y_1;q)\overline{E}_{n_2,\dots,n_l;m_2,\dots,m_l;2o_2,\dots,2o_{l-1}}(x_1,\dots,x_l;y_1,\dots,y_l;q)\end{aligned} \quad (45)$$

$$\begin{aligned}&\overline{E}_{n_1,\dots,n_l;m_1,\dots,m_l;2(o_1+1),2o_2,\dots,2o_{l-1}}(x_1,\dots,x_l;y_1,\dots,y_l;q) = \\ &\qquad \int_0^q \frac{dq'}{q'} \overline{E}_{n_1,\dots,n_l;m_1,\dots,m_l;2o_1,\dots,2o_{l-1}}(x_1,\dots,x_l;y_1,\dots,y_l;q')\end{aligned} \quad (46)$$

holds.

The integral over the product of two more general elliptic polylogarithms is given by

$$\begin{aligned}\int_0^q \frac{d\bar{q}}{\bar{q}} \mathrm{ELi}_{m,n}(x,\bar{q}^a,\bar{q}^b)\mathrm{ELi}_{m',n'}(x',\bar{q}^{a'},\bar{q}^{b'}) &= \sum_{k=1}^\infty \sum_{l=1}^\infty \sum_{k'=1}^\infty \sum_{l'=1}^\infty \frac{x^k}{k^m} \frac{x'^k}{k'^{m'}} \frac{q^{al}}{l^n} \frac{q^{a'l'}}{l'^n} \\ &\times \frac{q^{bkl+b'k'l'}}{al+a'l'+bkl+bk'l'}.\end{aligned} \quad (47)$$

Integrals over other products are obtained accordingly.

In the derivation often the argument q^m, $m \in \mathbb{N}, m > 0$, appears, which shall be mapped to the variable q. We do this for the Lambert series using the replacement

$$\mathrm{Li}_0(x^m) = \frac{x^m}{1-x^m} = \frac{1}{m}\sum_{k=1}^{m} \frac{\rho_m^k x}{1-\rho_m^k x} = \frac{1}{m}\sum_{k=1}^{m} \mathrm{Li}_0(\rho_m^k x), \tag{48}$$

with

$$\rho_m = \exp\left(\frac{2\pi i}{m}\right). \tag{49}$$

One has

$$\sum_{k=1}^{\infty} \frac{k^\alpha q^{mk}}{1-q^{mk}} = \mathrm{ELi}_{-\alpha;0}(1;1;q^m) = \frac{1}{m^{\alpha+1}} \sum_{n=1}^{m} \mathrm{ELi}_{-\alpha;0}(\rho_m^n;1;q)\,. \tag{50}$$

Relations like (48, 50) and similar ones are the sources of the mth roots of unity, which correspondingly appear in the parameters of the elliptic polylogarithms through the Lambert series.

Furthermore, the following sums occur

$$\sum_{m=1}^{\infty} \frac{(am+b)^l q^{am+b}}{1-q^{am+b}} = \sum_{n=1}^{l} \binom{l}{n} a^n b^{l-n} \sum_{m=1}^{\infty} \frac{m^n q^{am+b}}{1-q^{am+b}}, \quad a,l \in \mathbb{N}, \quad b \in \mathbb{Z} \tag{51}$$

and

$$\sum_{m=1}^{\infty} \frac{m^n q^{am+b}}{1-q^{am+b}} = \mathrm{ELi}_{-n;0}(1;q^b;q^a) = \frac{1}{a^{n+1}} \sum_{\nu=1}^{a} \mathrm{ELi}_{-n;0}(\rho_a^\nu;q^b;q)\,. \tag{52}$$

Likewise, one has

$$\begin{aligned}\sum_{m=1}^{\infty} \frac{(-1)^m m^n q^{am+b}}{1-q^{am+b}} &= \mathrm{ELi}_{-n;0}(-1;q^b;q^a) \qquad (53)\\ &= \frac{1}{a^{n+1}} \left\{ \sum_{\nu=1}^{2a} \mathrm{ELi}_{-n;0}(\rho_{2a}^\nu;q^b;q) - \sum_{\nu=1}^{a} \mathrm{ELi}_{-n;0}(\rho_a^\nu;q^b;q) \right\}.\end{aligned}$$

In intermediate representations also Jacobi symbols appear, obeying the identities

$$\left(\frac{-1}{(2k)\cdot n + (2l+1)}\right) = (-1)^{k+l}; \qquad \left(\frac{-1}{ab}\right) = \left(\frac{-1}{a}\right)\left(\frac{-1}{b}\right). \tag{54}$$

In the case of an even value of the denominator one may factor $\left(\frac{-1}{2}\right) = 1$ and consider the case of the remaining odd-valued denominator.

We found also Lambert series of the kind

$$\sum_{m=1}^{\infty} \frac{q^{(c-a)m}}{1-q^{cm}} = \mathrm{ELi}_{0;0}(1; q^{-a}; q^c) = \frac{1}{c}\sum_{n=1}^{c} \mathrm{ELi}_{0;0}(\rho_c^n; q^{-a}; q) \tag{55}$$

$$\sum_{m=1}^{\infty}(-1)^m \frac{q^{(c-a)m}}{1-q^{cm}} = \mathrm{ELi}_{0;0}(1; -q^{-a}; q^c) = \frac{1}{c}\sum_{n=1}^{c} \mathrm{ELi}_{0;0}(\rho_c^n; -q^{-a}; q),$$
$$a, c \in \mathbb{N}\backslash\{0\} \tag{56}$$

in intermediate steps of the calculation.

Also the functions

$$\begin{aligned} Y_{m,n,l} &:= \sum_{k=0}^{\infty} \frac{(mk+n)^{l-1} q^{mk+n}}{1-q^{mk+n}} \\ &= n^{l-1}\mathrm{Li}_0(q^n) + \sum_{j=0}^{l-1} \binom{l-1}{j} n^{l-1-j} m^j \mathrm{ELi}_{-j;0}(1; q^n; q^m) \end{aligned} \tag{57}$$

$$Z_{m,n,l} := \sum_{k=1}^{\infty} \frac{k^{m-1} q^{nk}}{1-q^{lk}} = \mathrm{ELi}_{0;-(m-1)}(1; q^{n-l}; q^l) \tag{58}$$

$$\begin{aligned} T_{m,n,l,a,b} &:= \sum_{k=0}^{\infty} \frac{(mk+n)^{l-1} q^{a(mk+n)}}{1-q^{b(mk+n)}} = n^{l-1} q^{n(a-b)} \mathrm{Li}_0\left(q^{nb}\right) \\ &\quad + q^{n(a-b)} \sum_{j=0}^{l-1} \binom{l-1}{j} m^j n^{l-1-j} \mathrm{ELi}_{-j;0}\left(q^{m(a-b)}; q^{nb}; q^{mb}\right) \end{aligned} \tag{59}$$

contribute. Note that (part of) the parameters $(x; y)$ of the elliptic polylogarithms can become q-dependent, unlike the case in [54, 61]. The elliptic polylogarithms rather form a suitable frame here, while we give preference to the Lambert-Eisenstein series. The q-dependence of $x(y)$ does not spoil the integration relations, which can be generalized in the case the factors $1/\eta(\tau)$ do not occur in addition.

5.2 *The q-Representation of the Inhomogeneous Solution*

Now we turn to (6) again and express all quantities in terms of the variable q.

The modulus is given by, cf. Eq. (32),

$$k = \frac{4\eta^8(2\tau)\eta^4\left(\frac{\tau}{2}\right)}{\eta^{12}(\tau)}, \qquad k' = \frac{\eta^4(2\tau)\eta^8\left(\frac{\tau}{2}\right)}{\eta^{12}(\tau)}, \tag{60}$$

which implies the following relation by $k' = \sqrt{1-k^2}$ for η functions

$$1 = \frac{\eta^8\left(\frac{\tau}{2}\right)\eta^8(2\tau)}{\eta^{24}(\tau)}\left[16\eta^8(2\tau) + \eta^8\left(\frac{\tau}{2}\right)\right] . \tag{61}$$

The elliptic integral of the first kind has the representation [78], sometimes also written using Jacobi's ϑ_i-functions [117],

$$\mathbf{K}(k^2) = \frac{\pi}{2}\frac{\eta^{10}(\tau)}{\eta^4\left(\frac{1}{2}\tau\right)\eta^4(2\tau)}, \qquad \mathbf{K}'(k^2) = -\frac{1}{\pi}\mathbf{K}(k^2)\ \ln(q) . \tag{62}$$

The elliptic integrals of the 2nd kind, $\mathbf{E}$ and $\mathbf{E}'$ are given by [118, 119]

$$\mathbf{E}(k^2) = \mathbf{K}(k^2) + \frac{\pi^2 q}{\mathbf{K}(k^2)}\frac{d}{dq}\ln\left[\vartheta_4(q)\right] \tag{63}$$

and the Legendre identity [120]

$$\mathbf{K}(z)\mathbf{E}(1-z) + \mathbf{E}(z)\mathbf{K}(1-z) - \mathbf{K}(z)\mathbf{K}(1-z) = \frac{\pi}{2}, \tag{64}$$

to express $\mathbf{E}'$,

$$\mathbf{E}'(k^2) = \frac{\pi}{2\mathbf{K}(k^2)}\left[1 + 2\ln(q)\, q\frac{d}{dq}\ln\left[\vartheta_4(q)\right]\right], \tag{65}$$

where the Jacobi ϑ functions are given by

$$\vartheta_2(q) = \frac{2\eta^2(2\tau)}{\eta(\tau)}, \quad \vartheta_3(q) = \frac{\eta^5(\tau)}{\eta^2\left(\frac{1}{2}\tau\right)\eta^2(2\tau)}, \quad \vartheta_4(q) = \frac{\eta^2\left(\frac{\tau}{2}\right)}{\eta(\tau)}. \tag{66}$$

We have now to determine the kinematic variable $x = x(q)$ analytically. This is not always possible for other choices of the definition of q, cf. [59]. In the present case, however, a cubic Legendre-Jacobi transformation [121, 122][6] allows the solution. Following [51, 52, 126, 127]

$$\frac{16y}{(1-y)(1+3y)^3} = \frac{\vartheta_2^4(q)}{\vartheta_3^4(q)} \tag{67}$$

is solved by

$$y = \frac{\vartheta_2^2(q^3)}{\vartheta_2^2(q)} \equiv= \frac{1}{3x}. \tag{68}$$

[6]This is, besides the well-know Landen transformation [78, 123], the next higher modular transformation; for a survey cf. [124]. Also for the hypergeometric function ${}_2F_1\left[\begin{matrix}\frac{1}{r}, 1-\frac{1}{r} \\ 1\end{matrix}; z(x)\right]$ there are rational modular transformations [125].

Both the expressions (67, 68) are modular functions. For definiteness, we consider the range in q

$$q \in [-1, 1] \quad \text{which corresponds to} \quad y \in \left[0, \tfrac{1}{3}\right], \quad x \in [1, +\infty] \tag{69}$$

in the following. Here the variable x lies in the unphysical region. However, the nome q has to obey the condition (69). Other kinematic regions can be reached by performing analytic continuations.

One obtains

$$x = \frac{1}{3}\frac{\eta^4(2\tau)\eta^2(3\tau)}{\eta^2(\tau)\eta^4(6\tau)}. \tag{70}$$

By this all ingredients of the inhomogeneous solution (6) can now be rewritten in q. Using the on-line encyclopedia of integer sequences [128] one finds in particular for entry `A256637`

$$\sqrt{(1-3x)(1+x)} = \frac{1}{i\sqrt{3}} \left. \frac{\eta\left(\frac{\tau}{2}\right)\eta\left(\frac{3\tau}{2}\right)\eta(2\tau)\eta(3\tau)}{\eta(\tau)\eta^3(6\tau)}\right|_{q\to -q} \tag{71}$$

and for terms in the inhomogeneity and the Wronskian `A187100, A187153` [128]

$$\frac{1}{1-x} = -3\frac{\eta^2(\tau)\eta\left(\frac{3}{2}\tau\right)\eta^3(6\tau)}{\eta^3\left(\frac{1}{2}\tau\right)\eta(2\tau)\eta^2(3\tau)} \tag{72}$$

$$\frac{1}{1-3x} = -\frac{\left[\eta(\tau)\eta\left(\frac{3}{2}\tau\right)\eta^2(6\tau)\right]^3}{\eta\left(\frac{1}{2}\tau\right)\eta^2(2\tau)\eta^9(3\tau)}. \tag{73}$$

This method can be applied since the q-series of the associated holomorphic modular form to these expressions factoring off a power of $1/\eta(\tau)$ is determined by a finite number of expansion coefficients since the dimension of the associated linear space is finte, cf. Lemma 1.

Next we would like to investigate which kind of modular form the solution $\psi(x)$ is. Some of its building blocks, like $\mathbf{K}$, are holomorphic modular forms [88, 89], while others, like $\mathbf{E}$, are meromorphic modular forms. In the case in which a solution can be thoroughly expressed by holomorphic modular forms, as e.g. in the case of the sun-rise graph studied in Refs. [54, 59], one has then the possibility to express the result in terms of polynomials of Lambert–Eisenstein series [114, 115], which are given by elliptic polylogarithms [116] and their generalizations, cf. e.g. [61] and references therein.

The elliptic integral of the first kind can be expressed by E or $\overline{E}$-functions only.

$$\mathbf{K}(z) = \frac{\pi}{2}\left[1 + 2\overline{E}_{0;0}(i;1;q)\right], \tag{74}$$

On the other hand, this is not the case for $1/\mathbf{K}(z)$, a function needed to represent $\mathbf{E}$:

$$\begin{aligned}
\frac{1}{\mathbf{K}(z)} = & \frac{2}{\pi\eta^{12}(\tau)}\left\{\frac{5}{48}\left\{1-24\mathrm{ELi}_{0;-1}(1;1;q)-4\left[1-\frac{3}{2}\left[\mathrm{ELi}_{0;-1}(1;1;q)\right.\right.\right.\right.\\
& \left.\left.\left.\left.+\mathrm{ELi}_{0;-1}(1;i;q)+\mathrm{ELi}_{0;-1}(1;-1;q)+\mathrm{ELi}_{0;-1}(1;-i;q)\right]\right]\right\}\right\}\left\{-1\right.\\
& +4\left[-\frac{1}{2}\left[\mathrm{ELi}_{-2;0}(i;1/q;q)+\mathrm{ELi}_{-2,0}(-i;1/q;q)\right]+\left[\mathrm{ELi}_{-1;0}(i;1/q;q)\right.\right.\\
& \left.\left.\left.+\mathrm{ELi}_{-1;0}(-i;1/q;q)\right]-\frac{1}{2}\left[\mathrm{ELi}_{0,0}(i;1/q;q)+\mathrm{ELi}_{0,0}(-i;1/q;q)\right]\right]\right\}\\
& -\frac{1}{16}\left\{5+4\left[-\frac{1}{2}\left[\mathrm{ELi}_{-4;0}(i;1/q;q)+\mathrm{ELi}_{-4;0}(-i;1/q;q)\right]\right.\right.\\
& +2\left[\mathrm{ELi}_{-3;0}(i;1/q;q)+\mathrm{ELi}_{-3,0}(-i;1/q;q)\right]-3\left[\mathrm{ELi}_{-2;0}(i;1/q;q)\right.\\
& \left.+\mathrm{ELi}_{-2,0}(-i;1/q;q)\right]+2\left[\mathrm{ELi}_{-1;0}(i;1/q;q)+\mathrm{ELi}_{-1;0}(-i;1/q;q)\right]\\
& \left.\left.-\frac{1}{2}\left[\mathrm{ELi}_{0;0}(i;1/q;q)+\mathrm{ELi}_{0,0}(-i;1/q;q)\right]\right]\right\}.
\end{aligned} \tag{75}$$

Here and in a series of other building blocks the factor $1/\eta^{12}(\tau)$ emerges through which the corresponding quantity becomes a meromorphic modular form [43].

Still one has to express the inhomogeneities of the corresponding differential equations. They are given by harmonic polylogarithms $H_{\mathbf{a}}(x)$ and rational pre-factors in x. In the variable $q = q(x)$ they will be different, cf. [43, 59], depending on the definition of q.

Since for the q-series of $1/\eta(\tau)$ no closed form expression of the expansion coefficients is known, one cannot write down a closed form integration relation for polynomials out of quantities like this, unlike the case for polynomials out of Lambert-Eisenstein series, see Ref. [43] for details. Therefore, a closed analytic solution of the inhomogeneous solution using structures like elliptic polylogarithms, cf. Sect. 5.1, cannot be given. Yet, one may use q-series in the numerical representation expanding to a certain power. This, however, is equivalent to the numerical representation given in Sect. 4, where no further analytic continuation is necessary.

6 The ρ-Parameter

Finally we would like to present numerical results on the ρ-parameter with a finite quark mass ratio, given in Ref. [44]. The ρ-parameter is defined by

$$\rho = 1 + \frac{\Pi_T^Z(0)}{M_Z^2} - \frac{\Pi_T^W(0)}{M_W^2} \equiv 1 + \Delta\rho, \tag{76}$$

with $\Pi_T^k(0)$ the respective transversal self energies at zero momentum and M_k the masses of the Z and W bosons. Here the correction is given by

$$\Delta\rho = \frac{3G_F m_t^2}{8\pi^2\sqrt{2}}\left(\delta^{(0)} + \frac{\alpha_s}{\pi}\delta^{(1)} + \left(\frac{\alpha_s}{\pi}\right)^2\delta^{(2)} + \mathscr{O}(\alpha_s^3)\right), \tag{77}$$

where G_F is the Fermi-constant, m_t denotes the heavy fermion mass, and $x = m_b^2/m_t^2$ the ratio of the masses of the light and the heavy partner squared.

The radiative corrections allow to set limits on heavy fermions in the case of doublet mass splitting, which was important to determine the precise mass region of the top-quark [129]. Radiative corrections were calculated in Refs. [67, 129–135]. In Ref. [43] we calculated the analytic form of the yet missing master integrals. They can now be evaluated numerically starting from a complete analytic representation. We insert our results into the representation given in [67].

The expression for the $\delta^{(2)}$, Eq. (77), in terms of the master integrals in the $\overline{\text{MS}}$ scheme, is given by Eq. (78), where we only show the contributions due to the iterative non-iterative integrals.

$$\begin{aligned}
\delta^{(2)}(x) = \cdots + C_F\left(C_F - \frac{C_A}{2}\right)&\left[\frac{11-x^2}{12(1-x^2)^2} f_{8a}(x) + \frac{9-x^2}{3(1-x^2)^2} f_{9a}(x)\right.\\
&\left.+\frac{1}{12} f_{10a}(x) + \frac{5-39x^2}{36(1-x^2)^2} f_{8b}(x) + \frac{1-9x^2}{9(1-x^2)^2} f_{9b}(x) + \frac{x^2}{12} f_{10b}(x)\right]\\
&+\frac{C_F T_F}{9(1-x^2)^3}\left[(5x^4 - 28x^2 - 9) f_{8a}(x) + \frac{1-3x^2}{3x^2}(9x^4 + 9x^2 - 2) f_{8b}(x)\right.\\
&\left.+(9-x^2)(x^4 - 6x^2 - 3) f_{9a}(x) + \frac{1-9x^2}{3x^2}(3x^4 + 6x^2 - 1) f_{9b}(x)\right].
\end{aligned} \tag{78}$$

The different functions $f_i(a)$ are given in Ref. [43]. The behaviour of the correction term $\delta^{(2)}(x)$ is shown in Fig. 2. The color factor signals that it stems from the

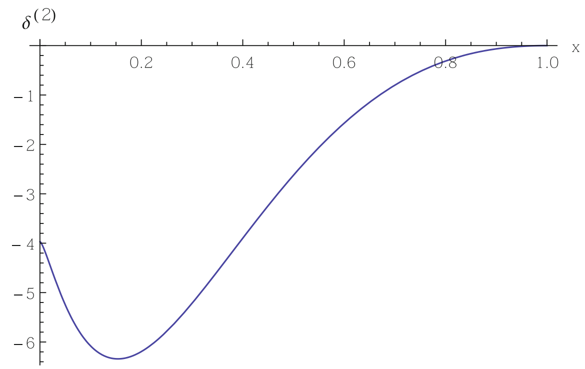

Fig. 2 The two-mass contributions to $\delta^{(2)}$ as a function of x

non-planar part of the problem. In the limit of $m_t \to \infty$ the numerical value $\delta^{(2)}(0) = -3.969$ is obtained in agreement with [131]. In the limit of zero mass splitting the correction vanishes.

7 Conclusions

In the analytic calculation of zero- and single-scale Feynman diagrams in the most simple cases iterative integral and indefinite nested sum representations are sufficient. Here either the system of differential or difference equations factorizes to first-order [29]. All these cases can be solved algorithmically, cf. [23], in whatsoever basis. The function spaces, which represent the solutions for the cases having been studied so far, are completely known and the associated numerical implementations are widely available.

At present an important target of research are the cases in which the level of non-factorization is of second- or higher order. Also in these cases the general structure of the formal solutions is known. In the case of the differential equations they are given by the variation of constant, over the solutions of the homogeneous equations. Here the latter ones have no iterative solutions. They can be written as (multiple) Mellin-Barnes [136] integrals [137] and by this cast into a multiple integral representation in which the next integration variable cannot be completely transformed into the integral boundaries. Therefore, these integrals are of non-iterative character. In summary, one obtains iterative integrals over these non-iterative integrals as the main structure [41, 43].

From the mathematical point of view one would like to understand the non-iterative integrals emerging on the different levels of non-factorization in more detail. In the 2nd order case the corresponding differential equations have ${}_2F_1$-solutions with specific rational parameters and rational functions in x as argument. This is generally due to the fact that the corresponding differential equations have more than three singularities. There is a decision algorithm, cf. [43, 76, 77], whether or not the ${}_2F_1$-solutions can be mapped on complete elliptic integrals or not. Furthermore, one may investigate, using the criteria given in [79, 80], whether representations in terms of complete elliptic integrals of the first kind are sufficient in special cases. In the elliptic case one may consider representations in terms of modular forms, which are in general meromorphic. A sub-class of only holomorphic modular forms, cf. e.g. [54, 61], also exists in a series of interesting cases. Finally, complete elliptic integrals of the first and second kind with argument x or $(1-x)$ do not form a 2nd order problem, if considered in N space, where they have a representation in hypergeometric terms.

The level of non-factorization for single-scale Feynman integrals at second order is widely understood and throughly tied up with ${}_2F_1$-solutions. Their properties allow to derive also analytic solutions. Corresponding series expansions in the complex plane allow for numerical implementations since their convergence regions do overlap sufficiently.

Much less is known in the case of third and higher order non-factorization. Cases of this kind will emerge in future calculations. Here one is not advised to apply the pure *integral* approach of differential equations [23, 27]. To recognize the nature of the integrals contributing here it is useful to apply the dispersive approach to the corresponding integrals first [138]. Even multiple cuts may be necessary to unravel the emerging structures. In this way, once again, *non-iterative* integrals are obtained. This has been the easiest approach to solve the sun-rise graph also, cf. [48]. This method will be of use to unravel further levels and to establish the links needed to known mathematical structures or at least to guide the way to work out the corresponding mathematics, if it is not know yet.

Again the analytic calculation of Feynman integrals shows the rich mathematical structures behind these quantities and leads to an intense cooperation between theoretical physics, different branches of mathematics and computer algebra. During the last 30 years an enormous development has been taking place, but much more is going to come.

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Analytic Continuation of the Kite Family

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Abstract We consider results for the master integrals of the kite family, given in terms of ELi-functions which are power series in the nome q of an elliptic curve. The analytic continuation of these results beyond the Euclidean region is reduced to the analytic continuation of the two period integrals which define q. We discuss the solution to the latter problem from the perspective of the Picard–Lefschetz formula.

1 Introduction

In this talk, we consider the family of Feynman integrals associated to the kite graph, shown in Fig. 1c. Certain master integrals of this family have recently served as interesting showcases for the problem that multiple polylogarithms are not always sufficient to express the coefficients of Feynman integrals in the Laurent expansion in ε of dimensional regularization. Elliptic generalizations of (multiple) polylogarithms can be used to express these integrals instead. In [5] a way to recursively obtain the master integrals of this family to arbitrary order in ε was presented for the Euclidean kinematic region. This computation and previous related work on the sunrise integral [6–9] rely crucially on properties of an underlying elliptic curve and its periods, which were pointed out in [17]. The results for the master integrals of the kite family are expressed in terms of a class of functions defined in [9] as power series in the nome q of this elliptic curve. Alternative expressions in terms of iterated integrals of modular

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forms were found in [12] and results for the first order of the Laurent expansion were previously derived in [42].

Here we focus on the analytic continuation of the results for the kite family [18] beyond the Euclidean region. By considering the periods of the underlying elliptic curve, we can reduce the analytic continuation of the Feynman integrals to the question how cycles on the elliptic curve behave under the variation of a kinematic invariant. The answer to this question is then very simple and can be deduced from an application of the Picard–Lefschetz formula [35], as we want to emphasise with this presentation. In this way we arrive at analytic results for the master integrals which can be evaluated numerically at any real value of the kimematic invariant, the singular points being the only exceptions.

Under certain conditions, which are met in our problem, the Picard–Lefschetz formula determines the variation undergone by integration domains when an unintegrated variable of the integral is sent on a path in the complex plane around a value, where a pinch singularity of the integral occurs. It was known for a long time that at least in some well behaved cases, the formula would apply to Feynman integrals and predict their analytic structure. With this motivation in mind, the theory was extended by Fotiadi, Froissart, Lascoux and especially by Pham [29, 38, 39] in the sixties, using results of Thom [44] and Leray [36]. Related literature from the sixties and seventies shows that already for rather simple Feynman integrals a practical application of Picard–Lefschetz theory is far from trivial.

Since then, other methods to determine the analytic properties of Feynman integrals have become more important. Cutkosky rules predict the discontinuities in a handy, graphical way in terms of cut-integrals. Furthermore, if the Feynman integral can be computed in the Euclidean region in terms of sufficiently well-known functions such as multiple polylogarithms, the analytic continuation to other regions can be deduced from the analytic properties of these functions. However, the mentioned theory framework around the Picard–Lefschetz theorem seems to experience new attention in the recent literature on Feynman integrals. Extended Picard–Lefschetz theory was used in a recent proof of the Cutkosky rules in [16]. Furthermore, in a series of articles [2–4] which employs Leray's residue theory for the definition of cut integrals, it is suggested that the discontinuities play a crucial role in a conjectured co-product structure on Feynman integrals, motivated from the co-product on polylogarithms. We take these recent developments as additional motivation to emphasise the role of homology in our application.

Our presentation is organized as follows: In the next section, we review the family of Feynman integrals associated to the kite graph and its underlying family of elliptic curves. In Sect. 3 we reduce the problem of the analytic continuation of the master integrals of the kite family to the question how the periods of the elliptic curve behave under a particular variation of a kinematic parameter. Section 4 discusses the latter problem as an application of the Picard–Lefschetz formula.

2 The Kite Family and Its Elliptic Curve

We consider the family of Feynman integrals associated to the kite graph of Fig. 1c. The same particle mass m is assigned to each of the three solid internal edges while the propagators drawn with dashed lines are massless. The graph has one external momentum p and we define $t = p^2$. The integrals of this family in D-dimensional Minkowski space are

$$I(\nu_1, \nu_2, \nu_3, \nu_4, \nu_5) = (-1)^{\nu} \int \frac{d^D l_1 d^D l_2}{\left(i\pi^{\frac{d}{2}}\right)^2} \prod_{i=1}^{5} D_i^{-\nu_i}$$

with inverse propagators $D_1 = l_1^2 - m^2$, $D_2 = l_2^2$, $D_3 = (l_1 - l_2)^2 - m^2$, $D_4 = (l_1 - p)^2$, $D_5 = (l_2 - p)^2 - m^2$ and $\nu = \sum_{i=1}^{5} \nu_i$. The integration is over loop-momenta l_1, l_2. These integrals are obviously functions of D, t and m^2 which is suppressed in our notation. By integration-by-parts reduction, the integrals of this family with $\nu_i \in \mathbb{Z}$ can be expressed as linear combinations of eight master integrals, which can be chosen as $I(2, 0, 2, 0, 0)$, $I(2, 0, 2, 1, 0)$, $I(0, 2, 2, 1, 0)$, $I(0, 2, 1, 2, 0)$, $I(2, 1, 0, 1, 2)$, $I(1, 0, 1, 0, 1)$, $I(2, 0, 1, 0, 1)$, $I(1, 1, 1, 1, 1)$. The first five of these integrals can be expressed in terms of multiple polylogarithms [30, 31]

$$\mathrm{Li}_{n_1,\dots,n_r}(z_1, \dots, z_r) = \sum_{j_1 > j_2 > \dots > j_r > 0} \frac{z_1^{j_1} \dots z_r^{j_r}}{j_1^{n_1} \dots j_r^{n_r}} \text{ for } |z_i| < 1.$$

The latter three integrals correspond to the graphs in Fig. 1 respectively. For the computation of these integrals, multiple polylogarithms are not sufficient. In particular the sunrise integral $I(1, 0, 1, 0, 1)$ has been essential in recent developments to extend the classes of functions applied in Feynman integral computations beyond multiple polylogarithms. We refer to [1, 10, 11, 13–15, 20–26, 37, 40, 41, 43] for some of these recent developments in quantum field theory and string theory.

The master integrals of the kite family can be computed by use of the method of differential equations, deriving a system of ordinary first-order differential equations in the variable t. It was shown in [5, 42] that certain changes of the basis of master integrals simplify the system of equations and in [13] it was shown that by a non-algebraic change of variables, the system can even be written in canonical form [32]. Results for the master integrals were given in terms of elliptic generalizations of (multiple) polylogarithms. In [5] it was shown that in the Euclidean region where $t < 0$ the master integrals can be expressed in terms of functions

$$\mathrm{ELi}_{n;m}(x; y; q) = \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \frac{x^j}{j^n} \frac{y^k}{k^m} q^{jk} = \sum_{k=1}^{\infty} \frac{y^k}{k^m} \mathrm{Li}_n(q^k x), \tag{1}$$

and multi-variable generalizations

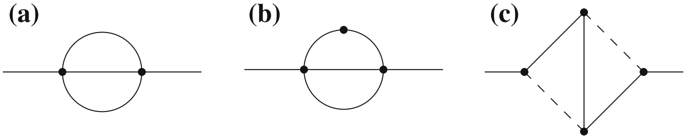

Fig. 1 The sunrise graph (**a**), the sunrise with one raised index (**b**), and the kite graph (**c**)

$$\mathrm{ELi}_{n_1,\dots,n_l;m_1,\dots,m_l;2o_1,\dots,2o_{l-1}}\left(x_1,\dots,x_l;y_1,\dots,y_l;q\right)$$
$$=\sum_{j_1=1}^{\infty}\cdots\sum_{j_l=1}^{\infty}\sum_{k_1=1}^{\infty}\cdots\sum_{k_l=1}^{\infty}\frac{x_1^{j_1}}{j_1^{n_1}}\cdots\frac{x_l^{j_l}}{j_l^{n_l}}\frac{y_1^{k_1}}{k_1^{m_1}}\cdots\frac{y_l^{k_l}}{k_l^{m_l}}\frac{q^{j_1k_1+\dots+j_lk_l}}{\prod_{i=1}^{l-1}\left(j_ik_i+\dots+j_lk_l\right)^{o_i}} \tag{2}$$

to all orders in $\varepsilon = (4-D)/2$. Results in terms of iterated integrals over modular forms were derived in [12]. For the purpose of this presentation, aiming at the analytic continuation of the results beyond the Euclidean region, the precise shape of the results for the master integrals is not relevant. The following discussion merely uses the fact that up to simple prefactors the results can be expressed as power series in $q = q(t)$ which is the nome of a family of elliptic curves, with the parameter of the family being the kinematic invariant t.

This family of elliptic curves is derived from the sunrise integral $I(1,0,1,0,1)$ following [17]. The second Symanzik polynomial reads

$$\mathscr{F} = -x_1x_2x_3t + m^2\left(x_1+x_2+x_3\right)\left(x_1x_2+x_2x_3+x_1x_3\right).$$

A change of variables transforms the equation $\mathscr{F} = 0$ to the Weierstrass normal form

$$y^2 = 4\left(x-e_1\right)\left(x-e_2\right)\left(x-e_3\right)$$

with the three roots

$$e_1 = \frac{1}{24}\left(-t^2+6m^2t+3m^4+3\left(m^2-t\right)^{\frac{3}{2}}\left(9m^2-t\right)^{\frac{1}{2}}\right)$$
$$e_2 = \frac{1}{24}\left(-t^2+6m^2t+3m^4-3\left(m^2-t\right)^{\frac{3}{2}}\left(9m^2-t\right)^{\frac{1}{2}}\right)$$
$$e_3 = \frac{1}{24}\left(2t^2-12m^2t-6m^4\right)$$

of the cubical polynomial in x, satisfying $e_1+e_2+e_3=0$. The family of elliptic curves degenerates at the values $0,\ m^2,\ 9m^2,\ \infty$ of the parameter t. In the Euclidean region $t<0$ the three roots are real and separated as $e_1 > e_3 > e_2$. Here we define the period integrals

$$\psi_1 = 2\int_{e_2}^{e_3}\frac{dx}{y},\ \ \psi_2 = 2\int_{e_1}^{e_3}\frac{dx}{y}$$

which evaluate to

$$\psi_1 = \frac{4}{\left(m^2-t\right)^{\frac{3}{4}}\left(9m^2-t\right)^{\frac{1}{4}}}K(k),\ \ \psi_2 = \frac{4i}{\left(m^2-t\right)^{\frac{3}{4}}\left(9m^2-t\right)^{\frac{1}{4}}}K(k')$$

with the complete elliptic integral of the first kind

$$K(k) = \int_0^1 \frac{dt}{\sqrt{\left(1-t^2\right)\left(1-k^2t^2\right)}} \tag{3}$$

where the modulus k and the complementary modulus k' are given by

$$k = \frac{e_3-e_2}{e_1-e_2},\ \ k'^2 = 1-k^2 = \frac{e_1-e_3}{e_1-e_2}.$$

With these periods we introduce

$$\tau = \frac{\psi_2}{\psi_1},\ \ q = e^{i\pi\tau}.$$

The mentioned results of [5] for the eight master integrals in the Euclidean region are expressed in terms of the functions of Eqs. 1 and 2 with the nome q. Up to simple general prefactors involving the first period ψ_1, this is their only dependence of the kinematic invariant t.

3 Analytic Continuation

The previous section has shown that the analytic continuation of the eight master integrals of the kite family can be reduced to the analytic continuation of the two period integrals ψ_1, ψ_2. We are interested in the analytic behaviour of the periods ψ_1, ψ_2 as t varies along the real axis beyond the Euclidean region. As singular points and branch cuts of the period integrals correspond to real values of t, we consider the variation of t in the complex t-plane and shift the contour of this variation slightly away from the real axis by Feynman's prescription $t \to t + i\delta$. Here δ is small, real, positive and sent to zero in the end for evaluations on the real axis. We choose the contour such that it furthermore circumvents the singular points in small half circles. Fig. 2 shows the contour of the variation of t.

In order to discuss the branch cut behaviour of the periods, it is furthermore useful to consider the complete elliptic integral of the first kind in Eq. 3 as a function of k^2 and note that it has only one branch cut $[1, \infty[$ in the complex k^2-plane. We study the question, where along the variation of t this branch cut is crossed for the two periods. Figure 3 shows the behaviour of k^2 and k'^2 as t is varied along the contour of Fig. 2.

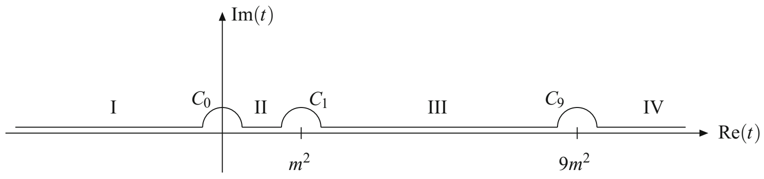

Fig. 2 Variation contour in the complex t-plane

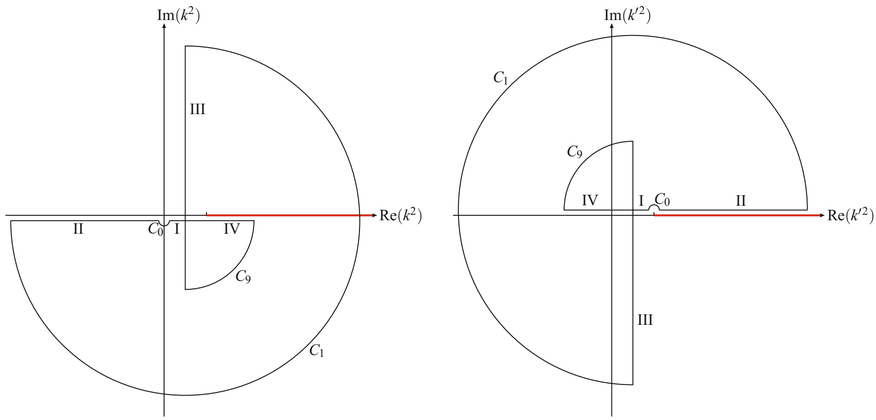

Fig. 3 Variations in the complex plane of k^2 and k'^2

We notice that k'^2 does not cross the branch cut of the complete elliptic integral at all. The variable k^2 crosses the branch cut only once. This happens as t is varied on the half circle C_1 around the singular point $t = m^2$. Therefore it is this piece of the contour of t along which we have to study the behaviour of the first period ψ_1 more closely.

The three quarters of the circle which k^2 takes in Fig. 3 may be deformed to a full circle for convenience. In order to study this variation, we consider the Legendre form

$$y^2 = x(x - \lambda)(x - 1)$$

of the family of elliptic curves, where $\lambda = k^2$. As t varies along C_1, the parameter λ moves in a small circle around 1. Equivalently, we can describe this variation by

$$y^2 = x(x - e_1(\varphi))(x - e_2(\varphi))$$

with $e_1(\varphi) = 1 - re^{i\varphi}, \quad e_2(\varphi) = 1 + re^{i\varphi}$ where r is a small, positive, real number and φ is an angle whose value is 0 in the beginning and monotonously rises to 2π. In order to observe the change of the two periods along this variation, it is convenient to write them as integrals over cycles δ_1, δ_2 which form a basis of the first homology group of the elliptic curve. We introduce

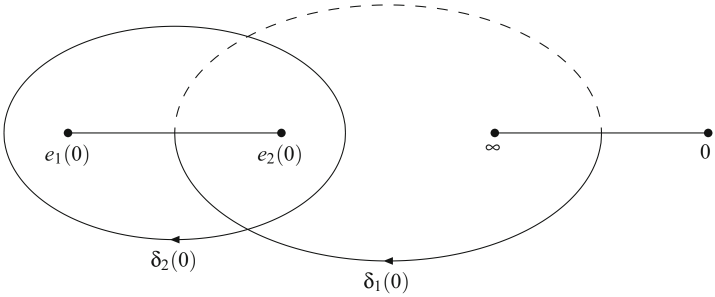

Fig. 4 The cycles δ_1 and δ_2 before the variation

$$P_1(\varphi) = \int_{\delta_1} \frac{dx}{y}, \quad P_2(\varphi) = \int_{\delta_2} \frac{dx}{y}, \quad y = -\sqrt{x}\sqrt{x - e_1(\varphi)}\sqrt{x - e_2(\varphi)},$$

where the cycles δ_1, δ_2 are oriented such that

$$P_1(0) = 2\int_0^{e_1(0)} \frac{dx}{y} = -2\int_{e_2(0)}^{\infty} \frac{dx}{y} \quad \text{and} \quad P_2(0) = 2\int_{e_2(0)}^{e_1(0)} \frac{dx}{y}$$

with the integration contour on the right-hand side slightly shifted by a negative imaginary part for x. Figure 4 shows the cycles δ_1, δ_2 on the elliptic curve. The use of dashed and straight lines indicates that δ_1 has two parts in two different Riemann sheets of the elliptic curve, separated by the branch cuts. The question is: How do the two cycles change under the mentioned variation? This will be discussed in Sect. 4. There we will see that δ_1 becomes $\delta_1 - 2\delta_2$ while δ_2 remains unchanged. We therefore obtain:

$$P_1(2\pi) = P_1(0) - 2P_2(0) \quad \text{and} \quad P_2(2\pi) = P_2(0).$$

This is the behaviour of the periods as t varies around the critical point $t = m^2$. The above discussion has shown that the behaviour along all other pieces of the variation is trivial. We hence arrive at the analytic continuation of the two period integrals:

$$\begin{pmatrix} \psi_2(t + i\delta) \\ \psi_1(t + i\delta) \end{pmatrix} = \frac{4}{\left(m^2 - t - i\delta\right)^{\frac{3}{4}} \left(9m^2 - t - i\delta\right)^{\frac{1}{4}}} M_t \begin{pmatrix} iK\left(k'\left(t + i\delta\right)\right) \\ K\left(k\left(t + i\delta\right)\right) \end{pmatrix}$$

with

$$M_t = \begin{cases} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \text{for } -\infty < t < m^2, \\ \begin{pmatrix} 1 & 0 \\ -2 & 1 \end{pmatrix} & \text{for } m^2 < t < \infty. \end{cases}$$

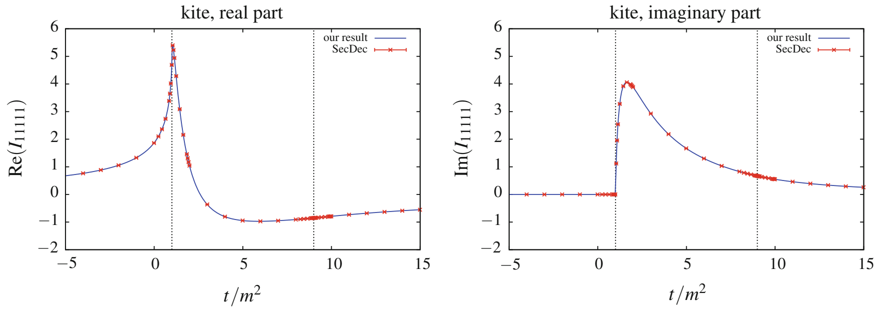

Fig. 5 The real and imaginary parts of the ε^0-term of the kite integral. The dashed vertical lines indicate $t = m^2$ and $t = 9m^2$. The blue line is our analytic result and the red dots are numerical data produced with the program SecDec [19]

Applying this result in terms of

$$q(t + i\delta) = e^{i\pi \frac{\psi_2(t+i\delta)}{\psi_1(t+i\delta)}}$$

to the functions in Eqs. 1 and 2, we obtain the analytic continuation of the results for the master integrals of the kite family. As an example, the results for the ε^0-term for the kite integral $I(1, 1, 1, 1, 1)$ in $4 - 2\varepsilon$ dimensions are plotted in Fig. 5.

4 An Application of the Picard–Lefschetz Formula

Before we discuss the deformation of δ_1 which was left open in the previous section, let us recall the main idea of the Picard–Lefschetz formula with the help of a classical example[1] [34]. We consider the integral

$$I(\lambda) = \int_a^b \frac{1}{x^2 - \lambda} dx = \frac{1}{2\sqrt{\lambda}} \ln\left(\frac{\left(a + \sqrt{\lambda}\right)\left(b - \sqrt{\lambda}\right)}{\left(a - \sqrt{\lambda}\right)\left(b + \sqrt{\lambda}\right)}\right)$$

with real $b > a > 0$ depending on a complex parameter λ. We are interested in the point $\lambda = 0$ where the two singular points $e_1 = -\sqrt{\lambda}$ and $e_2 = \sqrt{\lambda}$ coincide. As long as the integration contour from a to b is not in between e_1 and e_2, this contour is not trapped when the two singular points approach each other. This is the situation of Fig. 6a, corresponding to the principal sheet of the logarithm. There is no square-root singularity in this case.

The more interesting situation is shown in Fig. 6b where the integration contour is in between the points e_1 and e_2 and will be trapped for $\lambda = 0$. (This picture is

[1] Thorough introductions to Picard–Lefschetz theory can be found in [28, 39].

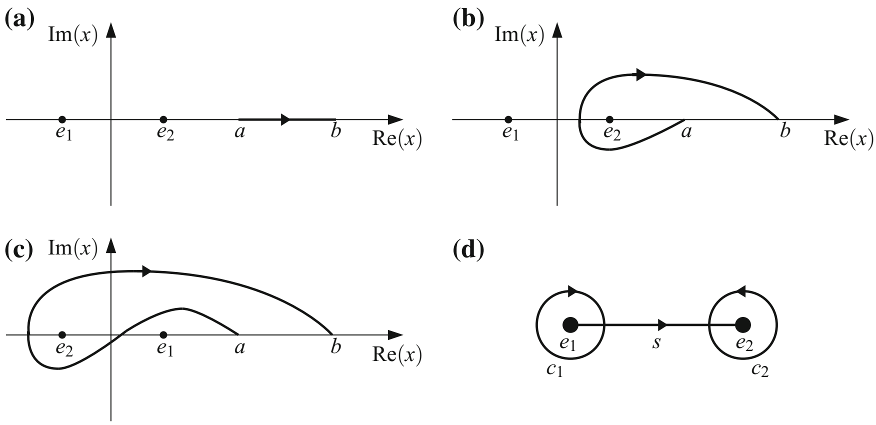

Fig. 6 Contours in the complex x-plane

obtained after sending λ in a small circle around a^2 in anti-clockwise direction.) The situation at $\lambda = 0$ is known as a simple pinch and it gives rise to a square-root singularity.

Let us now send λ in a small circle around 0 in anti-clockwise direction. We will call this the variation of λ. This causes the points e_1 and e_2 to rotate around each other in anti-clockwise direction until they have changed positions. The result of this movement is shown in Fig. 6c. The integration contour is deformed by this rotation as shown in the figure. Along the variation of λ, the integral $I(\lambda)$ picks up a discontinuity, which is an integral with the same integrand and the integration contour given by two small cycles c_1, c_2 around e_1, e_2 with orientations shown in Fig. 6d. It is easy to see that these two cycles are in a homological sense the difference between the integration contours of $I(\lambda)$ before and after the variation of λ.

It is this change of integration contours after variations around a simple pinch which is computed in the Picard–Lefschetz formula. The formula can be written as

$$c \to c + k \cdot h, \tag{4}$$

where c is a path or cycle, in our case the contour of integration of $I(\lambda)$, the arrow indicates the change along the variation of λ, k is an integer and h is another cycle. Both, the integer k and the cycle h are determined from a so-called vanishing cycle associated to the pinch situation. In our simple example, the relevant vanishing cycle is the straight line s oriented from e_1 to e_2 as shown in Fig. 6d. This line is indeed vanishing if λ goes to zero and it is a relative cycle in the relative homology of the complex plane modulo the set of points $\{e_1, e_2\}$. We may consider s as an oriented 1-simplex and obtain its boundary as

$$\partial s = e_2 - e_1. \tag{5}$$

The last ingredient in the construction of the cycle h is the co-boundary operator δ of Leray [36]. The co-boundary of an n-dimensional cycle can be thought of as an $(n+1)$-dimensional tube wrapped around the cycle. In our case, we only need to construct the co-boundary of a point, which is a small circle around this point with anti-clockwise orientation. We obtain

$$h = \delta\,(\partial s) = c_1 + c_2$$

where the minus sign in Eq. 5 is reflected in the clockwise orientation of c_1.

It remains to determine the integer k in the Picard–Lefschetz formula. Up to a sign, which depends on the dimension of the problem, this number is an intersection number or Kronecker index, depending only on the relative orientation of the cycle c and the vanishing cycle at their intersection. In our case one simply obtains $k = 1$. In conclusion, the Picard–Lefschetz formula predicts $c \to c + c_1 + c_2$ which is precisely what we have deduced from the figures above.

We are only two steps away from the answer to the question left open in Sect. 3. On the elliptic curve, the points $e_1(\lambda)$, $e_2(\lambda)$ coincide for $\lambda = 1$ and trap the cycle δ_1 in a simple pinch, similar to the above example. In contrast to the warm-up example, these two points make not half of a rotation but a full rotation around each other as λ is sent around the pinch point. We therefore have an additional factor 2 in the Picard–Lefschetz formula and obtain

$$\delta_1(0) \to \delta_1(2\pi) = \delta_1(0) + 2\,(c_1 + c_2)$$

where c_1 and c_2 are the small circles around e_1 and e_2 again. The series of snapshots in Fig. 7 shows in more detail how after half of a rotation, these circles arise in the deformation of δ_1 and from these pictures it is clear, that c_1 and c_2 are located in different Riemann sheets. In order to express the change of δ_1 in terms of the basis of the first homology group, $\delta_1(0)$, $\delta_2(0)$, we may pull c_1 over to the same sheet as c_2. This is the step from in Fig. 7c to d. We see that they combine to the cycle $-\delta_2(0)$ and arrive at the result

$$\delta_1(0) \to \delta_1(2\pi) = \delta_1(0) - 2\delta_2(0)$$

applied in Sect. 3.

We remark that this deformation on the elliptic curve is also a well-known example. Detailed discussions with slightly different visualizations can be found e.g. in [27, 45] where the Riemann sheets, glued together to a torus, are viewed as twisted against each other.

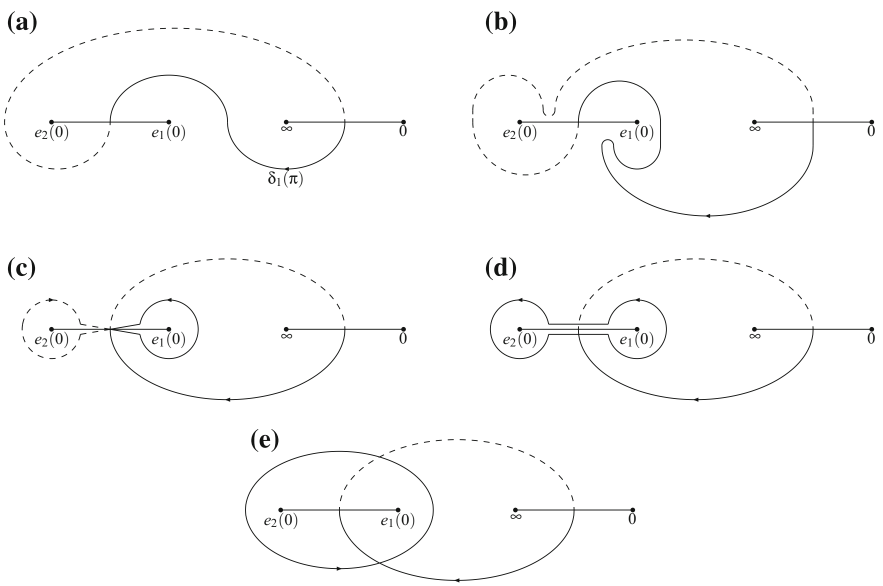

Fig. 7 The deformation of δ_1 on the elliptic curve

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A Four-Point Function for the Planar QCD Massive Corrections to Top-Antitop Production in the Gluon-Fusion Channel

Roberto Bonciani, Matteo Capozi and Paul Caucal

Abstract In these proceedings we present the study of a four-point function that is involved in the evaluation of the Master Integrals necessary to compute the two-loop massive QCD planar corrections to $t\bar{t}$ production in the gluon fusuin channel, at hadron colliders. The solution involves complete elliptic integrals of the first and second kind and one- or two-fold integrations of such elliptic integrals multiplied by ratios of polynomials, inverse square roots and logarithms or dilogarithms.

1 Introduction

The NNLO QCD corrections to the production of a $t\bar{t}$ pair in hadronic collisions are known since some years [1–8]. In these works, all the calculations used to evaluate the different ingredients contributing to the corrections to inclusive and more exclusive observables, were done using semi-numerical methods. A complete analytic computation of the cross section at that perturbative order is not yet available, although many ingredients are present in the literature. In particular, the matrix elements for the one-loop $2 \to 3$ process are known since the work in [9–12]; progresses are also done in the determination of the infra-red (IR) subtraction terms [13–16], needed to cure IR divergences in collinear and soft regions of the phase space during the integration; finally the one-loop squared matrix elements were calculated in

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[17–19]. The genuinely two-loop part of the calculation, i.e. the interference between the two-loop $2 \to 2$ diagrams and the tree-level, are known only partially.

At NNLO in QCD, two-loop contributions to the $t\bar{t}$ production process in hadronic collisions come from two partonic channels: $q\bar{q} \to t\bar{t}$ (quark-annihilation channel) and $gg \to t\bar{t}$ (gluon fusion channel).

The interference of the two-loop amplitude in the quark-annihilation channel with the corresponding tree-level amplitude can be expressed in terms of ten gauge independent color factors. The color structure in the gluon-fusion channel is more complicated, and it can be expressed in terms of sixteen color factors.

All the ten color coefficients of the $q\bar{q}$ channel are known numerically [20] and their infrared poles are known analytically [21, 22]. For eight out of the ten color coefficients a complete analytic expression, written in terms of generalized harmonic polylogarithms (GPLs) [23–26], was found in [27, 28].

All of the sixteen color coefficients appearing in the two-loop corrections in the gluon-fusion channel are known numerically [29] and the analytic expression of all the infrared poles was evaluated in [21, 22]. In addition, a complete analytic expression (again written in terms of GPLs) is known for ten out of the sixteen color coefficients [30–32]. The remaining six color coefficients in this partonic channel are known to involve elliptic integrals. Very recently, the master integrals (MIs) for planar topologies that involve a closed heavy fermionic loop were evaluated in [33–35]. They contribute to one of the six unknown color coefficients.

In these proceedings, we give a short description of the computation of one of the four-point functions at 5 denominators that enter the calculation of the massive two-loop QCD planar corrections to the $t\bar{t}$-pair production at hadron colliders.

2 Notations

We consider the process $g(p_1) + g(p_2) \to t(p_3) + \bar{t}(p_4)$ in which the external particles are on their mass-shell $p_1^2 = p_2^2 = 0$, $p_3^2 = p_4^2 = m_t^2$ and where m_t is the mass of the top quark.

The squared matrix element, summed over spin and colour, can be expanded in powers of the strong coupling constant α_s according to

$$\sum \left| \mathscr{M}\left(s, t, m_t^2, \varepsilon\right) \right|^2 = 16\pi^2 \alpha_s^2 \left[\mathscr{A}_0 + \frac{\alpha_s}{\pi} \mathscr{A}_1 + \left(\frac{\alpha_s}{\pi}\right)^2 \mathscr{A}_2 + \mathscr{O}\left(\alpha_s^3\right) \right], \quad (1)$$

where $\varepsilon = (4 - d)/2$ indicates the dimensional regulator and where the functions $\mathscr{A}_i$ depend upon s, t, m_t^2, ε. After UV renormalization, the terms $\mathscr{A}_i$ still include IR divergences, which appear as poles in ε. These divergences cancel only after the virtual corrections are added to the real emission ones.

The term $\mathscr{A}_2$ in Eq. (1) can be further split in the sum of two contributions

$$\mathscr{A}_2 = \mathscr{A}_2^{(2\times 0)} + \mathscr{A}_2^{(1\times 1)} . \quad (2)$$

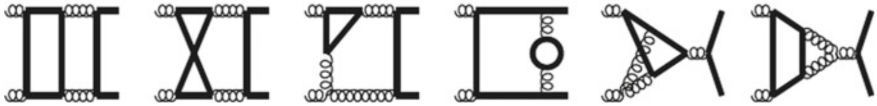

Fig. 1 Examples of Feynman diagrams contributing to the calculation of the color coefficients E_h, F_h, G_h

$\mathscr{A}_2^{(1\times 1)}$ arises from the interference of one loop diagrams and was evaluated in [17–19]. The color structure of the interference of two-loop and tree-level diagrams, $\mathscr{A}_2^{(2\times 0)}$, is the following

$$\begin{aligned}\mathscr{A}_2^{(2\times 0)} = \left(N_c^2-1\right)\Big\{ & N_c^3 A + N_c B + \frac{1}{N_c} C + \frac{1}{N_c^3} D + N_c^2 N_l E_l + N_c^2 N_h E_h + N_l F_l + N_h F_h \\ & + \frac{N_l}{N_c^2} G_l + \frac{N_h}{N_c^2} G_h + N_c N_l^2 H_l + N_c N_h^2 H_h + N_c N_l N_h H_{lh} + \frac{N_l^2}{N_c} I_l \\ & + \frac{N_h^2}{N_c} I_h + \frac{N_l N_h}{N_c} I_{lh} \Big\}, \end{aligned} \tag{3}$$

where N_c indicates the number of colors, N_l the number of massless flavor quarks (in our case $N_l = 5$) and N_h the number of quarks of mass m_t ($N_h = 1$). The sixteen gauge-invariant color coefficients $A, B, \ldots, I_{lh}$ are functions of s, t, m_t^2 and ε. To date, only the leading color coefficient, A and the seven color coefficients proportional to N_l: E_l, F_l, G_l, H_l, H_{lh}, I_l and I_{lh} were calculated analytically [30–32].

In these proceedings, we focus on the QCD corrections at two loops in which a top-quark loop is present. Some examples of Feynman diagrams belonging to this set are shown in Fig. 1. These contributions enter the calculation of the color coefficients E_h, F_h, G_h. In particular, the planar diagrams, such as the ones in Fig. 1a, c, d, f … contribute to all of the three color coefficients, while the crossed diagrams, b, e, … contribute only to F_h and G_h. This means that, computing the planar diagrams we are able to give an analytic expression for the coefficient E_h. In these proceedings we focus on the planar corrections.

We introduce the Mandelstam invariants

$$s = (p_1+p_2)^2\,, \quad t = (p_1-p_3)^2\,, \quad u = (p1-p_4)^2\,, \tag{4}$$

where $s+t+u = 2m_t^2$.

The interference of the two-loop Feynman diagrams contributing to the NNLO QCD planar heavy-loop corrections to $g+g \to t+\bar{t}$ can be expressed in terms of scalar integrals belonging to the following 9-denominators family:

$$\int \mathscr{D}^d k_1 \mathscr{D}^d k_2 \frac{1}{D_1^{a_1} D_2^{a_2} D_3^{a_3} D_4^{a_4} D_5^{a_5} D_6^{a_6} D_7^{a_7} D_8^{a_8} D_9^{a_9}}\,, \tag{5}$$

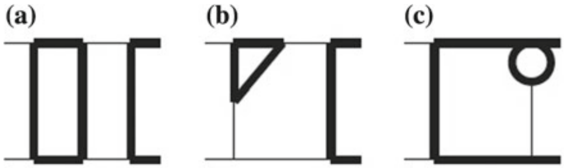

Fig. 2 Seven- and six-denominator topologies

where a_i, with $i = 1, \ldots, 9$, are integer numbers. The D_i, $i = 1, \ldots, 9$, are the denominators involved, d is the dimension of the space-time, and the normalization is such that

$$\mathscr{D}^d k_i = \frac{d^d k_i}{i\pi^{\frac{d}{2}}} e^{\varepsilon \gamma_E} \left(\frac{m_t^2}{\mu^2} \right)^{\varepsilon} . \tag{6}$$

The routing that we used for the propagators is the following:

$$\Big\{ -k_1^2 + m_t^2, -(p_1 + k_1)^2 + m_t^2, -k_2^2 + m_t^2, -(p_1 + k_1 - k_2)^2,$$
$$-(p_1 - p_3 + k_1 - k_2)^2 + m_t^2, -(p_2 - k_1 + k_2)^2, -(p_2 - k_1)^2 + m_t^2,$$
$$-(k_1 - k_2)^2, -(p_3 + k_1)^2 \Big\} , \tag{7}$$

where the momenta k_1 and k_2 are the loop momenta.

There are two 7-denominator and one 6-denominator new topologies involved in this calculation. They are shown in Fig. 2. Other topologies at 6 denominators that enter the calculation are the three-point functions studied for the NLO QCD corrections to Higgs production in gluon fusion [36, 37].

The reduction to the MIs of the families in Eq. (5) was performed using the computer programs[1] `FIRE` [42–44] and `Reduze 2` [45, 46], that implement integration-by-parts identities [47–49] and Lorentz-invariance identities [50]. We find 55 MIs, shown in Fig. 3. Some of these MIs were known in the literature from previous works [27, 28, 30–32, 51–60].

3 The Differential Equations

The MIs shown in Fig. 3 were calculated using the differential equations method [50, 61–64]. Some of the MIs lead to differential equations that admit solutions defined by elliptic integrals. Therefore, for some of the MIs in Fig. 3 a second order linear differential equation has to be solved. With this respect is worth to notice that we can distinguish among three different groups of MIs. The first group of MIs is constituted by the diagrams in Fig. 3 ($\mathscr{T}_1$)–($\mathscr{T}_6$), ($\mathscr{T}_9$)–($\mathscr{T}_{14}$), ($\mathscr{T}_{17}$)–($\mathscr{T}_{27}$),

[1] Other public programs for the reduction to the MIs can be found in [38–41].

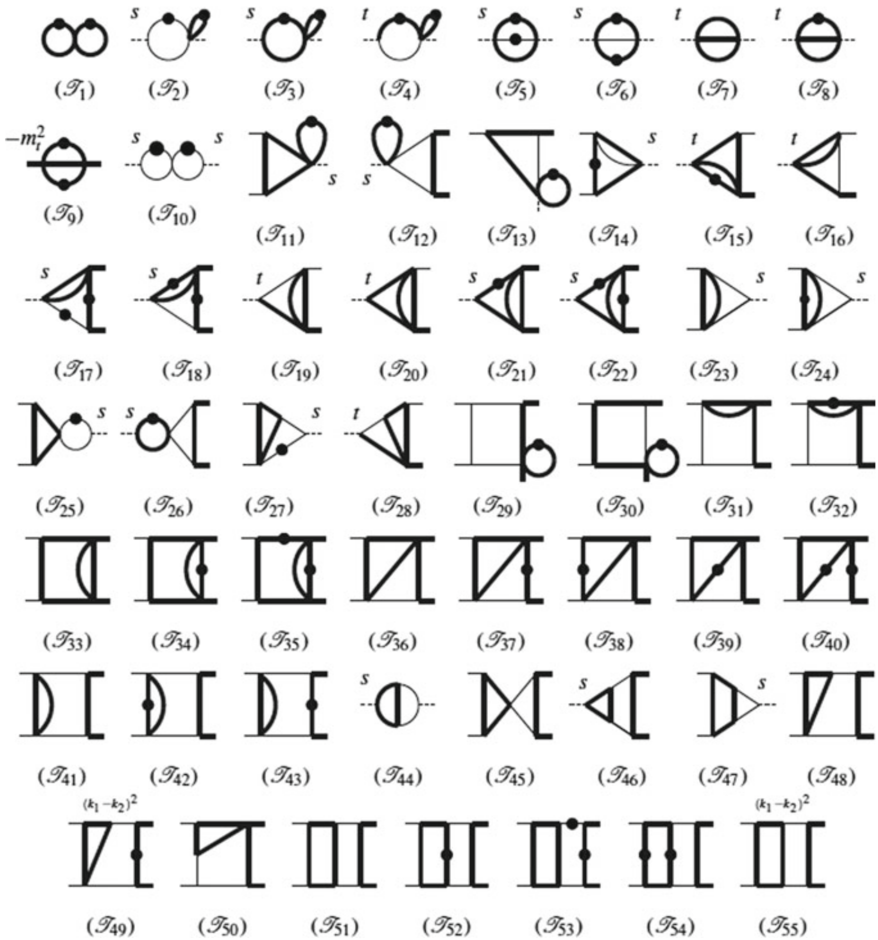

Fig. 3 Master integrals in pre-canonical form. Internal plain thin lines represent massless propagators, while thick lines represent the top propagator. External plain thin lines represent massless particles on their mass-shell. External thick lines represents the top quark on its mass-shell

$(\mathcal{T}_{29})$–$(\mathcal{T}_{32})$, $(\mathcal{T}_{44})$–$(\mathcal{T}_{47})$. For these MIs, the system of differential equations can be cast in canonical form [65] (see also [66–75]). The solution is expressed in terms of GPLs with maximum weight 4. We checked our results against the numerical program FIESTA4 [76–78] finding complete agreement within the error quoted by FIESTA4 both in the Euclidean and Minkowski regions. The analytic continuation to Minkowski region was done numerically, adding to s a small imaginary part, $s + i0^+$, according to the causal prescription.

The second group of MIs is constituted by the diagrams in Fig. 3 $(\mathcal{T}_{15})$, $(\mathcal{T}_{16})$, $(\mathcal{T}_{28})$, $(\mathcal{T}_{48})$–$(\mathcal{T}_{50})$. These MIs have homogeneous equation with solution that do not involve elliptic integrals, but in the non-homogeneous part of the differential equation they contain elliptic integrals, in particular the equal-mass sunrise diagrams ($\mathscr{T}_7$) and ($\mathscr{T}_8$).

The last group is constituted by the diagrams in Fig. 3 ($\mathscr{T}_{33}$)–($\mathscr{T}_{43}$) and ($\mathscr{T}_{51}$)–($\mathscr{T}_{55}$). These MIs have solutions of the homogeneous part of the differential equations that are expressed in terms of elliptic integrals and, moreover, also the non homogeneous parts contain elliptic integrals.

In these proceedings we will focus on the study of the MIs ($\mathscr{T}_{33}$)–($\mathscr{T}_{35}$).

3.1 Second Order Differential Equation

The three MIs ($\mathscr{T}_{33}$)–($\mathscr{T}_{35}$) satisfy a system of coupled first-order linear differential equations. With the basis choice presented in Fig. 3 we are able to decouple one of the three, the scalar $\mathscr{T}_{33}$, from the other two, that remain coupled. This is the best we can do, and therefore, order-by-order in ε, we have to solve a second-order linear differential equation in s and one in t. The differential equation in s for $\mathscr{T}_{34}$ at $\mathscr{O}(\varepsilon^0)$ is the following:

$$\frac{d^2}{ds^2}F + p(s,t)\frac{d}{ds}F + q(s,t)F = \Omega(s,t)\,, \tag{8}$$

where

$$p(s,t) = -\frac{1}{(s-4)} - \frac{2}{s} - \frac{1}{\left(s - 4\frac{t-1}{t-9}\right)} - \frac{1}{\left(s + \frac{(t-1)^2}{t}\right)} + \frac{1}{\left(s + 4\frac{t+1}{t+3}\right)}\,, \tag{9}$$

$$\begin{aligned} q(s,t) = &-\frac{1}{4s^2} - \frac{(t-9)^5}{(256(t-3)^3(4-9s-4t+st))} \\ &-\frac{(3+t)^5}{(64(-4+3s+4t+st)(-3-2t+t^2)^2)} \\ &+\frac{(5-10t+2t^2)}{(4s(t-1)^2)} + \frac{(-25-77t-27t^2+t^3)}{(128(-4+s)(1+t)^2)} \\ &-\frac{((t-9)^2(-1971+1944t-534t^2+48t^3+t^4))}{(256(4+s(t-9)-4t)(t-3)^3(t-1))} \\ &+\frac{(9t^2+6t^3+2t^4-6t^5+t^6)}{((t-3)^2(t-1)^2(1+t)^2(1-2t+st+t^2))} \\ &-\frac{((3+t)^2(135+192t-10t^2-72t^3+11t^4))}{(64(t-3)^2(t-1)(1+t)^2(-4+4t+s(3+t)))}\,, \end{aligned} \tag{10}$$

and where the non-homogeneous part $\Omega(s,t)$ contains the master integrals of the subtopologies, namely $\mathscr{T}_1$, $\mathscr{T}_3$, $\mathscr{T}_7$, $\mathscr{T}_8$, $\mathscr{T}_9$, $\mathscr{T}_{11}$, $\mathscr{T}_{15}$, $\mathscr{T}_{21}$, $\mathscr{T}_{22}$. The differential equation in t has an analogous structure.

Equation (8) is complicated to solve. The rational functions $p(s,t)$ and $q(s,t)$ have many divergence points and it is not easy in general to find two independent solutions of the homogeneous part. A strategy for the reduction of the number of singularities in $p(s,t)$ and $q(s,t)$, like the one used in [79], does not work in this case. Therefore, we have to find another approach in order to be able to solve the homogeneous part of Eq. (8) and then integrate the particular solution with the Euler method.

3.2 Homogeneous Solution and Maximal Cut

A possibility to find the solution of the second-order linear differential equation was pointed out in [80–83]. It is based on the fact that the maximal cuts of the diagrams we are interested on are a solution of the homogeneous part of the system of first-order linear differential equations they satisfy and, therefore, of the associated second-order differential equations for the single MIs. In particular, the MI $\mathcal{T}_{34}$ is finite, and therefore we use directly the technique proposed in [81]. The four-dimensional maximal cut can be expressed as follows:

$$Cut(s,t) = \frac{1}{R(s,t)}\, K(\omega)\,, \tag{11}$$

where

$$K(\omega) = \int_0^1 \frac{dx}{\sqrt{(1-x^2)(1-\omega x^2)}} \tag{12}$$

is the complete elliptic integral of the first kind and where

$$\omega(s,t) = \frac{N(s,t)}{D(s,t)}\,, \tag{13}$$

$$R(s,t) = 2\sqrt{s\, D(s,t)} \tag{14}$$

with

$$N(s,t) = 16\sqrt{s(t^2+(s-2)t+1)}\,, \tag{15}$$

$$\begin{aligned} D(s,t) = {} & 4(t-1)\left(2\frac{t-1}{s+t-1}\sqrt{s(t^2+(s-2)t+1)} - t + 1\right) \\ & + s\left(t^2 + 8\frac{\sqrt{s(t^2+(s-2)t+1)}}{(s+t-1)} - 6t - 3\right). \end{aligned} \tag{16}$$

In Eqs. (15), (16) we considered $m_t^2 = 1$.

The two independent solutions of the homogeneous part of Eq. (8) are then

$$\psi_1(s,t) = \frac{1}{R(s,t)}\, K(\omega)\,, \qquad \psi_2(s,t) = \frac{1}{R(s,t)}\, K(1-\omega) \tag{17}$$

and they are solution also for the homogeneous part of the second-order linear differential equation in t.

3.3 Complete Solution

Once the solutions for the homogeneous differential equations are found, we can proceed to the integration of the particular solution using the Euler method of variation of the arbitrary constants. For convenience we introduce the two dimensionless variables, x and y, such that

$$s = -m_t^2 \frac{(1-x)^2}{x}\,, \qquad t = -m_t^2 y\,. \tag{18}$$

x and y are useful for the removal of the square roots in the differential equations for the MIs belonging to sub-topologies that appear in the non-homogeneous part of Eq. (8).

The particular solution is then written as

$$\begin{aligned} F(x,y) = c_1\psi_1 + c_2\psi_2 - \psi_1 \int \frac{d\xi}{W(\xi,y)} \psi_2(\xi,y)\Omega(\xi,y) \\ +\psi_2 \int \frac{d\xi}{W(\xi,y)} \psi_1(\xi,y)\Omega(\xi,y), \end{aligned} \tag{19}$$

where c_1, c_2 are arbitrary functions of y and $W(x,y)$ is the Wronskian of the two solutions ψ_1 and ψ_2:

$$W(x,y) = \frac{\pi}{32} \frac{x^2[y-3-2x(3y-1)+x^2(y-3)]}{(x-1)^3(x+1)(x+y+x^2y+xy^2)[y+9+2x(y-7)+x^2(y+3)]}\,. \tag{20}$$

Imposing the regularity in $s=0$, forces $c_1 = c_2 = 0$. Therefore, the solution of the MI $\mathscr{T}_{34}$ is given by

$$\begin{aligned} F(x,y) = -\psi_1(x,y) \int \frac{d\xi}{W(\xi,y)} \psi_2(\xi,y)\Omega(\xi,y) \\ + \psi_2(x,y) \int \frac{d\xi}{W(\xi,y)} \psi_1(\xi,y)\Omega(\xi,y)\,. \end{aligned} \tag{21}$$

3.3.1 Structure of the Integrals

Let us comment briefly on the structure of the integral solution in Eq. (21).

Firstly, we remark the fact that the solution we found is given in terms of a single integration in the variable x. The other variable, y, is not involved in the integration procedure. The functional dependence on t is exact. At this order in ε, $\Omega(x, y)$ is a function that can be expressed in terms of rational functions, logarithms (or at most Li_2 functions for the following order in ε) and elliptic integrals of the first and second kind (or one-fold integration over the elliptic kernel for the following order in ε). These latters come from the solution of the sunrise with equal masses, which is present as subtopology. However, the equal-mass sunrise appears as a function of y only and, therefore, it is not directly involved in the integration, which is done in x. At this order in ε we have to perform one-dimensional integrals of the product of the homogeneous solution and rational or logarithmic functions

$$F(x, y) \sim \int_1^x d\xi \left\{ \frac{P(\xi, y)}{Q(\xi, y)} \, ; \, \log \xi \right\} \frac{1}{R(\xi, y)} K(\omega(\xi, y)) \, . \tag{22}$$

The numeric integration of a form such as the one in Eq. (22) is extremely fast. Moreover, it is suitable for the analytic continuation in the Minkowski space. For the computation of the color factors, the following order in ε of $\mathscr{T}_{34}$ (as well as of $\mathscr{T}_{33}$ and $\mathscr{T}_{35}$) is needed. We do not consider the order ε in these proceedings.

We checked our results against the results obtained with the program FIESTA4 [76–78] and we found complete agreement, within the number of digits given by FIESTA4, in the Euclidean region.

The structure of the functions that appear in our result as iterated integrals over elliptic kernels was studied very recently in [84–88].

3.4 *The MIs $\mathscr{T}_{33}$ and $\mathscr{T}_{35}$*

Once the solution for $\mathscr{T}_{34}$ is found, we have to find the solution for the other two masters of the same topology. In principle, the problem is solved. Knowing the solution for $\mathscr{T}_{34}$ we can find, for instance, the solution for $\mathscr{T}_{35}$, which is the MI directly coupled to $\mathscr{T}_{34}$ in the system of differential equations, using the first-order differential equation for $\mathscr{T}_{34}$ and therefore expressing $\mathscr{T}_{35}$ as a combination of $\mathscr{T}_{34}$ and its derivative with respect to x. This implies that $\mathscr{T}_{35}$ can be expressed as a combination of the same kind of integrals encountered in the expression of $\mathscr{T}_{34}$ with the addition of complete elliptic integrals of the second kind. For $\mathscr{T}_{33}$, however, the situation is different. Since it is decoupled from the other two MIs, $\mathscr{T}_{33}$ can be calculated using a first-order linear differential equation, in which the non homogeneous part contains the other two MIs $\mathscr{T}_{34}$ and $\mathscr{T}_{35}$. A direct consequence of this fact is that $\mathscr{T}_{33}$ has an additional integration with respect to $\mathscr{T}_{34}$ and $\mathscr{T}_{35}$ and therefore its functional structure is more complicated, employing up to three-fold integrations in x. This problem can affect the speed of the numeric integration.

In order to have an homogeneous number of parametric integrations for all the three MIs, we adopted the following strategy. We know that the basis of the MIs chosen is completely arbitrary. Therefore, we can find different basis in which one MI is decoupled from the other two, that are coupled between each other. We chose two different basis, the first one constituted by $\mathcal{T}_{33}$, $\mathcal{T}_{34}$ and $\mathcal{T}_{35}$ and the second one constituted by $\mathcal{T}_{33}$, $\mathcal{T}_{34}$ and another master, which is finite in four dimensions, that we will call $\mathcal{T}_{35bis}$. In both sets, $\mathcal{T}_{33}$ is decoupled from the other two. Having calculated $\mathcal{T}_{34}$ with the maximal cut and then with parametric integrations as in Eq. (22), we can find both $\mathcal{T}_{34}$ and $\mathcal{T}_{35bis}$ from simple derivative with respect to x. The basis constituted by $\mathcal{T}_{34}$, $\mathcal{T}_{35}$ and $\mathcal{T}_{35bis}$ is then expressed in terms of a numeric integration of a form such as the one in Eq. (22).

We checked our results for the remaining two MIs, $\mathcal{T}_{35}$ and $\mathcal{T}_{35bis}$, against the results obtained with the program FIESTA4 and we found complete agreement in the Euclidean region.

4 Conclusions

In these proceedings, we presented the calculation of three 5-denominators two-loop box diagrams that enter the computation of the NNLO QCD corrections to three of the sixteen color coefficients in terms of which we can express the partonic cross section for the production of a top-antitop pair in gluon fusion.

The calculation was performed using the differential equations method. A part of the MIs could be calculated using standard methods that involve the construction of the canonical basis and its solution in terms of GPLs of maximum weight 4. For some MIs, however, this was not possible and we had to solve second-order linear differential equations that admit solutions in terms of iterated integrations over elliptic kernels. In particular, we focused on the study of an elliptic box. Calculating its maximal cut, we were able to find two independent solutions for the homogeneous part of the second-order differential equations (one in s and the other in t) that this MI has to satisfy. Imposing initial conditions, then, we found a suitable representation for this class of integrals, which is based on one- or two-fold integration of elliptic integrals multiplied by rational functions, logarithms and dilogarithms, in the single variable s. The dependence on t remains exact. This form is particularly good for fast numeric integrations and allows for a straightforward analytic continuation of the formulas in the physical region of the phase space.

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From Modular Forms to Differential Equations for Feynman Integrals

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Abstract In these proceedings we discuss a representation for modular forms that is more suitable for their application to the calculation of Feynman integrals in the context of iterated integrals and the differential equation method. In particular, we show that for every modular form we can find a representation in terms of powers of complete elliptic integrals of the first kind multiplied by algebraic functions. We illustrate this result on several examples. In particular, we show how to explicitly rewrite elliptic multiple zeta values as iterated integrals over powers of complete elliptic integrals and rational functions, and we discuss how to use our results in the context of the system of differential equations satisfied by the sunrise and kite integrals.

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1 Introduction

Recently, a lot of progress has been made in understanding elliptic multiple polylogarithms (eMPLs) [20], and in particular their use in the calculation of multiloop Feynman integrals [11–13]. As of today, a clear formulation for these functions is available in two different languages. The first, as iterated integrals over a set of kernels defined on a torus, is preferred in the mathematics community and finds natural applications in the calculation of one-loop open-string scattering amplitudes [14–16]. The second, as iterated integrals on an elliptic curve defined as the zero-set of a polynomial equation of degree three or four, is more natural in the context of the calculation of multiloop Feynman integrals by direct integration (for example over their Feynman-Schwinger parameter representation). In spite of this impressive progress, it remains not obvious how to connect these two languages to that of the differential equations method [23–25, 30], which constitutes one of the most powerful tools for the computation of large numbers of complicated multiloop Feynman integrals.

It is well known that Feynman integrals fulfil systems of linear differential equations with rational coefficients in the kinematical invariants and the dimensional regularization parameter ε. Once the differential equations are expanded in ε, a straightforward application of Euler's variation of constants allows one to naturally write their solutions as iterated integrals over rational functions and (products of) their homogeneous solutions. The homogeneous solutions can in turn be inferred by the study of the maximal cut of the corresponding Feynman integrals [29] and are in general given by non-trivial transcendental functions of the kinematical invariants. When dealing with Feynman integrals which evaluate to ordinary multiple polylogarithms (MPLs), the homogeneous solutions are expected to be algebraic functions (or at most logarithms). In the ellipitic case, they are instead given by (products of) complete elliptic integrals [5, 6, 10, 26, 28, 31, 33]. The iterated integrals arising naturally from this construction have been studied in the literature in different special cases [4, 32], and are particular instances of the 'iterative non-iterative integrals' considered in Refs. [3, 4]. A natural question is how and when these new types of iterated integrals can be written in terms of the eMPLs defined in the mathematical literature. In other words, is it possible to phrase the solution of the differential equations for elliptic Feynman integrals directly in terms of eMPLs, and if yes under which conditions? An obstacle when trying to address this question is that the kernels defining eMPLs do not present themselves in terms of complete elliptic integrals. A first possible hint to an answer to this apparent conundrum comes from the observation that elliptic polylogarithms evaluated at some special points can always be written as iterated integrals of modular forms [17], and a representation of the equal-mass sunrise in terms of this class of iterated integrals also exists [7, 8, 17]. It is therefore tantalising to speculate that the new class of iterated integrals showing up in Feynman integrals are closely connected to iterated integrals of modular forms and generalisations thereof.

In these proceedings, we start investigating the fascinating problem of how to relate iterated integrals of modular forms to iterated integrals over rational/algebraic functions and products of complete elliptic integrals. We mostly focus here on a simpler subproblem, namely on how to express modular forms in terms of powers of complete elliptic integrals, multiplied by suitable algebraic functions. This is a first step towards classifying the new classes of integration kernels that show up in Feynman integral computations, and how these new objects are connected to classes of iterated integrals studied in the mathematics literature. As a main result, we will show that, quite in general, modular forms admit a representation in terms of linearly independent products of elliptic integrals and algebraic functions. The advantage of this formulation of modular forms (for applications to Feynman integrals) lies in the fact that we can describe them in "purely algebraic terms", where all quantities are parametrised by variables constrained by polynomial equations – a setting more commonly encountered in physics problems than the formulation in terms of modular curves encountered in the mathematics (and string theory) literature. At the same time, since this formulation is purely algebraic, it lends itself more directly to generalisations to cases that cannot immediately be matched to the mathematics of modular forms, e.g., in cases of Feynman integrals depending on more than one kinematic variable.

This contribution to the proceedings is organised as follows: in Sect. 2 we provide a brief survey of the necessary concepts such as congruence subgroups of $\mathrm{SL}(2,\mathbb{Z})$, modular forms, Eisenstein and cuspidal subspaces and modular curves. Section 3 contains the main part of our contribution: we will show that one can indeed find suitable one-forms in an algebraic way, which we demonstrate to be in one-to-one correspondence with a basis of modular forms. Finally, we briefly discuss three applications in Sect. 4 and present our conclusions in Sect. 5.

2 Terms and Definitions

2.1 *The Modular Group* $\mathrm{SL}(2,\mathbb{Z})$ *and Its Congruence Subgroups*

In these proceedings we are going to consider functions defined on the extended upper half-plane $\overline{\mathbb{H}} = \mathbb{H} \cup \mathbb{Q} \cup \{i\infty\}$, where $\mathbb{H} = \{\tau \in \mathbb{C} \,|\, \mathrm{Im}\,\tau > 0\}$. The modular group $\mathrm{SL}(2,\mathbb{Z})$ acts on the points in $\overline{\mathbb{H}}$ through Möbius transformations of the form

$$\gamma \cdot \tau = \frac{a\tau + b}{c\tau + d}, \quad \gamma = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \mathrm{SL}(2,\mathbb{Z}). \tag{1}$$

In the following, we will be interested in subgroups of the full modular group. Of particular interest are the so-called *congruence subgroups of level* N of $\mathrm{SL}(2,\mathbb{Z})$,

$$\begin{aligned}
\Gamma_0(N) &= \left\{ \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \mathrm{SL}(2,\mathbb{Z}) \;:\; c = 0 \mod N \right\} ,\\
\Gamma_1(N) &= \left\{ \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \mathrm{SL}(2,\mathbb{Z}) \;:\; c = 0 \mod N \text{ and } a = d = 1 \mod N \right\} ,\\
\Gamma(N) &= \left\{ \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \mathrm{SL}(2,\mathbb{Z}) \;:\; b = c = 0 \mod N \text{ and } a = d = 1 \mod N \right\} .
\end{aligned} \tag{2}$$

It is easy to see that $\Gamma \subseteq \mathrm{SL}(2,\mathbb{Z})$ acts separately on $\mathbb{H}$ and $\mathbb{Q} \cup \{i\infty\}$. The action of Γ decomposes $\mathbb{Q} \cup \{i\infty\}$ into disjoint orbits. We refer to the elements of the coset-space $(\mathbb{Q} \cup \{i\infty\})/\Gamma$ (i.e., the space of all orbits) as *cusps* of Γ. By abuse of language, we usually refer to the elements of the orbits also as cusps. We note here that the number of cusps is always finite for any of the congruence subgroups considered in Eq. (2).

Example 1 One can show that for every rational number $\frac{a}{c} \in \mathbb{Q}$, there is a matrix $\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \mathrm{SL}(2,\mathbb{Z})$ such that $\frac{a}{c} = \lim_{\tau \to i\infty} \frac{a\tau+b}{c\tau+d}$. Hence, under the action of the group $\Gamma(1) \simeq \mathrm{SL}(2,\mathbb{Z})$ every rational number lies in the orbit of the point $i\infty$, and so $\Gamma(1)$ has a single cusp which we can represent by the point $i\infty \in \overline{\mathbb{H}}$, often referred to as the cusp at infinity.

At higher levels a congruence subgroup usually has more than one cusp. For example, the group $\Gamma(2)$ has three cusps, which we may represent by $\tau = i\infty$, $\tau = 0$ and $\tau = 1$. Representatives for the cusps of congruence subgroups of general level N can be obtained from SAGE [1].

2.2 Modular Curves

Since the action of any congruence subgroup Γ of $\mathrm{SL}(2,\mathbb{Z})$ allows us to identify points in the (extended) upper half-plane $\mathbb{H}$ ($\overline{\mathbb{H}}$), it is natural to consider its quotient by Γ, commonly referred to as a *modular curve*,

$$X_\Gamma = \overline{\mathbb{H}}/\Gamma \quad \text{and} \quad Y_\Gamma = \mathbb{H}/\Gamma \,. \tag{3}$$

In the cases where Γ is any of the congruence subgroups in Eq. (2), the corresponding modular curves are usually denoted by $X_0(N) = X_{\Gamma_0(N)}$, $X_1(N) = X_{\Gamma_1(N)}$ and $X(N) = X_{\Gamma(N)}$.

There is a vast mathematical literature on modular curves (see, for example Ref. [22]), and we content ourselves here to summarise the main results which we will use in the remainder of these proceedings. It can be shown that Y_Γ always defines a Riemann surface, which can be compactified by adding a finite number of points to Y_Γ, which are precisely the cusps of Γ. In other words, while Y_Γ is in general not compact, X_Γ always defines a *compact* Riemann surface. Hence, we can apply very general results from the theory of compact Riemann surfaces to the study of modular curves, as we review now.

In principle, there are two ways to describe the modular curve X_Γ: either as the quotient of the extended upper half plane, or as the projective curve $\mathscr{C}$ in $\mathbb{CP}^2$ defined by the polynomial equation $\Phi(x, y) = 0$. Hence, there must be a map from $\overline{\mathbb{H}}/\Gamma$ to $\mathscr{C}$ which assigns to $\tau \in \overline{\mathbb{H}}/\Gamma$ a point $(x(\tau), y(\tau)) \in \mathscr{C}$ such that $\Phi(x(\tau), y(\tau)) = 0$. Since two points in $\overline{\mathbb{H}}/\Gamma$ are identified if they are related by a Möbius transformation for Γ, the functions $x(\tau)$ and $y(\tau)$ must be invariant under modular transformations for Γ, e.g.,

$$x\left(\frac{a\tau + b}{c\tau + d}\right) = x(\tau)\,, \qquad \forall \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \Gamma\,, \tag{4}$$

and similarly for $y(\tau)$. A meromorphic function satisfying Eq. (4) is called a *modular function* for Γ. Equivalently, the modular functions for Γ are precisely the meromorphic functions on X_Γ. Note that since X_Γ is compact, there are no non-constant holomorphic functions on X_Γ (because they would necessarily violate Liouville's theorem). Modular functions can easily be described in terms of the algebraic curve $\mathscr{C}$: they are precisely the rational functions in (x, y) subject to the constraint $\Phi(x, y) = 0$. Equivalently, the field of modular functions for X_Γ is the field $\mathbb{C}(x(\tau), y(\tau))$. In particular, we see that the field of meromorphic functions of a modular curve (or of any compact Riemann surface) has always (at most) two generators x and y.

Example 2 It can be shown that the modular curve $X_0(2)$ is isomorphic to the algebraic variety $\mathscr{C}$ described by the zero-set of the polynomial

$$\begin{aligned}\Phi_2(x, y) &= x^3 + y^3 - 162000(x^2 + y^2) + 1488xy(x + y) - x^2y^2 + 8748000000(x + y)\\ &\quad + 40773375xy - 157464000000000\,.\end{aligned} \tag{5}$$

In general, the coefficients of the polynomials describing modular curves are very large numbers, already for small values of the level N. The map from the quotient space $\overline{\mathbb{H}}/\Gamma_0(2)$ to the curve $\mathscr{C}$ is given by[1]

$$\tau \mapsto (x, y) = (j(\tau), j'(\tau)) = (j(\tau), j(2\tau))\,, \tag{6}$$

where $j : \mathbb{H} \to \mathbb{C}$ denotes Klein's j-invariant. The field of meromorphic functions of $X_0(2)$ is the field of rational functions in two variables (x, y) subject to the constraint $\Phi_2(x, y) = 0$, or equivalently the field $\mathbb{C}(j(\tau), j'(\tau))$ of rational functions in $(j(\tau), j'(\tau))$.

In general, the polynomials $\Phi_N(x, y)$ describing the *classical modular curves* $X_0(N)$ can be constructed explicitly, cf. e.g. Refs. [18, 21], and they are available in computer-readable format up to level 300 [2]. The zeroes of $\Phi_N(x, y)$ are parametrised by $(j(\tau), j'(\tau)) = (j(\tau), j(N\tau))$, the field of meromorphic functions is $\mathbb{C}(j(\tau), j'(\tau))$.

In some cases it is possible to find purely rational solutions to the polynomial equation $\Phi(x, y) = 0$, i.e., one can find rational functions $(X(t), Y(t))$ such that

[1]The notation $j'(\tau) = j(2\tau)$ is standard in this context in the mathematics literature, though we emphasise that $j'(\tau)$ *does not* correspond to the derivative of $j(\tau)$.

$\Phi(X(t), Y(t)) = 0$ for all values of $t \in \widehat{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$. In such a scenario we have constructed a map from the Riemann sphere $\widehat{\mathbb{C}}$ to the curve $\mathscr{C}$, and so we can identify the curve $\mathscr{C}$, and thus the corresponding modular curve X_Γ, with the Riemann sphere. By a very similar argument one can conclude that there must be a modular function $t(\tau)$ for Γ which allows us to identify the quotient $\overline{\mathbb{H}}/\Gamma$ with the Riemann sphere. Such a modular function is called a *Hauptmodul* for Γ. It is easy to see that in this case the field of meromorphic functions reduces to the field $\mathbb{C}(t(\tau))$ of rational functions in the Hauptmodul, in agreement with the fact that the meromorphic functions on the Riemann sphere are precisely the rational functions.

Example 3 It is easy to check that Eq. (5) admits a purely rational solution of the form [27]

$$(x, y) = (X(t), Y(t)) = \left(\frac{(t+16)^3}{t}, \frac{(t+256)^3}{t^2}\right). \tag{7}$$

We have thus constructed a map from the Riemann sphere to the modular curve $X_0(2)$, and so $X_0(2)$ is a curve of genus zero. A Hauptmodul for $X_0(2)$ can be chosen to be [27]

$$t_2(\tau) = 2^{12}\left(\frac{\eta(2\tau)}{\eta(\tau)}\right)^{24}, \tag{8}$$

where η denotes Dedekind's η-function.

It is possible to compute the genus of a modular curve. In particular, it is possible to decide for which values of the level N the modular curves associated to the congruence subgroups in Eq. (2) have genus zero. Here is a list of results:

- $X_0(N)$ has genus 0 iff $N \in \{1, \dots, 10, 12, 13, 16, 18, 25\}$.
- $X_1(N)$ has genus 0 iff $N \in \{1, \dots, 10, 12\}$.
- $X(N)$ has genus 0 iff $N \in \{1, 2, 3, 4, 5\}$.

Hauptmodule for these modular curves have been studied in the mathematics literature. In particular, the complete list of Hauptmodule for the modular curves $X_0(N)$ of genus zero can be found in Ref. [27] in terms of η-quotients. Other cases are also known in the literature, but they may involve Hauptmodule that require generalisations of Dedekind's η-function, see e.g. Ref. [35].

Example 4 The modular curves $X(1)$ and $X(2)$ have genus zero, and the respective Hauptmodule are Klein's j-invariant $j(\tau)$ and the modular λ-function,

$$\lambda(\tau) = \theta_2^4(0,\tau)/\theta_3^4(0,\tau) = 2^4\left(\frac{\eta(\tau/2)\,\eta(2\tau)^2}{\eta(\tau)^3}\right)^8, \tag{9}$$

where $\theta_n(0, \tau)$ are Jacobi's θ-functions.

2.3 Modular Forms

One of the deficiencies when working with modular curves is the absence of holomorphic modular functions on X_Γ. We can, however, introduce a notion of holomorphic functions by relaxing the condition on how the functions should transform under Γ. For every non-negative integer k, we can define an action of Γ on functions on $\overline{\mathbb{H}}$ by

$$(f|_k\gamma)(\tau) = (c\tau + d)^{-k} f(\gamma \cdot \tau)\,, \quad \gamma = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \Gamma\,. \tag{10}$$

A meromorphic function $\overline{\mathbb{H}} \to \mathbb{C}$ is called *weakly modular of weight k* for Γ if it is invariant under this action,

$$(f|_k\gamma)(\tau) = f(\tau). \tag{11}$$

Note that weakly modular functions of weight zero are precisely the modular functions for Γ.

A *modular form* of weight k for Γ is, loosely speaking, a weakly modular function of weight k that is holomorphic on $\overline{\mathbb{H}}$. In particular it is holomorphic at all the cusps of Γ. We denote the $\mathbb{Q}$-vector space of modular forms of weight k for Γ by $\mathcal{M}_k(\Gamma)$. It can be shown that this space is always finite-dimensional. We summarise here some properties of spaces of modular forms that are easy to prove and that will be useful later on.

1. The space of all modular forms is a graded algebra,

$$\mathcal{M}_\bullet(\Gamma) = \bigoplus_{k=0}^{\infty} \mathcal{M}_k(\Gamma), \quad \text{with} \quad \mathcal{M}_k(\Gamma) \cdot \mathcal{M}_\ell(\Gamma) \subseteq \mathcal{M}_{k+\ell}(\Gamma). \tag{12}$$

2. If $\Gamma' \subseteq \Gamma$, then $\mathcal{M}_k(\Gamma) \subseteq \mathcal{M}_k(\Gamma')$.
3. If $\left(\begin{smallmatrix} -1 & 0 \\ 0 & -1 \end{smallmatrix}\right) \in \Gamma$, then there are no modular forms of odd weight for Γ.

A modular form that vanishes at all cusps of Γ is called a *cusp form*. The space of all cusp forms of weight k for Γ is denoted by $\mathcal{S}_k(\Gamma)$. The space of all cusp forms $\mathcal{S}_\bullet(\Gamma) = \bigoplus_{k=0}^{\infty} \mathcal{S}_k(\Gamma)$ is obviously a graded subalgebra of $\mathcal{M}_\bullet(\Gamma)$ and an ideal in $\mathcal{M}_\bullet(\Gamma)$. The quotient space is the *Eisenstein subspace*:

$$\mathcal{E}_\bullet(\Gamma) \simeq \mathcal{M}_\bullet(\Gamma)/\mathcal{S}_\bullet(\Gamma). \tag{13}$$

Note that at each weight the dimension of the Eisenstein subspace for Γ is equal[2] to the number of cusps of Γ.

Example 5 Let us analyse modular forms for $\Gamma(1) \simeq SL(2, \mathbb{Z})$. There are no modular forms for $\Gamma(1)$ of odd weight. Since $\Gamma(1)$ has only one cusp, there is one Eisenstein series for every even weight, the Eisenstein series G_{2m},

[2] There are exceptions for small values of the weight and the level.

$$G_{2m}(\tau) = \sum_{(\alpha,\beta)\in\mathbb{Z}^2\setminus\{(0,0)\}} \frac{1}{(\alpha+\beta\tau)^{2m}}. \tag{14}$$

It is easy to check that $G_{2m}(\tau)$ transforms as a modular form of weight 2 m, except when $m = 1$, which will be discussed below. The first cusp form for $\Gamma(1)$ appears at weight 12, known as the modular discriminant,

$$\Delta(\tau) = 2^{12}\,\eta(\tau)^{24} = 10\,800\left(20\,G_4(\tau)^3 - 49\,G_6(\tau)^2\right)\,. \tag{15}$$

In the same way as the Eisenstein subspace for $\Gamma(1)$ is generated by the Eisenstein series $G_{2m}(\tau)$, there exist analogues for the Eisenstein subspaces for congruence subgroups.

$G_2(\tau)$ is an example of a quasi-modular form. A *quasi-modular form of weight n and depth p for Γ* is a holomorphic function $f : \overline{\mathbb{H}} \to \mathbb{C}$ that transforms as,

$$(f|_n\gamma)(\tau) = f(\tau) + \sum_{r=1}^{p} f_r(\tau)\left(\frac{c}{c\tau+d}\right)^r\,, \quad \gamma = \left(\begin{smallmatrix} a & b \\ c & d\end{smallmatrix}\right) \in \Gamma\,, \tag{16}$$

where $f_1,\dots,f_p$ are holomorphic functions. In the case of the Eisenstein series $G_2(\tau)$ we have,

$$G_2\left(\frac{a\tau+b}{c\tau+d}\right) = (c\tau+d)^2\Big(G_2(\tau) - \frac{1}{4\pi i}\frac{c}{c\tau+d}\Big). \tag{17}$$

Comparing Eqs. (17) to (16), we see that $G_2(\tau)$ is a quasi-modular form of weight two and depth one.

It is easy to check that any congruence subgroup Γ of level N contains the element

$$T^N = \left(\begin{smallmatrix} 1 & N \\ 0 & 1\end{smallmatrix}\right), \tag{18}$$

which generates the Möbius transformation $\tau \to \tau + N$. Consequently, modular forms of level N are periodic functions with period N and thus admit Fourier expansions of the form

$$f(\tau) = \sum_{m=0}^{\infty} a_m e^{2\pi i m\tau/N} = \sum_{m=0}^{\infty} a_m q_N^m, \tag{19}$$

with $q = \exp(2\pi i\tau)$ and $q_N = q^{1/N}$, which are called *q-expansions*.

Example 6 The Eisenstein series for $\Gamma(1)$ admit the q-expansion

$$G_{2m}(\tau) = 2\zeta_{2m} + \frac{2\,(2\pi i)^{2m}}{(2m-1)!}\sum_{n=1}^{\infty}\sigma_{2m-1}(n)\,q^n\,, \tag{20}$$

where $\sigma_p(n) = \sum_{d|n} d^p$ is the divisor sum function.

In the previous section we have argued that modular curves admit a purely algebraic description in terms of zeroes of polynomials in two variables. For practical applications in physics such an algebraic description is often desirable, because concrete applications often present themselves in terms of polynomial equations. Such an algebraic description also exists for (quasi-)modular forms. In particular, every modular form of positive weight k satisfies a linear differential equation of order $k+1$ with algebraic coefficients. More precisely, consider a modular form $f(\tau)$ of weight k for Γ. We can pick a modular function $t(\tau)$ for Γ and locally invert it to express τ as a function of t. Then the function $F(t) = f(\tau(t))$ satisfies a linear differential equation in t of degree $k+1$ with coefficients that are algebraic functions in t. In the case where Γ has genus zero[3] we can choose $t(\tau)$ to be a Hauptmodul, in which case the coefficients of the differential equation are rational functions. We emphasise that the function $F(t)$ is only defined *locally*, and in general it has branch cuts.

One of the goals of these proceedings is to make this algebraic description of modular forms concrete and to present a way how it can be obtained in some specific cases. For simplicity we only focus on the genus zero case, because so far modular forms corresponding to congruence subgroups of higher genus have not appeared in Feynman integral computations. We emphasise, however, that this restriction is not essential and it is straightforward to extend our results to congruence subgroups of higher genus.

3 An Algebraic Representation of Modular Forms

3.1 General Considerations

In this section, we will make the considerations at the end of the previous section concrete, and we are going to construct a basis of modular forms of given weight for different congruence subgroups of $\mathrm{SL}(2,\mathbb{Z})$ in terms of objects that admit a purely algebraic description. More precisely, consider a modular form f of weight k for Γ, where Γ can be any of the congruence subgroups in Eq. (2). Then, at least *locally*, we can find a modular function $x(\tau)$ for Γ and an *algebraic* function A such that

$$f(\tau) = \mathrm{K}(\lambda(\tau))^k\, A(x(\tau))\,, \tag{21}$$

where λ denotes the modular λ function of Eq. (9) and K is the complete elliptic integral of the first kind,

$$\mathrm{K}(\lambda) = \int_0^1 \frac{1}{\sqrt{(1-t^2)(1-\lambda\, t^2)}}\, dt\,. \tag{22}$$

[3]We define the genus of a congruence subgroup Γ to be the genus of the modular curve X_Γ.

Note that locally we can write λ as an algebraic function of x, so that the argument of the complete elliptic integral can be written as an algebraic function of x. Since K satisfies a linear differential equation of order two, it is then easy to see that the right-hand side of Eq. (21) satisfies a linear differential equation of order $k+1$ in x with algebraic coefficients. The existence of the local representation in Eq. (21) can be inferred from the following very simple reasoning. First, since $\Gamma(N) \subseteq \Gamma_1(N) \subseteq \Gamma_0(N)$ it is sufficient to discuss the case of the group $\Gamma(N)$. Next, let $M = \mathrm{lcm}(4, N)$ be the least common multiple of 4 and N. Since $\Gamma(M) \subseteq \Gamma(N)$, f is a modular form of weight k for $\Gamma(M)$. One can check that $\mathrm{K}(\lambda(\tau))$ is a modular form of weight one for $\Gamma(4)$, and therefore also for $\Gamma(M)$. The ratio $f(\tau)/\mathrm{K}(\lambda(\tau))^k$ is then a modular form of weight zero for $\Gamma(M)$, and thus a modular function, i.e., an element of the function field $\mathbb{C}(x(\tau), y(\tau))$ of $\Gamma(M)$. Hence we have $f(\tau)/\mathrm{K}(\lambda(\tau))^k = R(x(\tau), y(\tau))$. y is an algebraic function of x (because they are related by the polynomial equation $\Phi(x, y) = 0$ that defines $X(M)$), and so we can choose $A(x(\tau)) = R(x(\tau), y(\tau))$ in Eq. (21).

While the previous argument shows that a representation of the form (21) exists for any modular form of level N, finding this representation in explicit cases can be rather hard. Our goal is to show that often one can find this representation using analytic constraints, which allow us to infer the precise form of the algebraic coefficient A. We focus here exclusively on congruence subgroups of genus zero, but we expect that similar arguments apply to higher genera. In the next paragraphs, we are going to describe the general strategy. In subsequent sections we will illustrate the procedure on concrete examples, namely the congruence subgroups $\Gamma(2)$ and $\Gamma_0(N)$ for $N \in \{2, 4, 6\}$, as well as the group $\Gamma_1(6)$ which is relevant for the sunrise graph [7, 9]. In particular, we will construct an explicit basis of modular forms for these groups for arbitrary weights.

Assume that we are given a modular form $B(\tau)$ of weight p for Γ, which we call *seed modular form* in the following. In the argument at the beginning of this section the seed modular form is $\mathrm{K}(\lambda(\tau))$, assuming that Γ contains $\Gamma(4)$ as a subgroup. It is however useful to formulate the argument in general without explicit reference to $\mathrm{K}(\lambda(\tau))$. Next, consider a modular form $f(\tau)$ of weight k for Γ with $p|k$. Then by an argument very similar to the one presented at the beginning of this section we conclude that there is a modular function $x(\tau)$ for Γ and an algebraic function $A(x)$ such that

$$A(x(\tau)) = \frac{f(\tau)}{B(\tau)^{k/p}}\,. \tag{23}$$

If Γ has genus zero and x is a Hauptmodul for Γ, then the function A is a rational function of x. From now on we assume for simplicity that we work within this setting.

Up to now the argument was similar to the one leading to the form (21), and we have not constrained the form of the rational function A. We now discuss how this can be achieved. Being a modular form, $f(\tau)$ needs to be holomorphic everywhere. Correspondingly, the rational function $A(x(\tau))$ can have poles at most for $B(\tau) = 0$. In applications, the location of the poles is usually known (see the next sections). Let us denote them by τ_i, and we set $x_i = x(\tau_i)$ (with $x_i \neq \infty$). We must have

$$A(x) = \frac{P(x)}{\prod_i (x - x_i)^{n_i}}\,, \tag{24}$$

where $P(x)$ is a polynomial. The degree of P is bounded by analysing the behaviour of the seed modular form at points where $x(\tau) = \infty$, where both f and B must be holomorphic. Finally, the modular form $f(\tau)$ can be written as

$$f(\tau) = \frac{B(\tau)^{k/p}}{\prod_i (x(\tau) - x_i)^{n_i}} \left[d_0 + d_1\, x(\tau) + \cdots + d_m\, x(\tau)^m\right], \tag{25}$$

where the d_i are free coefficients. In the next sections we illustrate this construction explicitly on the examples of the congruence subgroups $\Gamma(2)$, $\Gamma_0(N)$, $N \in \{2, 4, 6\}$ and $\Gamma_1(6)$. However, before we do so, let us make a few comments about Eq. (25). First, we see that we can immediately recast Eq. (25) in the form (21) if we know how to express the seed modular form B in terms of the complete elliptic integral of the first kind. While we do not know any generic way of doing this a priori, in practical applications the seed modular form will usually be given by a Picard–Fuchs equation whose solutions can be written in terms of elliptic integrals. Second, we see that Eq. (25) depends on $m + 1$ free coefficients, and so $\dim \mathscr{M}_k(\Gamma) = m + 1$. Finally, let us discuss how cusp forms arise in this framework. Let us assume that Γ has n_C cusps, which we denote by τ_r, $1 \le r \le n_C$. For simplicity we assume that $c_r = x(\tau_r) \neq \infty$, though the conclusions will not depend on this assumption. Then f is a cusp form if $f(\tau_r) = 0$ for all $1 \le r \le n_C$. It can easily be checked that, by construction, the ratio multiplying the polynomial in Eq. (25) can never vanish. Hence, all the zeroes of f are encoded into the zeroes of the polynomial part in Eq. (25). Therefore f is a cusp form if and only if it can locally be written in the form

$$f(\tau) = \frac{B(\tau)^{k/p}}{\prod_i (x(\tau) - x_i)^{n_i}} \left[\prod_{\substack{r=1\\ c_r \neq \infty}}^{n_C} (x(\tau) - c_r)\right] \left[\sum_{j=1}^{m-n_c-\delta_\infty} d_j\, x(\tau)^j\right], \tag{26}$$

with

$$\delta_\infty = \begin{cases} 1\,, & \text{if } c_r = \infty \text{ for some } r\,, \\ 0\,, & \text{otherwise}\,. \end{cases} \tag{27}$$

3.2 A Basis for Modular Forms for $\Gamma(2)$

In this section we derive an algebraic representation for all modular forms of weight $2k$ for the group $\Gamma(2)$, and we present an explicit basis for such modular forms for arbitrary weights. As already mentioned in Example 4, the modular curve $X(2)$ has genus zero and the associated Hauptmodul is the modular λ-function. Since $\left(\begin{smallmatrix} -1 & 0 \\ 0 & -1 \end{smallmatrix}\right) \in \Gamma(2)$, there are no modular forms of odd weight. The group $\Gamma(2)$ has three cusps, which are represented by $\tau = i\infty$, $\tau = 1$ and $\tau = 0$. Under the modular λ function the cusps are mapped to

$$\lambda(i\infty) = 0\,, \qquad \lambda(0) = 1\,, \qquad \lambda(1) = \infty\,. \tag{28}$$

Next, we need to identify our seed modular form. One can easily check that $B(\tau) = \mathrm{K}(\lambda(\tau))^2$ is a modular form of weight two for $\Gamma(2)$. If f denotes a modular form of weight $2k$ for $\Gamma(2)$, then we can form the ratio

$$R(\lambda(\tau)) = \frac{f(\tau)}{B(\tau)^k} = \frac{f(\tau)}{\mathrm{K}(\lambda(\tau))^{2k}}\,, \tag{29}$$

where R is a rational function in the Hauptmodul λ.

In order to proceed, we need to determine the pole structure of R, or equivalently the zeroes of the seed modular form B, i.e., of the complete elliptic integral of the first kind. The elliptic integral $\mathrm{K}(\ell)$ has no zeroes in the complex plane. Furthermore, it is not difficult to show that $\mathrm{K}(\ell)$ behaves like $1/\sqrt{\ell}$ for $\ell \to \infty$. So the function $B(\tau)$ becomes zero only at $\lambda(\tau) = \infty$, which corresponds to $\tau = 1 \bmod \Gamma(2)$. We thus conclude that $R(\lambda(\tau))$ cannot have poles at finite values of $\lambda(\tau)$, and so it must be a polynomial. The degree of the polynomial is bounded by the requirement that the ratio in Eq. (29) has no pole at $\tau = 1$. Starting from a polynomial ansatz

$$R(\lambda(\tau)) = \sum_{n=0}^{m} a_n \lambda(\tau)^n \tag{30}$$

we find

$$f(\tau) = \mathrm{K}(\lambda(\tau))^{2k} \sum_{n=0}^{m} a_n \lambda(\tau)^n \overset{\tau\to 1}{\sim} \left(\frac{1}{\sqrt{\lambda(\tau)}}\right)^{2k} a_m \lambda(\tau)^m = a_m \lambda(\tau)^{m-k}\,. \tag{31}$$

We see that $f(\tau)$ is holomorphic at $\tau = 1$ if and only if the degree of R is at most k. Thus, we can write the most general ansatz for the modular form of weight $2k$ for $\Gamma(2)$:

$$f(\tau) = \mathrm{K}(\lambda(\tau))^{2k} \sum_{n=0}^{k} c_n \lambda(\tau)^n\,. \tag{32}$$

In turn, this allows to infer the dimension of the space of modular forms of weight $2k$:

$$\dim \mathscr{M}_{2k}(\Gamma(2)) = k + 1, \quad k > 1\,, \tag{33}$$

and we see that the modular forms

$$\mathrm{K}(\lambda(\tau))^{2k}\, \lambda(\tau)^n\,, \quad 0 \le n \le k+1\,, \tag{34}$$

form a basis for $\mathscr{M}_{2k}(\Gamma(2))$.

Finally, let us comment on the space of cusp forms of weight $2k$ for $\Gamma(2)$. Using Eq. (26), we conclude that the most general element of $\mathscr{S}_{2k}(\Gamma(2))$ has the form

$$\mathrm{K}(\lambda(\tau))^{2k}\,\lambda(\tau)\,(1-\lambda(\tau))\sum_{n=0}^{k-3}a_n\,\lambda(\tau)^n\,. \tag{35}$$

We see that there are $k-2$ cups forms for $\Gamma(2)$ of weight $2k > 2$. This number agrees with the data for the dimensions of Eisenstein and cuspidal subspaces delivered by SAGE [1]. Moreover, we can easily read off a basis of cusp forms for arbitrary weights.

Example 7 Every Eisenstein series for $\Gamma(1)$ (see Eq. (14)) is a modular form for $\Gamma(2)$, and so we can write them locally in the form

$$G_{2k}(\tau) = \mathrm{K}(\lambda(\tau))^{2k}\,\mathscr{G}_{2k}(\lambda(\tau))\,,\quad k>1\,, \tag{36}$$

where $\mathscr{G}_{2k}(\ell)$ is a polynomial of degree k. For example, for low weights we find

$$\begin{aligned}\mathscr{G}_4(\ell) &= \frac{16}{45}\,(\ell^2-\ell+1)\,,\\ \mathscr{G}_6(\ell) &= \frac{64}{945}\,(\ell-2)(\ell+1)(2\ell-1)\,,\\ \mathscr{G}_8(\ell) &= \frac{256}{4725}\,(\ell^2-\ell+1)^2\,.\end{aligned} \tag{37}$$

In this basis the modular discriminant of Eq. (15) takes the form

$$\Delta(\tau) = 65\,536\,\mathrm{K}(\lambda(\tau))^{12}\,\lambda(\tau)^2\,(1-\lambda(\tau))^2\,, \tag{38}$$

in agreement with Eq. (35). Finally, the Eisenstein series of weight two is not modular, so it cannot be expressed in terms of the basis in Eq. (34). We note however that one can write

$$G_2(\tau) = 4\,\mathrm{K}(\lambda(\tau))\,\mathrm{E}(\lambda(\tau)) + \frac{4}{3}\,(\lambda(\tau)-2)\,\mathrm{K}(\lambda(\tau))^2\,, \tag{39}$$

where E denotes the complete elliptic integral of the second kind

$$\mathrm{E}(\lambda) = \int_0^1 dt\,\sqrt{\frac{1-\lambda\,t^2}{1-t^2}}\,. \tag{40}$$

3.3 A Basis for Modular Forms for $\Gamma_0(2)$

In this section we perform the same analysis for the congruence subgroup $\Gamma_0(2)$. The analysis will be very similar to the previous case, so we will not present all the steps in detail. However, there are a couple of differences which we want to highlight.

We start by reviewing some general facts about $\Gamma_0(2)$. First, there are no modular forms of odd weight. Second, $\Gamma_0(2)$ has genus zero (cf. Sect. 2.2), and a Hauptmodul for $\Gamma_0(2)$ is the function t_2 defined in Eq. (8). Since $\Gamma(2) \subseteq \Gamma_0(2)$, the Hauptmodul t_2 is a modular function for $\Gamma(2)$, and so it can be written as a rational function of λ, the Hauptmodul for $\Gamma(2)$. Indeed, one finds

$$t_2(\tau) = 16\frac{\lambda(\tau)^2}{1-\lambda(\tau)}\,. \tag{41}$$

Inverting the previous relation, we find

$$\lambda(\tau) = \frac{1}{32}\left[\sqrt{t_2(\tau)(t_2(\tau)+64)} - t_2(\tau)\right] - 2\,. \tag{42}$$

We see that $\lambda(\tau)$ is an *algebraic* function of the Hauptmodul t_2.

Next, let us identify a seed modular form $B_0(\tau)$. As can be checked for example with SAGE, there is a unique modular form of weight 2 for $\Gamma_0(2)$ (up to rescaling). Since $\Gamma(2) \subseteq \Gamma_0(2)$, this form has to be in the space $\mathscr{M}_2(\Gamma(2))$, so we can – using the results from the previous subsection – write the ansatz

$$B_0(\tau) = \mathrm{K}(\lambda(\tau))^2(c_0 + c_1\lambda(\tau))\,. \tag{43}$$

The coefficients can be fixed by matching q-expansions with the expression delivered by SAGE and one finds that $\mathscr{M}_2(\Gamma_0(2))$ is generated by

$$B_0(\tau) = \mathrm{K}(\lambda(\tau))^2(\lambda(\tau) - 2)\,. \tag{44}$$

Equipped with the seed modular form B_0, we can now repeat the analysis from the previous subsection. For a modular form $f(\tau)$ of weight $2k$ for $\Gamma_0(2)$, the function

$$R(t_2(\tau)) = \frac{f(\tau)}{B_0(\tau)^k} \tag{45}$$

is meromorphic and has weight 0, thus it must be a rational function of the Hauptmodul t_2. In order to fix the precise form of $R(t_2)$, let us again consider the pole structure of the right-hand side of Eq. (45): since both $f(\tau)$ and $B_0(\tau)$ are holomorphic, poles in $R(\tau)$ can appear only for $B_0(\tau) = 0$, which translates into

$$\lambda(\tau) = 2 \quad \text{or} \quad \mathrm{K}(\lambda(\tau)) = 0\,. \tag{46}$$

As spelt out in the previous subsection, the second situation is realised for $\lambda \to \infty$, i.e., for $\tau \to 1$. Considering this limit, we find

$$\lim_{\tau\to 1} B_0(\tau) = \lim_{\tau\to 1} \mathrm{K}(\lambda(\tau))^2(\lambda(\tau)-2) \sim \lambda(\tau)\Big(\frac{1}{\sqrt{\lambda(\tau)}}\Big)^2 = \mathcal{O}(1)\,, \tag{47}$$

and we see that $B_0(\tau)$ does not vanish in the limit $\mathrm{K}(\lambda(\tau)) \to 0$. As $\mathrm{K}(\lambda(\tau))$ is finite for $\lambda(\tau) = 2$, B_0 will have a simple zero there. As a function of the Hauptmodul t_2, however, $B_0(t_2)$ behaves like

$$B_0(t_2) \overset{t_2\to -64}{\sim} \sqrt{t_2+64}\,, \tag{48}$$

which can be seen by expanding Eq. (42) around $t_2 = -64$. Accordingly, $R(t_2)$ can at most have a pole of order $\lfloor k/2 \rfloor$ at $t_2 = -64$. Hence, we can write down the following ansatz for $R(t_2)$,

$$R(t_2) = \frac{P(t_2)}{(t_2+64)^{\lfloor k/2 \rfloor}}\,, \tag{49}$$

where $P(t_2)$ is a polynomial in the Hauptmodul. Its degree can be bounded by demanding regularity for $t_2 \to \infty$. We obtain in this way the most general form for a modular form of weight $2k$ for $\Gamma_0(2)$:

$$f(\tau) = \mathrm{K}(\lambda(\tau))^{2k} \frac{(\lambda(\tau)-2)^k}{(t_2(\tau)+64)^{\lfloor k/2 \rfloor}} \sum_{m=0}^{\lfloor k/2 \rfloor} c_m t_2(\tau)^m\,. \tag{50}$$

In particular we see that

$$\dim \mathcal{M}_{2k}(\Gamma_0(2)) = \lfloor k/2 \rfloor + 1\,, \tag{51}$$

and an explicit basis for $\mathcal{M}_{2k}(\Gamma_0(2))$ is

$$\mathrm{K}(\lambda(\tau))^{2k} \frac{(\lambda(\tau)-2)^k\, t_2(\tau)^m}{(t_2(\tau)+64)^{\lfloor k/2 \rfloor}}\,, \qquad 0 \le m \le \lfloor k/2 \rfloor\,. \tag{52}$$

We have checked up to weight 10 that our results are in agreement with the explicit basis for modular forms for $\Gamma_0(2)$ obtained by SAGE. Finally, let us comment on the cusp forms for $\Gamma_0(2)$. $\Gamma_0(2)$ has two cusps, which can be represented by $\tau = i\infty$ and $\tau = 0$. The Hauptmodul t_2 maps the cusps to

$$t_2(i\infty) = 0 \;\text{ and }\; t_2(0) = \infty\,. \tag{53}$$

We then see from Eq. (26) that a basis for $\mathscr{S}_{2k}(\Gamma_0(2))$ is

$$K(\lambda(\tau))^{2k}\,\frac{(\lambda(\tau)-2)^k\,t_2(\tau)^m}{(t_2(\tau)+64)^{\lfloor k/2\rfloor}}\,,\qquad 1\le m\le \lfloor k/2\rfloor-1\,. \tag{54}$$

Example 8 Since $\Gamma(2)\subseteq\Gamma_0(2)$, we have $\mathscr{M}_{2k}(\Gamma_0(2))\subseteq\mathscr{M}_{2k}(\Gamma(2))$. In particular, this means that we must be able to write every basis element for $\mathscr{M}_{2k}(\Gamma_0(2))$ in Eq. (52) in terms of the basis for $\mathscr{M}_{2k}(\Gamma(2))$ in Eq. (34). Indeed, inserting Eq. (41) into (52), we find,

$$\frac{(\lambda-2)^k\,t_2^m}{(t_2+64)^{\lfloor k/2\rfloor}}=16^{m-\lfloor k/2\rfloor}\,\lambda^{2m}\,(1-\lambda)^{\lfloor k/2\rfloor-m}\,(\lambda-2)^{k-2\lfloor k/2\rfloor}\,. \tag{55}$$

It is easy to see that the previous expression is polynomial in λ provided that $0\le m\le\lfloor k/2\rfloor$. Hence, we see that every element in Eq. (52) can be written in terms of the basis in Eq. (34).

3.4 A Basis for Modular Forms for $\Gamma_0(4)$ and $\Gamma_0(6)$

In this section we discuss the congruence subgroups $\Gamma_0(4)$ and $\Gamma_0(6)$. The analysis is identical to the case of $\Gamma_0(2)$ in the previous section, so we will be brief. There are no modular forms of odd weight and both groups have genus zero. The respective Hauptmodule t_4 and t_6 can be found in Ref. [27] in terms of η-quotients, though their explicit forms are irrelevant for what follows. Here we only mention that we can write the Hauptmodul t_2 as a rational function in either t_4 or t_6 [27]

$$t_2=t_4(t_4+16)=\frac{t_6(t_6+8)^3}{t_6+9}\,. \tag{56}$$

Since $\Gamma_0(2N)\subseteq\Gamma_0(2)$, the modular form $B_0(\tau)$ in Eq. (44) is a modular form of weight two for $\Gamma_0(2N)$ for any value of N. Hence, we can choose $B_0(\tau)$ as our seed modular form, and so if $f\in\mathscr{M}_{2k}(\Gamma_0(2N))$, then $f(\tau)/B_0^k(\tau)$ is a modular function for $\Gamma_0(2N)$. In the cases $N=2,3$ which we are interested in this implies that $f(\tau)/B_0^k(\tau)$ is a rational function in the Hauptmodul t_{2N},

$$R(t_{2N}(\tau))=\frac{f(\tau)}{B_0(\tau)^k}\,,\qquad N=4,6\,. \tag{57}$$

Let us now analyse the pole structure of $R(t_4)$. From the last section we know that $B_0(\tau)$ has a simple zero at $\lambda(\tau)=2$, or equivalently $t_2=-64$, and Eq. (56) then implies $t_4=-8$. Writing down an ansatz for $R(t_4)$ and bounding the degree of the polynomial in the numerator in the usual way, one finds that a basis of modular forms of weight $2k$ for $\Gamma_0(4)$ is

$$\mathrm{K}(\lambda(\tau))^{2k}\left(\frac{\lambda(\tau)-2}{t_4(\tau)+8}\right)^k t_4(\tau)^m\,,\qquad 0\le m\le k\,. \tag{58}$$

$\Gamma_0(4)$ has three cusps which can be represented by $\tau\in\{i\infty, 1, 1/2\}$ and which under t_4 are mapped to

$$t_4(i\infty)=0\qquad t_4(1)=\infty\,,\qquad t_4(1/2)=-16\,. \tag{59}$$

Hence a basis for $\mathscr{S}_{2k}(\Gamma_0(4))$ is

$$\mathrm{K}(\lambda(\tau))^{2k}\left(\frac{\lambda(\tau)-2}{t_4(\tau)+8}\right)^k t_4(\tau)^m\,(t_4(\tau)+16)\,,\qquad 1\le m\le k-2\,. \tag{60}$$

As a last example, let us have a short peek at $\Gamma_0(6)$. Equation (56) implies that $B_0(\tau)$ has simple poles for

$$t_6(\tau)=-6\pm 2\sqrt{3}\,. \tag{61}$$

The argument proceeds in the familiar way, with the only difference that now there are two distinct poles. The most general ansatz for a modular form of weight $2k$ for $\Gamma_0(6)$ reads

$$\frac{f(\tau)}{B_0^k(\tau)}=\frac{P(t_6(\tau))}{[(t_6(\tau)+6-2\sqrt{3})(t_6(\tau)+6+2\sqrt{3})]^k}=\frac{P(t_6(\tau))}{(t_6(\tau)^2+12t_6(\tau)+24)^k}\,, \tag{62}$$

where the degree of the polynomial P can again be bounded by the common holomorphicity argument. This leads to the following basis for modular forms of weight $2k$ for $\Gamma_0(6)$,

$$\mathrm{K}(\lambda(\tau))^{2k}\left(\frac{\lambda(\tau)-2}{t_6(\tau)^2+12t_6(\tau)+24}\right)^k t_6(\tau)^m\,,\qquad 0\le m\le 2k\,. \tag{63}$$

The cusps of $\Gamma_0(6)$ are represented by $\tau\in\{i\infty, 1, 1/2, 1/3\}$, or equivalently

$$t_6(i\infty)=0\,,\qquad t_6(1)=\infty\,,\qquad t_6(1/2)=-8\,,\qquad t_6(1/3)=-9\,. \tag{64}$$

Hence a basis for $\mathscr{S}_{2k}(\Gamma_0(6))$ is, with $1\le m\le 2k-3$,

$$\mathrm{K}(\lambda(\tau))^{2k}\left(\frac{\lambda(\tau)-2}{t_6(\tau)^2+12t_6(\tau)+24}\right)^k t_6(\tau)^m\,(t_6(\tau)+8)\,(t_6(\tau)+9)\,. \tag{65}$$

3.5 A Basis for Modular Forms for $\Gamma_1(6)$

As a last application we discuss the structure of modular forms for $\Gamma_1(6)$, which is known to be relevant for the sunrise and kite integrals [7, 9]. The general story will be very similar to the examples in previous sections. In particular, $\Gamma_1(6)$ has genus zero, and $\Gamma_1(6)$ and $\Gamma_0(6)$ have the same Hauptmodul t_6 [9]. Here we find it convenient to work with an alternative Hauptmodul t which is related to t_6 by a simple Möbius transformation [7, 27],

$$t = \frac{t_6}{t_6 + 8} \,. \tag{66}$$

The main difference in comparison to the previous examples – in particular to $\Gamma_0(6)$ – lies in the fact that $\left(\begin{smallmatrix} -1 & 0 \\ 0 & -1 \end{smallmatrix}\right) \notin \Gamma_1(6)$, and so $\Gamma_1(6)$ admits modular forms of odd weight. In particular, it is known that $\mathscr{M}_1(\Gamma_1(6))$ is two-dimensional (this can easily be checked with SAGE for example). Therefore, we would like to choose our seed modular form to have weight one. We find it convenient to choose as seed modular form a solution of the Picard–Fuchs operator associated to the sunrise graph [9, 26]. A particularly convenient choice is

$$B_1(\tau) = \Psi_1(t(\tau))\,, \tag{67}$$

where

$$\Psi_1(t) = \frac{4}{[(t-9)(t-1)^3]^{1/4}}\, \mathrm{K}\left(\frac{t^2 - 6t - 3 + \sqrt{(t-9)(t-1)^3}}{2\sqrt{(t-9)(t-1)^3}}\right) . \tag{68}$$

It can be shown that $\Psi_1(t(\tau))$ is indeed a modular form of weight one for $\Gamma_1(6)$ [7].

Next consider a modular form $f(\tau)$ of weight k for $\Gamma_1(6)$. Following the usual argument, the ratio

$$R(t(\tau)) = \frac{f(\tau)}{B_1(\tau)^k} \tag{69}$$

is a rational function in the Hauptmodul t with poles at most at points where $\Psi_1(t)$ vanishes. It is easy to check that the only zero of $\Psi_1(t)$ is at $t = \infty$, and we have

$$\Psi_1(t) \overset{t\to\infty}{\sim} 1/t \,. \tag{70}$$

Hence, $R(t)$ must be a polynomial in t whose degree is bounded by requiring that $\Psi_1(t)^k\, R(t)$ be free of poles at $t = \infty$. It immediately follows that a basis of modular forms of weight k for $\Gamma_1(6)$ is

$$\Psi_1(t(\tau))^k\, t(\tau)^m\,, \qquad 0 \le m \le k\,. \tag{71}$$

The cusps of $\Gamma_1(6)$ can be represented by $\tau \in \{i\infty, 1, 1/2, 1/3\}$, and they are mapped to

$$t(i\infty) = 0, \qquad t(1) = 1\,, \qquad t(1/2) = \infty\,, \qquad t(1/3) = 9\,. \tag{72}$$

So a basis of cusp forms of weight k for $\Gamma_1(6)$ is

$$\Psi_1(t(\tau))^k\, t(\tau)^m\, (t(\tau) - 1)\, (t(\tau) - 9)\,, \qquad 1 \leq m \leq k - 3\,. \tag{73}$$

Let us conclude by commenting on the structure of the modular forms for $\Gamma_1(6)$, and their relationship to modular forms for $\Gamma_0(6)$. Since $\Gamma_1(6) \subseteq \Gamma_0(6)$ we obviously have $\mathcal{M}_k(\Gamma_0(6)) \subseteq \mathcal{M}_k(\Gamma_1(6))$. Moreover, from Eqs. (63) to (71) we see that for even weights these spaces have the same dimension, and so we conclude that

$$\mathcal{M}_{2k}(\Gamma_1(6)) = \mathcal{M}_{2k}(\Gamma_0(6))\,. \tag{74}$$

There is a similar interpretation of the modular forms of odd weights. It can be shown that the algebra of modular forms for $\Gamma_1(N)$ admits the decomposition [34]

$$\mathcal{M}_k(\Gamma_1(N)) = \bigoplus_{\chi} \mathcal{M}_k(\Gamma_0(N), \chi)\,, \tag{75}$$

where the sum runs over all Dirichlet characters modulo N, i.e., all homomorphisms $\chi : \mathbb{Z}_N^\times \to \mathbb{C}^\times$. Here $\mathcal{M}_k(\Gamma_0(N), \chi)$ denotes the vector space of modular forms of weight k for $\Gamma_0(N)$ with character χ, i.e., the vector space of holomorphic functions $f : \overline{\mathbb{H}} \to \mathbb{C}$ such that

$$f\left(\frac{a\tau + b}{c\tau + d}\right) = \chi(d)\, (c\tau + d)^k\, f(\tau)\,, \qquad \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \Gamma_0(N)\,. \tag{76}$$

For $N = 6$ there are two Dirichlet characters modulo 6,

$$\chi_0(n) = 1 \qquad \text{and} \qquad \chi_1(n) = (-1)^n\,. \tag{77}$$

Hence, in the case we are interested in, Eq. (75) reduces to

$$\mathcal{M}_k(\Gamma_1(6)) = \mathcal{M}_k(\Gamma_0(6), \chi_0) \oplus \mathcal{M}_k(\Gamma_0(6), \chi_1) = \mathcal{M}_k(\Gamma_0(6)) \oplus \mathcal{M}_k(\Gamma_0(6), \chi_1)\,. \tag{78}$$

We then conclude that

$$\mathcal{M}_{2k}(\Gamma_0(6), \chi_1) = 0 \quad \text{and} \quad \mathcal{M}_{2k+1}(\Gamma_0(6), \chi_1) = \mathcal{M}_{2k+1}(\Gamma_1(6))\,. \tag{79}$$

4 Some Examples and Applications

4.1 Elliptic Multiple Zeta Values as Iterated Integrals Over Modular Forms for $\Gamma(2)$

Elliptic multiple zeta values have appeared in calculations in quantum field theory and string theory in various formulations during the last couple of years. While initially formulated as special values of elliptic multiple polylogarithms, they can be conveniently rewritten as iterated integrals over the Eisenstein series G_{2k} defined in Eq. (20) [16]. In other words, elliptic multiple zeta values are iterated integrals over modular forms for $\Gamma(1) = \mathrm{SL}(2, \mathbb{Z})$ (though it is known that not every such integral defines an element in the space of elliptic multiple zeta value [19]).

We have seen in Example 7 that every modular form for $\Gamma(1)$ is a modular form for $\Gamma(2)$. In particular, for $k > 1$ we can always write G_{2k} as the $2k$th power of $\mathrm{K}(\lambda(\tau))$ multiplied by a polynomial $\mathscr{G}_{2k}$ of degree k in $\lambda(\tau)$ (see Eq. (36)). The case $k = 1$ is special, and involves the elliptic integral of the second kind, see Eq. (39).

As a consequence, we can write every iterated integral of Eisenstein series of level $N = 1$, and thus every elliptic multiple zeta value, as iterated integrals over integration kernels that involve powers of complete elliptic integrals of the first kind multiplied by the polynomials $\mathscr{G}_{2k}(\lambda(\tau))$. More precisely, consider the one-forms $d\tau\, G_{2k}(\tau)$ which define iterated integrals of Eisenstein series of level one. Changing variables from τ to $\ell = \lambda(\tau)$, we obtain, for $k > 1$,

$$d\tau\, G_{2k}(\tau) = \frac{i\pi\, d\ell}{4\,\ell\,(\ell - 1)}\, \mathrm{K}(\ell)^{2k-2}\, \mathscr{G}_{2k}(\ell)\,, \tag{80}$$

where Jacobian is given by

$$2\pi\, i\partial_\tau \lambda(\tau) = 8\lambda(\tau)(\lambda(\tau) - 1)\mathrm{K}(\lambda(\tau))^2\,. \tag{81}$$

Note that we also need to include the Eisenstein series of weight zero, $G_0(\tau) = -1$, and Eq. (80) remains valid if we let $\mathscr{G}_0(\ell) = -1$. For $k = 1$ we can derive from Eq. (39) a similar relation involving the complete elliptic integral of the second kind. As a conclusion, we can always write iterated integrals of Eisenstein series of level one in terms of iterated integrals involving powers of complete elliptic integrals multiplied by rational functions. We stress that this construction is not specific to level $N = 1$ or to Eisenstein series, but using the results from previous sections it is possible to derive similar representations of 'algebraic type' for iterated integrals of general modular forms.

4.2 A Canonical Differential Equation for Some Classes of Hypergeometric Functions

As an example of how the ideas from previous sections can be used in the context of differential equations, let us consider the family of integrals

$$T(n_1,n_2,n_3) = \int_0^1 dx\, x^{-1/2+n_1+a\,\varepsilon}(1-x)^{-1/2+n_2+b\,\varepsilon}(1-z\,x)^{-1/2+n_3+c\,\varepsilon} . \quad (82)$$

This family is related to a special class of hypergeometric functions whose ε-expansion has been studied in detail in Refs. [11, 12]. It is easy to show that all integrals in Eq. (82), for any choice of n_1, n_2, n_3, can be expressed as linear combination of two independent master integrals, which can be chosen as

$$F_1 = T(0,0,0) \quad \text{and} \quad F_2 = T(1,0,0) . \quad (83)$$

The two masters satisfy the system of two differential equations,

$$\partial_z F = (A+\varepsilon B)F , \quad \text{with} \quad F = (F_1, F_2)^T , \quad (84)$$

where A, B are two 2×2 matrices

$$A = \frac{1}{z}\begin{pmatrix} 0 & 0 \\ 1/2 & -1 \end{pmatrix} + \frac{1}{z-1}\begin{pmatrix} -1/2 & 1/2 \\ -1/2 & 1/2 \end{pmatrix} , \quad (85)$$

$$B = \frac{1}{z}\begin{pmatrix} 0 & 0 \\ a & -a-b \end{pmatrix} + \frac{1}{z-1}\begin{pmatrix} -a & a+b+c \\ -a & a+b+c \end{pmatrix} . \quad (86)$$

A suitable boundary condition for the differential equations (84) can be determined by computing directly the integrals in Eq. (82) at $z=0$

$$\lim_{z\to 0} F = \frac{\Gamma\left(a\varepsilon+\frac{1}{2}\right)\Gamma\left(b\varepsilon+\frac{1}{2}\right)}{\Gamma(1+(a+b)\varepsilon)}\left(1, \frac{2a\varepsilon+1}{2\varepsilon(a+b)+2}\right)^T . \quad (87)$$

We are now ready to solve the differential equations. It is relatively easy to see that by performing the following change of basis

$$F = MG , \quad G = (G_1, G_2)^T , \quad (88)$$

with

$$M = \frac{1}{(2(a+b+c)\varepsilon+1)}\begin{pmatrix} 2K(z)(2(a+b+c)\varepsilon+1) & 0 \\ \frac{\varepsilon}{2zK(z)} - \frac{2E(z)}{z} + \frac{2((a+b)\varepsilon+(a+c)z\varepsilon+1)K(z)}{z} & \frac{\varepsilon}{2\,z\,K(z)} \end{pmatrix} , \quad (89)$$

the new master integrals G_1, G_2 fulfil the system of differential equations

$$\partial_z G = \frac{\varepsilon}{2\,z\,(z-1)\,K(z)^2}\,\Omega\,G\,, \tag{90}$$

where the matrix Ω can be written as

$$\Omega = \Omega_0 + \Omega_1 + \Omega_2\,, \tag{91}$$

with

$$\begin{aligned} \Omega_0 &= \frac{1}{4}\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}, \qquad \Omega_1 = (a+b+(c-a)z)\,K(z)^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \\ \Omega_2 &= 4\,\left((a+b)^2+(a+c)^2z^2-2\left(a^2+ba+ca-bc\right)z\right)\,K(z)^4\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \end{aligned} \tag{92}$$

We stress that the differential equations in Eq. (90) are ε-factorised.

In order to solve Eq. (90), let us change variable from z to τ via $z = \lambda(\tau)$, where λ denotes the modular λ-function. Using the form of the Jacobian in Eq. (81), we find that the differential equations become

$$\partial_\tau G = \frac{2\,\varepsilon}{\pi\,i}\,\Omega\,G\,. \tag{93}$$

As the last step, we know from the discussion in Sect. 3.2 that a basis of modular forms of weight $2k$ for $\Gamma(2)$ is given by $\lambda(\tau)^p K(\lambda(\tau))^{2k}$, with $0 \le p \le k$. Using this, we see that the entries of Ω are indeed linear combinations of modular forms of $\Gamma(2)$. The boundary condition at $z = 0$ in Eq. (87) translates directly into a boundary condition in $\tau = i\infty$. Hence, we have proved that the two entries of the vector G can be written, to all orders in ε, in terms of iterated integrals of modular forms for $\Gamma(2)$.

4.3 Modular Forms for $\Gamma_1(6)$ and the Sunrise and the Kite Integrals

In section 3 of Ref. [8] the kite integral family has been investigated, and it was shown that all the kernels presented in eq. (34) of Ref. [8] are modular forms for the congruence subgroup $\Gamma_1(6)$. This can also been seen upon integration of the Feynman parameters for the kite and the sunrise integral: the resulting elliptic curves agree.

The analysis of Ref. [8] relies on a direct matching of the kernels that appear in the sunrise and kite integrals to the basis of Eisenstein for $\Gamma_1(6)$ given in the mathematics literature. In Sect. 3.5 we have constructed an alternative basis for $\Gamma_1(6)$, and so we must be able to write all the integration kernels that appear in the sunrise integral in terms of our basis. This is the content of this section, and we argue that our basis makes the fact that the sunrise and kite integrals can be expressed in terms of iterated integrals of modular forms for $\Gamma_1(6)$ completely manifest.

In order to make our point, we proceed by example, and we consider in particular the function f_2 defined in eq. (34) of Ref. [8]. This function is one of the coefficients that appear in the differential equation satisfied by the master integrals of the kite topology, after the differential equations have been transformed to ε-form [8, 24]. All other coefficients appearing in the system of differential equations can be analysed in the same way. The function f_2 is defined as

$$f_2(x) = \frac{1}{24\pi^2}\Psi_1(x)^2\big(3x^2 - 10x - 9\big) \tag{94}$$

where $x = p^2/m^2$, with m the mass of the massive state flowing in the loop and p the external momentum, and (in our notations) Ψ_1 was defined in Eq. (68) (note that compared to Ref. [8] we have explicitly inserted the expression for the Wronskian W as a function of x into the definition of f_2). From the form of Eq. (94) we can immediately read off that f_2 defines a modular form for $\Gamma_1(6)$. Indeed, changing variables to $x = t(\tau)$, where $t(\tau)$ is the Hauptmodul for $\Gamma_1(6)$ introduced in Sect. 3.5, we see that $f_2(t(\tau))$ takes the form $\Psi_1(t(\tau))^2\, P(t(\tau))$, where P is a polynomial of degree two. Thus $f_2(t(\tau))$ can be written as a linear combination of the basis of modular forms of weight two for $\Gamma_1(6)$ given in Eq. (71), and so $f_2(t(\tau))$ itself defines a modular form of weight two for $\Gamma_1(6)$. It is easy to repeat the same analysis for all the coefficients that appear in the system of differential equations for sunrise and kite integrals, and we can conclude that the sunrise and kite integrals can be written in terms of iterated integrals of modular forms to all orders in ε. We emphasise that we have reached this conclusion solely based on the knowledge of the Hauptmodul of $\Gamma_1(6)$ and the fact that $\Psi_1(t(\tau))$ defines a modular form of weight one for $\Gamma_1(6)$. The rest follows from our analysis performed in Sect. 3.5, and we do not require any further input from the mathematics literature on the structure of modular forms for $\Gamma_1(6)$.

5 Conclusions and Outlook

In this contribution to the proceedings of the conference "Elliptic integrals, elliptic functions and modular forms in quantum field theory", we presented a systematic way of writing a basis of modular forms for congruence subgroups of the modular group $\mathrm{SL}(2,\mathbb{Z})$ in terms of powers of complete elliptic integrals of the first kind multiplied by algebraic functions. We considered congruence groups whose modular curves have genus zero and as such all modular forms can be written as powers of complete elliptic integrals of the first kind multiplied by rational functions of their corresponding Hauptmodule. Our construction relied simply on the knowledge of a seed modular form of lowest weight for each congruence group and its analytic properties. This, put together with the holomorphicity condition for modular forms, allowed us to write a general ansatz for a basis of modular forms.

We presented concrete examples for the congruence groups $\Gamma(2)$, $\Gamma_0(N)$ for $N = 2, 4, 6$, and finally $\Gamma_1(6)$ which features in physical applications such as the sunrise and kite integrals. By this method we showed how to write elliptic multiple zeta values as iterated integrals of rational functions weighted by complete elliptic integrals. Likewise, rewriting the differential equations of the sunrise and kite integrals, we were able to show that to all orders in ε these can be written as iterated integrals of modular forms for $\Gamma_1(6)$, confirming the findings of [7, 8].

We hope that our construction constitutes a first step into clarifying the connection between solutions of differential equations for elliptic Feynman integrals and elliptic multiple polylogarithms, allowing for a systematic application of this class of functions to realistic physical problems.

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One-Loop String Scattering Amplitudes as Iterated Eisenstein Integrals

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Abstract In these proceedings we review and expand on the recent appearance of iterated integrals on an elliptic curve in string perturbation theory. We represent the low-energy expansion of one-loop open-string amplitudes at multiplicity four and five as iterated integrals over holomorphic Eisenstein series. The framework of elliptic multiple zeta values serves as a link between the punctured Riemann surfaces encoding string interactions and the iterated Eisenstein integrals in the final results. In the five-point setup, the treatment of kinematic poles is discussed explicitly.

1 Introduction

Open-string scattering amplitudes at the one-loop level have proven to be a valuable laboratory for the application of techniques related to iterated elliptic integrals and elliptic multiple zeta values. Although elliptic curves and the classical elliptic integrals are one of the best-studied topics of 18th/19th-century mathematics, iterated integrals on elliptic curves and their associated special values are still a prominent topic in the recent mathematics literature, see for instance Refs. [1–3].

In high-energy physics, several integrals related to various scattering amplitudes in QCD have been solved using methods and techniques inherent to the elliptic curve. The concept of iterated integrals on an elliptic curve, however, made a first appearance in physics via one-loop scattering amplitudes in open-superstring theory

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in [4]. Since then, several refinements and extensions of the techniques have been put forward from different perspectives, see for examples Refs. [5–10].

Moreover, first connections between the open-string setup of iterated integrals and non-holomorphic modular invariants encountered in closed-string amplitudes have been investigated in Ref. [11]. The modular invariants in closed-string calculations are formulated in the framework of modular graph functions [12, 13], where tremendous progress in understanding their multiloop systematics has been made during the last couple of months [14, 15].

The low-energy expansion of one-loop scattering amplitudes in open-superstring theory gives rise to iterated elliptic integrals evaluated at special points: those functions of the modular parameter τ of the elliptic curve are called elliptic multiple zeta values and come in a twisted and an untwisted version. Both, untwisted and twisted elliptic multiple zeta values, however, allow for an alternative representation in terms of iterated integrals over the modular parameter τ: iterated Eisenstein integrals.

In these proceedings we are extending earlier results in two directions: we present low-energy expansions for the planar and non-planar five-point amplitudes, and we cast the four- and five-point expressions in the language of iterated Eisenstein integrals.

The current proceedings are structured as follows: in Sect. 2 we provide background information and define the mathematical setting for the calculation of one-loop open-string amplitudes at various multiplicities. We classify the occurring integrals and state the integral contributions to be evaluated at the four- and five-point level. In Sect. 3 a short introduction to twisted and untwisted elliptic multiple zeta values is provided. We relate these special values to iterated integrals over different flavors of Eisenstein series. This representation allows to infer relations between different twisted and untwisted elliptic multiple zeta values, which paves the way towards a canonical representation. Accordingly, in Sects. 4 and 5 we present and discuss the results of the four- and five-point integrals from Sect. 2 and represent them in terms of conventional elliptic multiple zeta values as well as iterated integrals over Eisenstein series.

2 One-Loop Open-String Amplitudes, Planar and Non-planar

2.1 General Setup, Planar and Non-planar

Scattering amplitudes in string theories are derived from punctured Riemann surfaces called worldsheets whose genus corresponds to the loop order in perturbation theory. In these proceedings we are going to consider the one-loop order exclusively, where the relevant topology for closed strings is a torus, and open-string amplitudes receive contributions from worldsheets of cylinder- and Mœbius-strip topologies. In all cases, the punctures correspond to the insertion of external states on the worldsheet via

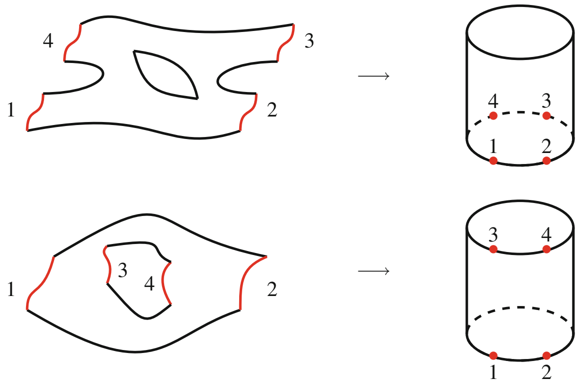

Fig. 1 The worldsheets for one-loop scattering of open strings include the topology of a cylinder. Conformal invariance on the worldsheet can be used to map external states to punctures on the cylinder boundaries. If vertex operators are inserted on one boundary only, the situation is referred to as the *planar cylinder* whereas the second topology is called the *non-planar cylinder*

vertex operators; those are conformal primary fields that carry the information on the external momenta and polarizations. For open strings, the vertex operators are inserted on the worldsheet boundaries, see Fig. 1. Moreover, each external open-string state carries additional degrees of freedom encoded in Lie-algebra generators t^a, called Chan–Paton factors. They enter scattering amplitudes in the form of traces, where the ordering of the generators reflects the distribution of vertex operators over the boundaries [16]. We will only consider massless vibration modes of the open superstring as an external state, i.e. one-loop scattering of gauge bosons and their superpartners. Accordingly, the Chan–Paton degrees of freedom of the external states are often referred to as color.

Having a single boundary only, the Mœbius strip can only contribute single traces to the n-point amplitude

$$M^n_{\mathrm{Moeb}} = -32 \sum_{\rho \in S_{n-1}} \mathrm{Tr}(t^1 t^{\rho(2)} t^{\rho(3)} \dots t^{\rho(n)}) A_{\mathrm{Moeb}}(1, \rho(2), \rho(3), \dots, \rho(n)) \,, \quad (1)$$

while the two boundary components of the cylinder admit double traces in the color decomposition. Accordingly, for a four-point amplitude the planar and non-planar cylinder contributions read

$$\begin{aligned} M^4_{\mathrm{cyl}} = \sum_{\rho \in S_3} \big\{ & N\, \mathrm{Tr}(t^1 t^{\rho(2)} t^{\rho(3)} t^{\rho(4)}) A_{\mathrm{cyl}}(1, \rho(2), \rho(3), \rho(4)) \\ & + \mathrm{Tr}(t^1 t^{\rho(2)}) \mathrm{Tr}(t^{\rho(3)} t^{\rho(4)}) A_{\mathrm{cyl}}(1, \rho(2) | \rho(3), \rho(4)) \big\} \\ & + \big\{ \mathrm{Tr}(t^1) \mathrm{Tr}(t^2 t^3 t^4) A_{\mathrm{cyl}}(1|2, 3, 4) + (1 \leftrightarrow 2, 3, 4) \big\} \,. \end{aligned} \quad (2)$$

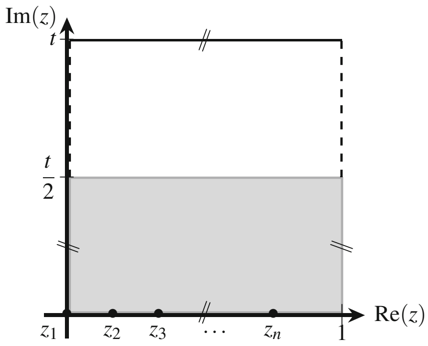

Fig. 2 In the boundary parametrization Eq. (4), worldsheets of cylinder topology are mapped to the shaded regions in the left (right) panel for the planar (non-planar) case. These regions cover half of a torus with modular parameter $\tau = it$ and identifications of edges marked by $\approx$ and $/\!/$, respectively. The Mœbius-strip topology is not drawn here as its contributions to the amplitude can be inferred from the planar cylinder [17], cf. Eqs. (6) and (8)

At higher multiplicity n, the analogous double-trace expressions in

$$M^n_{\text{cyl}} = N \sum_{\rho \in S_{n-1}} \text{Tr}(t^1 t^{\rho(2)} \dots t^{\rho(n)}) A_{\text{cyl}}(1, \rho(2), \dots, \rho(n)) + \text{double traces}\,, \quad (3)$$

comprise all partitions of the external states over the two boundaries along with all cyclically inequivalent arrangements. For instance, the double-trace sector of the five-point amplitude features permutations of $\text{Tr}(t^1t^2)\text{Tr}(t^3t^4t^5)A_{\text{cyl}}(1, 2|3, 4, 5)$ and $\text{Tr}(t^1)\text{Tr}(t^2t^3t^4t^5)A_{\text{cyl}}(1|2, 3, 4, 5)$, with an obvious generalization to higher multiplicity.

The number N of colors in the single-trace sector of Eqs. (2) and (3) arises from the trace over the identity matrix corresponding to the empty boundary component. The color-ordered amplitudes A_{Moeb} and A_{cyl} in Eqs. (1) and (3) are determined by integrating a correlation function of vertex operators over the punctures such that their cyclic ordering on each boundary component matches the accompanying color traces [16]. In the parametrization of the cylinder as half of a torus with purely imaginary modular parameter $\tau = it,\ t \in \mathbb{R}$, see Fig. 2, the integration domains for the punctures are of the form

$$\begin{aligned} D(1, 2, \dots, j|j{+}1, \dots, n) = \{&z_i \in \mathbb{C}\,,\ \text{Im}\, z_{1,2,\dots,j} = 0\,,\ \text{Im}\, z_{j+1,\dots,n} = \tfrac{t}{2}\,,\\ &0 \le \text{Re}\, z_1 < \text{Re}\, z_2 < \dots < \text{Re}\, z_j < 1\,,\ 0 \le \text{Re}\, z_{j+1} < \dots < \text{Re}\, z_n < 1\}\,. \end{aligned} \quad (4)$$

In particular, Eq. (4) refers to the non-planar amplitude $A_{\text{cyl}}(1, 2, \dots, j|j{+}1, \dots, n)$ along with the double trace $\text{Tr}(t^1t^2 \dots t^j)\text{Tr}(t^{j+1} \dots t^n)$ with $j = 1, 2, \dots, n{-}1$. We will also write $D(1, 2, \dots, n) = D(1, 2, \dots, n|\emptyset)$ for the integration domain of the planar cylinder amplitude $A_{\text{cyl}}(1, 2, \dots, n)$ in Eq. (3).

The correlation functions in the integrand will be denoted by $\mathcal{K}_n$. They depend on the punctures z_j, the modular parameter τ as well as the external polarizations and momenta of the gauge supermultiplet. For the cylinder topology, the integration domain for modular parameters $\tau = it$ is $t \in \mathbb{R}_+$ or

$$q = e^{2\pi i\tau} = e^{-2\pi t} \,, \qquad q \in (0,1)\,. \tag{5}$$

Then, the expression for color-ordered cylinder amplitudes reads

$$A_{\mathrm{cyl}}(1,2,\ldots,j|j{+}1,\ldots,n) = \int_0^1 \frac{\mathrm{d}q}{q} \int\limits_{D(1,2,\ldots,j|j+1,\ldots,n)} \mathrm{d}z_1\,\mathrm{d}z_2\,\ldots\,\mathrm{d}z_n\,\delta(z_1)\,\mathcal{K}_n\,, \tag{6}$$

where translation invariance on a genus-one surface has been used to fix $z_1 = 0$ through a delta-function insertion. We will also express the punctures in Eq. (4) in terms of real variables $x_i \in (0,1)$ and parametrize $D(1,2,\ldots,j|j{+}1,\ldots,n)$ via

$$z_i = \begin{cases} x_i & : i=1,2,\ldots,j \\ \frac{\tau}{2}+x_i & : i=j+1,\ldots,n \end{cases}, \quad 0 \le x_1 < x_2 < \cdots < x_j < 1\,, \quad 0 \le x_{j+1} < \cdots < x_n < 1\,. \tag{7}$$

For single-trace amplitudes in Eq. (6) with $j = n$, the integration over q introduces endpoint divergences as $q \to 0$. The latter cancel against the divergent contributions from the Mœbius strip in Eq. (1)

$$A_{\mathrm{Moeb}}(1,2,\ldots,n) = \int_0^{-1} \frac{\mathrm{d}q}{q} \int\limits_{D(1,2,\ldots,n)} \mathrm{d}z_1\,\mathrm{d}z_2\,\ldots\,\mathrm{d}z_n\,\delta(z_1)\,\mathcal{K}_n \tag{8}$$

if $N = 32$, i.e. if the gauge group[1] is taken to be $SO(32)$ [17]. The change of variables leading to the range $q \in (-1,0)$ in Eq. (8) can also be found in the reference.

In this work, we will be interested in the low-energy expansion of the integrals over the cylinder punctures in Eq. (6) at fixed value of q but unspecified choice of the gauge group. For instance, the integrals over $D(1,2,3|4)$ turn out to have an interesting mathematical structure, even though their coefficients $\sim\mathrm{Tr}(t^4)$ vanish for the physically preferable gauge group $SO(32)$. At the level of the integrand w.r.t. q, the Mœbius-strip results in Eq. (8) can be inferred from the planar instance of Eq. (6) by sending $q \to -q$ [17].

2.2 *Four-Point Amplitudes*

The four-point cylinder amplitude Eq. (6) of massless open-superstring states is governed by the correlation function

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[1]The choice of gauge group $SO(32)$ also ensures that the hexagon gauge anomaly in ($n \ge 6$)-point open-superstring amplitudes cancels [18, 19].

$$\mathcal{K}_4 = s_{12}\, s_{23}\, A^{\text{tree}}_{\text{SYM}}(1,2,3,4) \prod_{i<j}^{4} \exp\left(\tfrac{1}{2} s_{ij}\, G(z_{ij},\tau)\right), \tag{9}$$

which has firstly been derived for external bosons in 1982 [20]. The exponentials of Eq. (9) involve dimensionless Mandelstam variables s_{ij}

$$s_{ij} = 2\alpha' k_i \cdot k_j \tag{10}$$

with inverse string tension α'. Moreover, Eq. (9) features the bosonic Green function on a genus-one worldsheet

$$G(z,\tau) = \log\left|\frac{\theta_1(z,\tau)}{\theta_1'(0,\tau)}\right|^2 - \frac{2\pi}{\operatorname{Im}\tau}(\operatorname{Im} z)^2 \tag{11}$$

with $z_{ij} = z_i - z_j$ as its first argument, where θ_1 is the odd Jacobi function

$$\theta_1(z,\tau) = 2q^{1/8}\sin(\pi z)\prod_{n=1}^{\infty}(1-q^n)(1-2q^n\cos(2\pi z)+q^{2n}). \tag{12}$$

Finally, external polarizations enter Eq. (9) through the color-ordered (super-)Yang–Mills tree-level amplitude $A^{\text{tree}}_{\text{SYM}}(1,2,3,4)$.

With respect to relabeling of the external legs, there are three inequivalent representatives for the planar and non-planar four-point amplitudes. Using Eqs. (6) and (9), they can be written as

$$\begin{aligned}
A_{\text{cyl}}(1,2,3,4) &= s_{12}s_{23}A^{\text{tree}}_{\text{SYM}}(1,2,3,4)\int_0^1 \frac{\mathrm{d}q}{q}\, I_{1234}(s_{ij},q)\\
A_{\text{cyl}}(1,2,3|4) &= \frac{1}{2}s_{12}s_{23}A^{\text{tree}}_{\text{SYM}}(1,2,3,4)\int_0^1 \frac{\mathrm{d}q}{q}\, I_{123|4}(s_{ij},q)\\
A_{\text{cyl}}(1,2|3,4) &= \frac{1}{2}s_{12}s_{23}A^{\text{tree}}_{\text{SYM}}(1,2,3,4)\int_0^1 \frac{\mathrm{d}q}{q}\, I_{12|34}(s_{ij},q)\,,
\end{aligned} \tag{13}$$

where the integrals over the positions of the punctures defined in Eq. (7) read

$$\begin{aligned}
I_{1234}(s_{ij},q) &= \int_0^1 \mathrm{d}x_4 \int_0^{x_4}\mathrm{d}x_3\int_0^{x_3}\mathrm{d}x_2\int_0^{x_2}\mathrm{d}x_1\,\delta(x_1)\exp\left(\sum_{i<j}^{4}\frac{s_{ij}}{2}G(x_{ij})\right)\\
I_{123|4}(s_{ij},q) &= \left(\prod_{l=1}^{4}\int_0^1 \mathrm{d}x_l\right)\delta(x_1)\exp\left(\sum_{i<j}^{3}\frac{s_{ij}}{2}G(x_{ij})+\sum_{j=1}^{3}\frac{s_{j4}}{2}G(\tfrac{\tau}{2}+x_{ij})\right)\\
I_{12|34}(s_{ij},q) &= \left(\prod_{l=1}^{4}\int_0^1 \mathrm{d}x_l\right)\delta(x_1)\exp\left(\frac{s_{12}}{2}G(x_{12})+\frac{s_{34}}{2}G(x_{34})+\sum_{\substack{i=1,2\\ j=3,4}}\frac{s_{ij}}{2}G(\tfrac{\tau}{2}+x_{ij})\right).
\end{aligned} \tag{14}$$

Here and below, the dependence on τ in the Green functions is left implicit for ease of notation. The factors of $\frac{1}{2}$ in Eq. (13) are introduced to obtain a more convenient description of the integration domain for the non-planar cases $I_{123|4}(s_{ij}, q)$ and $I_{12|34}(s_{ij}, q)$: The natural integration domains $0 \leq x_1 < x_2 < x_3 < 1$ and $0 \leq x_3 < x_4 < 1$ expected from $\mathrm{Tr}(t^1 t^2 t^3)$ and $\mathrm{Tr}(t^3 t^4)$ can be rewritten to yield an independent integration of all the x_i over (0, 1) when taking the symmetry of the color factors or the integrands into account.

The integrals in Eq. (14) are the central four-point quantities in these proceedings. In Sect. 4, we are going to review and extend the results of Refs. [4, 6] on their low-energy expansion around $\alpha' = 0$, i.e. the Taylor expansion in the dimensionless Mandelstam invariants Eq. (10). Note that momentum conservation and the choice of massless external states in Eq. (9) with $k_j^2 = 0 \; \forall \; j = 1, 2, 3, 4$ relate the four-point Mandelstam invariants

$$\sum_{j=1}^{4} k_j = 0 \quad \Rightarrow \quad s_{12} = s_{34} \,, \quad s_{14} = s_{23} \,, \quad s_{13} = s_{24} = -s_{12} - s_{23} \,. \tag{15}$$

Accordingly, the integrand in Eq. (9) is unchanged if the Green function is shifted by $G(z, \tau) \to G(z, \tau) + f(\tau)$ as long as $f(\tau)$ does not depend on the position of the punctures.

2.3 Five-Point Amplitudes

The massless five-point correlator for the cylinder amplitude Eq. (6) is given by[2] [23, 24]

$$\mathcal{K}_5 = \left[f_{23}^{(1)} s_{23} \, C_{1|23,4,5} + (23 \leftrightarrow 24, 25, 34, 35, 45) \right] \prod_{i<j}^{5} \exp\left(\tfrac{1}{2} s_{ij} G(z_{ij}) \right) , \tag{16}$$

where the Green function is defined in Eq. (11) and we use the following shorthand for doubly-periodic functions of the punctures with a simple pole at $z_i - z_j \in \mathbb{Z} + \tau \mathbb{Z}$

$$f_{ij}^{(1)} = \partial_z \log \theta_1(z_{ij}, \tau) + 2\pi i \frac{\mathrm{Im}\, z_{ij}}{\mathrm{Im}\, \tau} = \partial_z G(z_{ij}, \tau) \,. \tag{17}$$

The kinematic factors in Eq. (16) obey symmetries $C_{1|23,4,5} = C_{1|23,5,4} = -C_{1|32,4,5}$ and can be expressed in terms of (super-)Yang–Mills tree-level amplitudes [24]

$$C_{1|23,4,5} = s_{45} \left[s_{24} \, A^{\mathrm{tree}}_{\mathrm{SYM}}(1, 3, 2, 4, 5) - s_{34} \, A^{\mathrm{tree}}_{\mathrm{SYM}}(1, 2, 3, 4, 5) \right] . \tag{18}$$

[2]Earlier work on five- and higher-point correlation functions for one-loop open-superstring amplitudes includes Refs. [21, 22].

The color decomposition of the five-point cylinder amplitude is a straightforward generalization of Eq. (2), and we collectively denote the color-ordered amplitudes by $A_{\mathrm{cyl}}(\lambda)$ with $\lambda = 1, 2, 3, 4, 5$ in the planar and $\lambda = 1, 2, 3, 4|5$ or $\lambda = 1, 2, 3|4, 5$ in the non-planar sector. Then, one can combine Eqs. (16) and (18) to bring all the cylinder contributions to the five-point amplitude into the form

$$A_{\mathrm{cyl}}(\lambda) = \int_0^1 \frac{\mathrm{d}q}{q} \big[I_\lambda^{23}(s_{ij}, q)\, A_{\mathrm{SYM}}^{\mathrm{tree}}(1, 2, 3, 4, 5) + I_\lambda^{32}(s_{ij}, q)\, A_{\mathrm{SYM}}^{\mathrm{tree}}(1, 3, 2, 4, 5) \big] \tag{19}$$

for some integrals $I_\lambda^{23}(s_{ij}, q)$ and $I_\lambda^{32}(s_{ij}, q)$ over the punctures whose domain $D(\lambda)$ is defined by Eq. (4). The color-ordered (super-)Yang–Mills amplitudes obtained from relabelings of Eq. (18) have been written in terms of a two-element basis of $A_{\mathrm{SYM}}^{\mathrm{tree}}(1, 2, 3, 4, 5)$ and $A_{\mathrm{SYM}}^{\mathrm{tree}}(1, 3, 2, 4, 5)$ using Bern–Carrasco–Johansson (BCJ) relations [25]. For planar choices of λ, for example, both $I_\lambda^{23}(s_{ij}, q)$ and $I_\lambda^{32}(s_{ij}, q)$ can be reduced to the following permutation-inequivalent integrals

$$H_{12345}^{12}(s_{ij}, q) = \int_0^1 \mathrm{d}x_5 \left(\prod_{l=1}^{4} \int_0^{x_{l+1}} \mathrm{d}x_l \right) \delta(x_1)\, f_{12}^{(1)}\, \exp\left(\sum_{i<j}^{5} \frac{s_{ij}}{2} G(x_{ij}) \right) \tag{20}$$

$$\widehat{H}_{12345}^{13}(s_{ij}, q) = \int_0^1 \mathrm{d}x_5 \left(\prod_{l=1}^{4} \int_0^{x_{l+1}} \mathrm{d}x_l \right) \delta(x_1)\, f_{13}^{(1)}\, \exp\left(\sum_{i<j}^{5} \frac{s_{ij}}{2} G(x_{ij}) \right). \tag{21}$$

The hat-notation in (21) and (23) below is used to distinguish integrals $\widehat{H}_\lambda^{ij}$ with a regular Taylor expansion around $s_{ij} = 0$ from cases H_λ^{ij} with kinematic poles of the form s_{ij}^{-1}, see Sect. 5.1. In the non-planar sector with $\lambda = 1, 2, 3|4, 5$, on the other hand, $I_\lambda^{23}(s_{ij}, q)$ and $I_\lambda^{32}(s_{ij}, q)$ can be assembled from permutations of

$$H_{123|45}^{12}(s_{ij}, q) = \left(\prod_{l=3}^{5} \int_0^1 \mathrm{d}x_l \right) \int_0^{x_3} \mathrm{d}x_2 \int_0^{x_2} \mathrm{d}x_1\, \delta(x_1)\, f_{12}^{(1)}\, \exp\left(\sum_{i<j}^{5} \frac{s_{ij}}{2} G(\delta_{ij} \tfrac{\tau}{2} + x_{ij}) \right) \tag{22}$$

$$\widehat{H}_{123|45}^{14}(s_{ij}, q) = \left(\prod_{l=3}^{5} \int_0^1 \mathrm{d}x_l \right) \int_0^{x_3} \mathrm{d}x_2 \int_0^{x_2} \mathrm{d}x_1\, \delta(x_1)\, f_{14}^{(1)}\, \exp\left(\sum_{i<j}^{5} \frac{s_{ij}}{2} G(\delta_{ij} \tfrac{\tau}{2} + x_{ij}) \right), \tag{23}$$

where $\delta_{12} = \delta_{13} = \delta_{23} = \delta_{45} = 0$ and $\delta_{ij} = 1$ if $i = 1, 2, 3$ and $j = 4, 5$. The analogous non-planar integral with $f_{45}^{(1)}$ in the place of $f_{12}^{(1)}$ and $f_{14}^{(1)}$ vanishes, because the integration measure is symmetric in 4, 5 while $f_{45}^{(1)} = -f_{54}^{(1)}$,

$$\left(\prod_{l=3}^{5} \int_0^1 \mathrm{d}x_l \right) \int_0^{x_3} \mathrm{d}x_2 \int_0^{x_2} \mathrm{d}x_1\, \delta(x_1)\, f_{45}^{(1)}\, \exp\left(\sum_{i<j}^{5} \frac{s_{ij}}{2} G(\delta_{ij} \tfrac{\tau}{2} + x_{ij}) \right) = 0. \tag{24}$$

Note that there are five independent Mandelstam variables for five massless particles, for example $s_{12}, s_{23}, s_{34}, s_{45}, s_{51}$,

$$\sum_{j=1}^{5} k_j = 0 \quad \Rightarrow \quad s_{13} = s_{45} - s_{12} - s_{23} \text{ and } \operatorname{cyc}(1, 2, 3, 4, 5)\,. \tag{25}$$

Similarly, the non-planar sector with $\lambda = 1, 2, 3, 4|5$ admits three topologies of permutation-inequivalent integrals: with insertions $f^{(1)}_{12}$, $f^{(1)}_{13}$ and $f^{(1)}_{45}$ beyond the Koba–Nielsen-factor, respectively.

2.4 Higher-Point Amplitudes

Starting from six external states, the correlators $\mathscr{K}_n$ no longer boil down to tree-level amplitudes $A^{\text{tree}}_{\text{SYM}}(\ldots)$ in (super-)Yang–Mills theory. Instead, one finds a more general class of kinematic factors, see Refs. [26, 27] for their precise form and the accompanying functions of the punctures at six points.

3 Mathematical Tools/Objects

Employing the form of the open-string one-loop propagator in Eq. (9) and expanding the exponentials of the propagators in powers of α' [cf. Eq. (10)], one finds all integrals in the previous section to boil down to iterated integrals on the elliptic curve. The integration kernels $f^{(1)}_{ij}$ in Eq. (17) and their higher-weight generalizations are canonical differentials on the elliptic curve that can be generated by a non-holomorphic extension of the Eisenstein–Kronecker series [1, 28]

$$\Omega(z, \alpha, \tau) = \exp\left(2\pi i \alpha \frac{\operatorname{Im} z}{\operatorname{Im} \tau}\right) \frac{\theta_1'(0, \tau)\theta_1(z + \alpha, \tau)}{\theta_1(z, \tau)\theta_1(\alpha, \tau)} = \sum_{n=0}^{\infty} \alpha^{n-1} f^{(n)}(z, \tau)\,. \tag{26}$$

The expansion in the second equality yields doubly-periodic functions

$$f^{(n)}(z, \tau) = f^{(n)}(z + 1, \tau) = f^{(n)}(z + \tau, \tau)\,, \qquad f^{(n)}(-z, \tau) = (-1)^n f^{(n)}(z, \tau)\,, \tag{27}$$

for example $f^{(0)} = 1$ and $f^{(1)}(z, \tau) = \partial_z \log \theta_1(z, \tau) + 2\pi i \frac{\operatorname{Im} z}{\operatorname{Im} \tau}$. Equation (17) arises from the shorthand $f^{(n)}_{ij} = f^{(n)}(z_i - z_j, \tau)$. The Fay relations of the Eisenstein–Kronecker series [1, 29]

$$\Omega(z_1, \alpha_1, \tau)\Omega(z_2, \alpha_2, \tau) = \Omega(z_1, \alpha_1 + \alpha_2, \tau)\Omega(z_2 - z_1, \alpha_2, \tau) + (z_1, \alpha_1 \leftrightarrow z_2, \alpha_2) \tag{28}$$

imply the following component relations when Laurent expanded in the bookkeeping variables α_i [4]:

$$f_{ij}^{(n)} f_{jl}^{(m)} = -f_{il}^{(m+n)} + \sum_{k=0}^{n} (-1)^k \binom{m-1+k}{k} f_{il}^{(n-k)} f_{jl}^{(m+k)} + \sum_{k=0}^{m} (-1)^k \binom{n-1+k}{k} f_{il}^{(m-k)} f_{ij}^{(n+k)} . \tag{29}$$

As already noted for the Green function after Eq. (14), all functions considered in these proceedings are functions of the modular parameter τ, which we will suppress here and below. Using the integration kernels $f^{(n)}(z)$ and the following definition of elliptic iterated integrals[3] with $\Gamma(\,;z) = 1$,

$$\Gamma\left(\begin{smallmatrix} n_1 & n_2 & \dots & n_\ell \\ b_1 & b_2 & \dots & b_\ell \end{smallmatrix} ; z \right) = \int_0^z \mathrm{d}t \; f^{(n_1)}(t-b_1) \; \Gamma\left(\begin{smallmatrix} n_2 & \dots & n_\ell \\ b_2 & \dots & b_\ell \end{smallmatrix} ; t \right) , \qquad z \in [0,1] , \tag{30}$$

one can solve the integrals over the punctures z_j in one-loop open-superstring amplitudes order by order in α'. In particular, it will be explained in detail in Sect. 4 how the mathematical tools of this section yield a recursive and algorithmic procedure to expand the four-point integrals Eq. (14) to any desired order in α'.

Allowing for rational values s_i and r_i in the fundamental elliptic domain only, twists $b_i = s_i + r_i \tau$ with $r_i, s_i \in [0,1)$ lead to the notion of twisted elliptic multiple zeta values or teMZVs [6]:

$$\begin{aligned} \omega\left(\begin{smallmatrix} n_1, & n_2, & \dots, & n_\ell \\ b_1, & b_2, & \dots, & b_\ell \end{smallmatrix} \right) &= \int\limits_{0 \leq z_i \leq z_{i+1} \leq 1} f^{(n_1)}(z_1 - b_1)\mathrm{d}z_1 \, f^{(n_2)}(z_2 - b_2)\mathrm{d}z_2 \, \dots f^{(n_\ell)}(z_\ell - b_\ell)\mathrm{d}z_\ell \\ &= \Gamma\left(\begin{smallmatrix} n_\ell & n_{\ell-1} & \dots & n_1 \\ b_\ell & b_{\ell-1} & \dots & b_1 \end{smallmatrix} ; 1 \right) . \end{aligned} \tag{31}$$

If there are no twists, that is, $b_i = 0 \; \forall \, i$, one obtains untwisted elliptic multiple zeta values or eMZVs, for which a simplified notation is used [4, 5]:

$$\omega(n_1, n_2, \dots, n_\ell) = \Gamma\left(\begin{smallmatrix} n_\ell & \dots & n_2 & n_1 \\ 0 & \dots & 0 & 0 \end{smallmatrix} ; 1 \right) = \Gamma(n_\ell, \dots, n_2, n_1; 1) . \tag{32}$$

For eMZVs and teMZVs defined in Eqs. (31) and (32), the quantities $w = \sum_{i=1}^{\ell} n_i$, and the number ℓ of integrations in are referred to as *weight* and *length* of the elliptic iterated integral and the corresponding (t)eMZV, respectively.

In view of the simple pole of $f^{(1)}(z,\tau)$ at $z = 0, 1$, eMZVs with entries $n_1 = 1$ or $n_\ell = 1$ suffer from endpoint divergences, whose regularization was discussed in

[3]The iterated integrals in Eq. (30) are not homotopy invariant. Still, one can find a homotopy-invariant completion for each $\Gamma\left(\begin{smallmatrix} n_1 & n_2 & \dots & n_\ell \\ b_1 & b_2 & \dots & b_\ell \end{smallmatrix} ; z \right)$ from the generating series in Ref. [1] (see also subsection 3.1 of Ref. [4]).

Ref. [4]. Similarly, a regularization scheme for the divergences caused by twists $b \in \mathbb{R}$ in Eq. (31) can be found in Ref. [6].

3.1 Elliptic Multiple Zeta Values in Terms of Iterated Eisenstein Integrals

While teMZVs can be represented as iterated integrals over the positions z_i of vertex operators, the analytically favorable way is to convert them to iterated integrals in the modular parameters τ. The main reason is, that the integration kernels appearing in this setting are very well-known objects: holomorphic Eisenstein series for congruence subgroups of $\mathrm{SL}_2(\mathbb{Z})$ of various levels M. For level 1, iterated τ-integrals over Eisenstein series do not satisfy any relations except for shuffle [30], hence, representing these (untwisted) eMZVs in terms of iterated Eisenstein integrals automatically exposes all their relations over the rational numbers. For levels $M > 1$, however, the Eisenstein series are not independent, when evaluated at rational points of the lattice. These relations have been investigated and discussed in Ref. [10] and allow to relate different iterated integrals, even between different levels M.

There does exist a straightforward method for converting iterated z-integrals underlying (t)eMZVs to iterated Eisenstein integrals $\mathcal{E}_0$ over Eisenstein series [2, 5, 6]: since the resulting "number" is still going to be a function of the modular parameter τ, one can conveniently take a derivative with respect to τ. Let us make this construction precise in the next paragraphs.

Given a teMZV of the form (31), let us take all of the twists b_i from a rational lattice $\Lambda_M = \left\{\frac{r}{M} + \tau\frac{s}{M} : r, s = 0, 1, 2, \ldots, M-1\right\}$ within the elliptic curve characterized by an integer level $M \in \mathbb{N}$. The derivative in τ of the teMZV is most conveniently expressed in terms of functions[4]

$$h^{(n)}(b_i, \tau) = (n-1) f^{(n)}(b_i, \tau)\,, \tag{33}$$

evaluated at lattice points $b_i \in \Lambda_M$, that is, Eisenstein series for congruence subgroups of $\mathrm{SL}_2(\mathbb{Z})$ [6]:

$$\begin{aligned}
2\pi i\,\partial_\tau\, \omega\left(\begin{smallmatrix} n_1, \ldots, n_\ell \\ b_1, \ldots, b_\ell \end{smallmatrix}\right) &= h^{(n_\ell+1)}(-b_\ell)\, \omega\left(\begin{smallmatrix} n_1, \ldots, n_{\ell-1} \\ b_1, \ldots, b_{\ell-1} \end{smallmatrix}\right) - h^{(n_1+1)}(-b_1)\, \omega\left(\begin{smallmatrix} n_2, \ldots, n_\ell \\ b_2, \ldots, b_\ell \end{smallmatrix}\right) \\
&+ \sum_{i=2}^{\ell} \left[\theta_{n_i \geq 1} \sum_{k=0}^{n_{i-1}+1} \binom{n_i + k - 1}{k} h^{(n_{i-1}-k+1)}(b_i - b_{i-1})\, \omega\left(\begin{smallmatrix} n_1, \ldots, n_{i-2}, n_i+k, n_{i+1}, \ldots, n_\ell \\ b_1, \ldots, b_{i-2}, \;\; b_i, \;\; b_{i+1}, \ldots, b_\ell \end{smallmatrix}\right) \right. \\
&\quad \left. - \theta_{n_{i-1} \geq 1} \sum_{k=0}^{n_i+1} \binom{n_{i-1} + k - 1}{k} h^{(n_i-k+1)}(b_{i-1} - b_i)\, \omega\left(\begin{smallmatrix} n_1, \ldots, n_{i-2}, n_{i-1}+k, n_{i+1}, \ldots, n_\ell \\ b_1, \ldots, b_{i-2}, \;\; b_{i-1}, \;\; b_{i+1}, \ldots, b_\ell \end{smallmatrix}\right)
\end{aligned}$$

[4]Note that the normalization conventions of the functions $h^{(n)}(b, \tau)$ in Eq. (33) and Ref. [6] differ from the definition of the Eisenstein series $h^{(n)}_{M,r,s} = f^{(n)}(\frac{r}{M} + \frac{s}{M}\tau, \tau)$ for congruence subgroups of $\mathrm{SL}_2(\mathbb{Z})$ in Ref. [10].

$$+(-1)^{n_i+1}\theta_{n_{i-1}\geq 1}\theta_{n_i\geq 1}h^{(n_{i-1}+n_i+1)}(b_i-b_{i-1})\,\omega\left(\begin{smallmatrix} n_1,\,\dots,\,n_{i-2},\,0,\,n_{i+1},\,\dots,\,n_\ell \\ b_1,\,\dots,\,b_{i-2},\,0,\,b_{i+1},\,\dots,\,b_\ell \end{smallmatrix}\right)\Big]\,. \tag{34}$$

We have introduced $\theta_{n\geq 1} = 1 - \delta_{n,0}$ for non-negative n, indicating that $n_i = 0$ cause certain terms in the last three lines to vanish. For teMZVs of length $\ell > 1$ on the left-hand side of Eq. (34), each teMZV on the right-hand side has lower length $\ell - 1$. Hence, Eq. (34) allows to recursively convert teMZVs to iterated integrals over the functions $h^{(k)}(b, \tau)$, terminating with a vanishing right-hand side for $\ell = 1$. Upon evaluation at fixed lattice points $b_i \in \Lambda_M$, the functions $h^{(k)}(b, \tau)$ are holomorphic in the modular parameter τ. For any $k > 2$, they can be conveniently represented as a lattice sum

$$h^{(k)}\left(\frac{r}{M} + \tau\frac{s}{M}, \tau\right) = (k-1)\sum_{(m,n)\neq(0,0)} \frac{e^{2\pi i\,\frac{rm-sn}{M}}}{(n+m\tau)^k}\,. \tag{35}$$

In order to render the corresponding expression finite for $k = 2$, the summation prescription has to be modified. Alternatively, level-M Eisenstein series have series expansions in $q^{1/M}$ [6], for example one finds

$$h^{(4)}\left(\frac{\tau}{2}, \tau\right) = \frac{\zeta_4}{4}\left(7 - 240\,q^{1/2} - 240\,q - 6720\,q^{3/2} - 240\,q^2 - 30240\,q^{5/2} + \cdots\right)\,. \tag{36}$$

For $r = s = 0$, one recovers the usual holomorphic Eisenstein series [cf. Eq. (35)]

$$\frac{h^{(k)}(0,\tau)}{1-k} = \mathrm{G}_k(\tau) = \sum_{(m,n)\neq(0,0)} \frac{1}{(n+m\tau)^k}\,, \qquad k \geq 3\,. \tag{37}$$

Correspondingly, Eq. (34) reduces to the differential equation for eMZVs stated in eq. (2.47) of Ref. [5]. Nicely, the situation $k = 2$ in the equation above does not occur, when considering the τ-derivative Eq. (34) of convergent eMZVs.

Considering the differential equation (34) and the identification (37), one can finally rewrite every eMZV in terms of iterated integrals of Eisenstein series [5]:

$$\begin{aligned}\mathcal{E}_0(k_1, k_2, \dots, k_r; q) &:= -\int_0^q \frac{\mathrm{d}q_r}{q_r}\,\frac{\mathrm{G}^0_{k_r}(q_r)}{(2\pi i)^{k_r}}\;\mathcal{E}_0(k_1, k_2, \dots, k_{r-1}; q_r) \\ &= (-1)^r \int\limits_{0\leq q_1\leq q_2\leq\cdots\leq q_r\leq q} \frac{\mathrm{d}q_1}{q_1}\cdots\frac{\mathrm{d}q_r}{q_r}\,\frac{\mathrm{G}^0_{k_1}(q_1)}{(2\pi i)^{k_1}}\cdots\frac{\mathrm{G}^0_{k_r}(q_r)}{(2\pi i)^{k_r}}\,.\end{aligned} \tag{38}$$

The recursion starts with $\mathcal{E}_0(;\tau) = 1$, and the non-constant parts of Eisenstein series are defined as

$$\mathrm{G}^0_{2n}(\tau) = \mathrm{G}_{2n}(\tau) - 2\,\zeta_{2n}\,, \qquad \mathrm{G}_0(\tau) = \mathrm{G}^0_0(\tau) = -1 \tag{39}$$

with $n \in \mathbb{N}$. For iterated integrals $\mathscr{E}_0(k_1, k_2, \dots, k_r; q)$ in Eq. (38), the number of non-zero entries ($k_j \neq 0$) is called the *depth* of the iterated Eisenstein integral.

The iterated Eisenstein integrals $\mathscr{E}_0(k_1, \dots, k_r; q)$ with $k_1 \neq 0$ are nicely convergent and do not need to be regularized. Even more, the conversion of untwisted eMZVs to iterated Eisenstein integrals provides an easy way to identify their relations [5, 30, 31]. Many of such eMZV relations are available in digital form [32] similar to the datamine of multiple zeta values [33].

In the same way as one can rewrite untwisted eMZVs as iterated integrals over the Eisenstein series Eq. (37), one can rewrite teMZVs as iterated integrals over the level-M Eisenstein series defined in Eq. (36). In contrast to the situation for usual holomorphic Eisenstein series, there are several linear relations between level-M Eisenstein series, which are discussed in Ref. [10] and which need to be taken into account when deriving functions relations in general. In the realm of string amplitudes discussed in the next subsection, we will however encounter only one particular Eisenstein series at level two, which does not require these additional relations in order to reach a canonical representation.

3.2 Eisenstein Series of Level two in the String Context

Although the differential equation (34) is applicable to Eisenstein series evaluated at points of any sublattice Λ_M, let us focus on the lattice Λ_2 suitable for string amplitudes. As will be elaborated in Sect. 4, the parametrization of the cylinder worldsheet in Fig. 2 gives rise to teMZVs with twists $b \in \{0, {}^{\tau}/_{2}\}$ in the non-planar amplitudes. Hence, the differential equation (34) allows to express the α'-expansion in terms of iterated Eisenstein integrals involving $h^{(k)}\left(\frac{\tau}{2}, \tau\right)$ and $h^{(k)}(0, \tau) = (1 - k)\mathrm{G}_k(\tau)$.

When expressing the teMZVs from the non-planar integrals in terms of a basis of iterated Eisenstein integrals, the contributions from $h^{(k)}\left(\frac{\tau}{2}, \tau\right)$ turn out to cancel. In other words, even for the non-planar integrals $I_{12|34}$ and $I_{123|4}$ of Eq. (14), the α'-expansions shown in the next section are expressible in terms of untwisted eMZVs or iterated integrals over $\mathrm{G}_k(\tau)$ exclusively. In spite of the cancellation of all non-trivial twists, the representation of intermediate results in terms of Eisenstein series for congruence subgroups of $\mathrm{SL}_2(\mathbb{Z})$ has been indispensable to attain a canonical form for all contributions.

As an example for the τ-derivative in Eq. (34), let us take the teMZVs

$$
\begin{aligned}
2\pi i \frac{\partial}{\partial \tau}\, \omega\left(\begin{smallmatrix} 0, & 1, & 1 \\ 0, & {}^{\tau}/_{2}, & {}^{\tau}/_{2} \end{smallmatrix}\right) &= h^{(2)}\left(\frac{\tau}{2}, \tau\right) \omega\left(\begin{smallmatrix} 0, & 1 \\ 0, & {}^{\tau}/_{2} \end{smallmatrix}\right) - \omega\left(\begin{smallmatrix} 2, & 1 \\ {}^{\tau}/_{2}, & {}^{\tau}/_{2} \end{smallmatrix}\right) \text{ and} \\
2\pi i \frac{\partial}{\partial \tau}\, \omega\left(\begin{smallmatrix} 0, & 1 \\ 0, & {}^{\tau}/_{2} \end{smallmatrix}\right) &= h^{(2)}\left(\frac{\tau}{2}, \tau\right) - \zeta_2 \,.
\end{aligned} \tag{40}
$$

Since intermediate steps in the expansion of $I_{123|4}$ and $I_{12|34}$ turn out to involve the rigid combination $2\,\omega\left(\begin{smallmatrix} 0, & 1, & 1 \\ 0, & {}^{\tau}/_{2}, & {}^{\tau}/_{2} \end{smallmatrix}\right) - \omega\left(\begin{smallmatrix} 0, & 1 \\ 0, & {}^{\tau}/_{2} \end{smallmatrix}\right)^2$, the contribution of $h^{(2)}\left(\frac{\tau}{2}, \tau\right)$ in

Eq. (40) cancels. Moreover, the relation $2\,\omega\left(\begin{smallmatrix}0, & 1, & 1\\ 0, & \tau/2, & \tau/2\end{smallmatrix}\right) - \omega\left(\begin{smallmatrix}0, & 1\\ 0, & \tau/2\end{smallmatrix}\right)^2 = \omega(0,0,2) + \frac{\zeta_2}{3}$ can be checked by taking higher τ-derivatives of the left-hand side.

Similarly, the τ-derivative Eq. (34) and the decomposition described in the previous subsection yield

$$\begin{aligned} \omega(0,0,2) &= -\frac{\zeta_2}{3} - 6\,\mathscr{E}_0(4,0;\tau) \\ \omega(0,1,0,0) &= \frac{3\zeta_3}{4\pi^2} - \frac{9}{2\pi^2}\,\mathscr{E}_0(4,0,0;\tau) \\ \omega(0,3,0,0) &= 180\,\mathscr{E}_0(6,0,0;\tau)\,. \end{aligned} \tag{41}$$

The terms $-\frac{\zeta_2}{3}$ and $\frac{3\zeta_3}{4\pi^2}$ at the order of q^0 exemplify that integration constants have to be taken into account when expressing teMZVs as integrals over their τ-derivatives Eq. (34). For the twists $b \in \{0, \tau/2\}$ of our interest, the integration constants are rational combinations of $(2\pi i)^{-1}$ and multiple zeta values that can be determined by the techniques in Section 2.3 of Ref. [5] and section 3.2 of Ref. [6].

4 Four-Point Results in Different Languages

In this section, we apply the mathematical framework of Sect. 3 to the α'-expansion of the four-point cylinder integrals Eq. (14). In order to relate the Green function Eq. (11) to the constituents of teMZVs, we use momentum conservation Eq. (15) to rewrite the target integrals[5] as

$$\begin{aligned} I_{1234}(s_{ij},q) &= \int_0^1 \mathrm{d}x_4 \int_0^{x_4} \mathrm{d}x_3 \int_0^{x_3} \mathrm{d}x_2 \int_0^{x_2} \mathrm{d}x_1\, \delta(x_1) \exp\left(\sum_{i<j}^4 s_{ij} P(x_{ij},q)\right) \\ I_{123|4}(s_{ij},q) &= \left(\prod_{l=1}^4 \int_0^1 \mathrm{d}x_l\right) \delta(x_1) \exp\left(\sum_{i<j}^3 s_{ij} P(x_{ij},q) + \sum_{j=1}^3 s_{j4} Q(x_{ij},q)\right) \\ I_{12|34}(s_{ij},q) &= q^{\frac{s_{12}}{4}} \left(\prod_{l=1}^4 \int_0^1 \mathrm{d}x_l\right) \delta(x_1) \exp\left(\sum_{\substack{(i,j)=\\(1,2),(3,4)}} s_{ij} P(x_{ij},q) + \sum_{\substack{i=1,2\\ j=3,4}} s_{ij} Q(x_{ij},q)\right), \end{aligned} \tag{42}$$

with the expressions

$$G(z,\tau),\quad \mathrm{Im}\, z = 0 \quad \rightsquigarrow \quad P(x,q) = \Gamma\left(\begin{smallmatrix}1\\0\end{smallmatrix};x\right) - \omega(1,0) \tag{43}$$

[5]The derivation of Eq. (42) from Eq. (14) is discussed on in Ref. [6]. The only difference is that the present definitions of $P(x,q)$ and $Q(x,q)$ in Eqs. (44) and (43) deviate from those in the reference by an additive constant. Instead, the objects $P(x,q)$ and $Q(x,q)$ defined in Eqs. (44) and (43) match the expressions in Ref. [11] up to an overall minus sign.

$$G(z,\tau), \quad \mathrm{Im}\, z = \frac{\mathrm{Im}\,\tau}{2} \quad \rightsquigarrow \quad Q(x,q) = \Gamma\left(\begin{smallmatrix}1\\ \tau/2\end{smallmatrix}; x\right) - \omega\left(\begin{smallmatrix}1, & 0\\ \tau/2, & 0\end{smallmatrix}\right), \tag{44}$$

where $x = Re z$ (cf. Eq. (7)), and the Green functions $P(x,q)$ and $Q(x,q)$ connect punctures on the same and on different cylinder boundaries, respectively. Both summands $\Gamma\left(\begin{smallmatrix}1\\ 0\end{smallmatrix}; x\right)$ and $\omega(1,0)$ in Eq. (44) individually represent divergent integrals whose regularization is discussed in detail in section 4.2 of [6]. As visualized in Fig. 2, the twists $\tau/2$ in Eq. (43) stem from the displacement of the two cylinder boundaries in our parametrization through a rectangular torus. Accordingly, the factor of $q^{s_{12}/4}$ in the above expression for the non-planar contribution $I_{12|34}(s_{ij},q)$ can be traced back to the term $\sim (\mathrm{Im}\, z)^2$ in the Green function Eq. (11).

When inserting the differences $x_{ij} = x_i - x_j$ of the cylinder punctures into the Green functions $P(x,q)$ and $Q(x,q)$, the following representations turn out to be particularly convenient for the α'-expansion of Eq. (42)

$$P(x_{ij},q) = \Gamma\left(\begin{smallmatrix}1\\ x_j\end{smallmatrix}; x_i\right) + \Gamma\left(\begin{smallmatrix}1\\ 0\end{smallmatrix}; x_j\right) - \omega(1,0), \qquad 1 < i < j \tag{45}$$

$$Q(x_{ij},q) = \Gamma\left(\begin{smallmatrix}1\\ x_j+\tau/2\end{smallmatrix}; x_i\right) + \Gamma\left(\begin{smallmatrix}1\\ \tau/2\end{smallmatrix}; x_j\right) - \omega\left(\begin{smallmatrix}1, & 0\\ \tau/2, & 0\end{smallmatrix}\right), \qquad 1 < i < j\,. \tag{46}$$

4.1 The Proof of Concept

The α'-expansion of the open-string integrals Eq. (42) at fixed[6] τ can be obtained by Taylor-expanding the exponentials in the integrand w.r.t. s_{ij} and employing the representations of the Green functions in Eqs. (44)–(46). The order-by-order integration can be reduced to the definitions of elliptic iterated integrals and teMZVs in Sect. 3 as soon as the following technical subtleties have been settled:

- The recursive definition Eq. (30) of elliptic iterated integrals cannot be used for integrands of the form $\mathrm{d}t\; f^{(n)}(t-b_1) f^{(m)}(t-b_2)$ with multiple occurrence of the integration variable t as arguments of different integration kernels in Eq. (26). This situation can be remedied by using the Fay relation (29), which can be viewed as the elliptic analogue of partial-fraction relations $\frac{1}{(t-b_1)(t-b_2)} + \mathrm{cyc}(t, b_1, b_2) = 0$. Then, each term on the right-hand side of the Fay relation can be recursively integrated via Eq. (30).
- The integration variable of Eq. (30) is not allowed to show up in the shifts b_i of the iterated integral Γ in the integrand. Therefore one has to derive functional relations between different iterated integrals. The main mechanism to derive relations like

$$\Gamma\left(\begin{smallmatrix}3, 1\\ 0, z\end{smallmatrix}; z\right) = -4\,\Gamma\left(\begin{smallmatrix}0, 4\\ 0, 0\end{smallmatrix}; z\right) + \Gamma\left(\begin{smallmatrix}1, 3\\ 0, 0\end{smallmatrix}; z\right) - \Gamma\left(\begin{smallmatrix}2, 2\\ 0, 0\end{smallmatrix}; z\right) - \Gamma\left(\begin{smallmatrix}4, 0\\ 0, 0\end{smallmatrix}; z\right) \tag{47}$$

[6]Given that the α'-expansions in this work are performed at fixed τ, our results do not expose the branch cuts of the loop amplitudes which result from the integral over q in Eqs. (13) and (19). In the terminology of the closed-string literature [12], the analysis of these proceedings is restricted to the analytic dependence of the one-loop amplitudes on the kinematic invariants.

consists of writing Γ as an integral over its own z-derivative and using again Fay relations on the integration kernels $f^{(n)}$ before integrating back [4]. The need for relations like Eq. (47) arises less frequently if the representations Eqs. (44) and (43) are used for propagators at argument x_{1j} with $j \neq 1$ and Eqs. (45) and (46) for propagators at argument x_{ij} with $1 < i < j$.

- The association of $1 < i < j$ with Eqs. (45) and (46) is adapted to an integration region where $0 < x_2 < x_3 < x_4 < 1$. The non-planar integrals $I_{123|4}$ and $I_{12|34}$, however, additionally involve situations where $x_j > x_{j+1}$. Still, the cubical integration region $x_{j=2,3,4} \in (0, 1)$ of $I_{123|4}$ and $I_{12|34}$ can be decomposed into six simplices $0 < x_i < x_j < x_k < 1$ with some permutations (i, j, k) of $(2, 3, 4)$. Each of these simplicial contributions in turn can then be reduced to the situation where $0 < x_2 < x_3 < x_4 < 1$ by simultaneous relabeling of the integration variables and the Mandelstam variables s_{ij}.

Further details and examples of this rather technical procedure can be found in Refs. [4, 6, 11]. For the purpose of these proceedings, let us just note that all integrals resulting from the α'-expansion of the integrands in Eq. (42) can be treated in this way; thus integration using Eq. (30) is possible.

Since the upper limit for the outermost integration in each term of Eq. (42) is $x_j = 1$, the elliptic iterated integrals in the α'-expansions ultimately boil down to teMZVs Eq. (31). Once the punctures x_2, x_3, x_4 are all integrated out, the leftover shifts b_j can take the values 0 and $\tau/2$. In the planar case I_{1234} with all integrations on the same boundary, there are no shifts; thus the α'-expansions are manifestly expressible in terms of untwisted eMZVs Eq. (32).

Note that the representation of the Green function used in the first discussion of the planar case [4] did not involve the subtraction of $\omega(1, 0)$ in Eqs. (44) and (45). As a virtue of the Green function $P(x_{ij}, q)$ including $-\omega(1, 0)$, divergent eMZVs $\omega(1, \ldots)$ or $\omega(\ldots, 1)$ (cf. the discussion prior to Sect. 3.1) automatically cancel from the α'-expansion along with each monomial in the s_{ij}. In other words, short-distance finiteness of the integrals is manifest term by term[7] without further use of momentum conservation.

Finally, the expansion of the non-planar integrals benefits from the particular choice of Green functions in Eqs. (44) and (43): The vanishing of $\int_0^1 \mathrm{d}x\, P(x, q)$ and $\int_0^1 \mathrm{d}x\, Q(x, q)$ [11] systematically bypasses various spurious terms, which appear in intermediate steps when using the representation of Green functions from Ref. [6].

4.2 Plain Results

Following the steps outlined in the previous section, the α'-expansion of the integral I_{1234} for the planar four-point cylinder amplitude Eq. (13) can be brought into the

[7]For instance, the contributions $s_{12}P(x_{12}, q)$ and $s_{13}P(x_{13}, q)$ from the exponentials in the representation Eq. (42) of $I_{1234}(s_{ij}, q)$ integrate to $\omega(1, 0, 0, 0) - \frac{1}{6}\,\omega(1, 0) = -\frac{1}{3}\,\omega(0, 1, 0, 0)$ and $\omega(1, 0, 0, 0) + \omega(0, 1, 0, 0) - \frac{1}{6}\,\omega(1, 0) = \frac{2}{3}\,\omega(0, 1, 0, 0)$, respectively.

following form [4]

$$\begin{aligned} I_{1234}(s_{ij},q) = \frac{1}{6} &+ 2\,\omega(0,1,0,0)\,s_{13} \\ &+ 2\,\omega(0,1,1,0,0)\big(s_{12}^2+s_{23}^2\big) - 2\,\omega(0,1,0,1,0)\,s_{12}s_{23} \\ &+ \beta_5\,(s_{12}^3{+}2s_{12}^2s_{23}{+}2s_{12}s_{23}^2{+}s_{23}^3) - \beta_{2,3}\,s_{12}s_{23}s_{13} + \mathcal{O}(\alpha'^4)\,, \end{aligned} \tag{48}$$

where we have used the following shorthands for the third order in α'

$$\begin{aligned} \beta_5 &= \frac{4}{3}\big[\omega(0,0,1,0,0,2)+\omega(0,1,1,0,1,0)-\omega(2,0,1,0,0,0)-\zeta_2\,\omega(0,1,0,0)\big] \\ \beta_{2,3} &= \frac{\zeta_3}{12}+\frac{8\zeta_2}{3}\,\omega(0,1,0,0)-\frac{5}{18}\,\omega(0,3,0,0)\,. \end{aligned} \tag{49}$$

In the non-planar four-point integrals of Eq. (13), the teMZVs obtained in intermediate steps are found to cancel by employing the canonical representation in terms of iterated Eisenstein integrals. With two punctures on each boundary, the cancellations of teMZVs in

$$\begin{aligned} q^{-\frac{s_{12}}{4}}I_{12|34}(s_{ij},q) &= 1+s_{12}^2\left(\frac{7\zeta_2}{6}+2\,\omega(0,0,2)\right)-2\,s_{13}s_{23}\left(\frac{\zeta_2}{3}+\omega(0,0,2)\right) \\ &-4\zeta_2\omega(0,1,0,0)s_{12}^3+s_{12}s_{13}s_{23}\left(\frac{5}{3}\,\omega(0,3,0,0)+4\zeta_2\omega(0,1,0,0)-\frac{\zeta_3}{2}\right)+\mathcal{O}(\alpha'^4) \end{aligned} \tag{50}$$

are guaranteed to extend to all orders in α' by the factorization argument in section 4.3.5 of [6]. The other non-planar topology with three punctures on the same boundary exhibits the same kinds of cancellations [6]

$$\begin{aligned} I_{123|4}(s_{ij},q) = 1 &+ (s_{12}^2+s_{12}s_{23}+s_{23}^2)\left(\frac{7\zeta_2}{6}+2\omega(0,0,2)\right) \\ &- s_{12}s_{23}s_{13}\left(4\zeta_2\omega(0,1,0,0)-\frac{5}{3}\,\omega(0,3,0,0)+\frac{\zeta_3}{2}\right)+\mathcal{O}(\alpha'^4) \end{aligned} \tag{51}$$

which might have an all-order explanation from the monodromy relations [34–36] among one-loop open-string amplitudes. The above results have been checked to reproduce the degeneration limits $q \to 0$ known from the literature, i.e. the zero'th order in the q-expansions of $I_{1234}(s_{ij},q)$, $I_{123|4}(s_{ij},q)$ and $q^{-\frac{s_{12}}{4}}I_{12|34}(s_{ij},q)$ agrees with the expressions in Refs. [37] and [35], respectively.

4.3 Results in Terms of Iterated Eisenstein Integrals

In this section, we rewrite the above α'-expansions in a canonical form by converting the eMZVs to a basis of iterated Eisenstein integrals (38). The planar integral Eq. (48) then takes the form

$$
\begin{aligned}
I_{1234}(s_{ij},q) &= \frac{1}{6} + \frac{3s_{13}}{2\pi^2}\big(\zeta_3 - 6\mathcal{E}_0(4,0,0;q)\big) + (s_{12}^2+s_{12}s_{23}+s_{23}^2)\left(\frac{\zeta_2}{6} - 2\mathcal{E}_0(4,0;q)\right)\\
&+ \frac{1}{\pi^2}(s_{12}^2+4s_{12}s_{23}+s_{23}^2)\left(60\mathcal{E}_0(6,0,0,0;q) - \frac{\zeta_4}{2}\right)\\
&+ s_{12}s_{13}s_{23}\left(2\mathcal{E}_0(4,0,0;q) + 50\mathcal{E}_0(6,0,0;q) - \frac{5\zeta_3}{12}\right) \qquad (52)\\
&+ \frac{1}{\pi^2}(s_{12}^3+2s_{12}^2s_{23}+2s_{12}s_{23}^2+s_{23}^3)\Big(216\mathcal{E}_0(4,0,4,0,0;q) + 648\mathcal{E}_0(4,4,0,0,0;q)\\
&\quad + \frac{3}{5}\mathcal{E}_0(4,0,0,0,0;q) - 108\mathcal{E}_0(4,0;q)\mathcal{E}_0(4,0,0;q) + 2016\mathcal{E}_0(8,0,0,0,0;q)\\
&\quad + 18\mathcal{E}_0(4,0;q)\zeta_3 - \frac{5\zeta_5}{2}\Big) + \mathcal{O}(\alpha'^4)\,,
\end{aligned}
$$

where the third order in α' exhibits integrals $\mathcal{E}_0(4,4,0,0,0;q)$ and $\mathcal{E}_0(4,0,4,0,0;q)$ of depth two. The non-planar integral Eq. (50) in turn contains shorter eMZVs and iterated Eisenstein integrals at the orders under consideration, cf. Eq. (41),

$$
\begin{aligned}
q^{-\frac{s_{12}}{4}} I_{12|34}(s_{ij},q) &= 1 + s_{12}^2\left(\frac{\zeta_2}{2} - 12\mathcal{E}_0(4,0;q)\right) + 12\, s_{13}s_{23}\mathcal{E}_0(4,0;q) \qquad (53)\\
&+ s_{12}^3\left(3\mathcal{E}_0(4,0,0;q) - \frac{\zeta_3}{2}\right) + s_{12}s_{13}s_{23}\,\big(300\mathcal{E}_0(6,0,0;q) - 3\mathcal{E}_0(4,0,0;q)\big) + \mathcal{O}(\alpha'^4)\,,
\end{aligned}
$$

and a similar structure can be found for Eq. (51):

$$
\begin{aligned}
I_{123|4}(s_{ij},q) &= 1 + (s_{12}^2 + s_{12}s_{23} + s_{23}^2)\left(\frac{\zeta_2}{2} - 12\mathcal{E}_0(4,0;q)\right) \qquad (54)\\
&+ s_{12}s_{23}s_{13}\Big(300\mathcal{E}_0(6,0,0;q) + 3\mathcal{E}_0(4,0,0;q) - \zeta_3\Big) + \mathcal{O}(\alpha'^4)\,.
\end{aligned}
$$

Note that the α'-expansions of both non-planar integrals $q^{-\frac{s_{12}}{4}} I_{12|34}(s_{ij},q)$ and $I_{123|4}(s_{ij},q)$ take a form very similar to the symmetrized version of the planar integral Eq. (52):

$$
\begin{aligned}
I_{1234}(s_{ij},q) + \text{perm}(2,3,4) &= 1 + (s_{12}^2 + s_{12}s_{23} + s_{23}^2)\Big(\zeta_2 - 12\mathcal{E}_0(4,0;q)\Big) \qquad (55)\\
&+ s_{12}s_{23}s_{13}\left(12\mathcal{E}_0(4,0,0;q) + 300\mathcal{E}_0(6,0,0;q) - \frac{5\zeta_3}{2}\right) + \mathcal{O}(\alpha'^4)\,.
\end{aligned}
$$

In fact, taking the differences between Eqs. (55) and (53) or (54), they are proportional to ζ_2, which might become visible only after using relations like $\zeta_2\,\omega(0,1,0,0) = \frac{\zeta_3}{8} - \frac{3}{4}\mathcal{E}_0(4,0,0)$. This observation is related to the expectation on the corresponding closed-string integral [12, 13] to follow from open-string quantities under a suitably chosen single-valued projection: The agreement of Eqs. (55) and (53) or (54) modulo

ζ_2 is argued in Ref. [11] to pave the way towards a tentative single-valued projection for eMZVs.

While there is no bottleneck in obtaining higher orders in α' from the same methods, it would be desirable to construct cylinder integrals directly from the elliptic associators [38]. This would generalize the representations of disk integrals in terms of the Drinfeld associator [39] and should explain the patterns of iterated Eisenstein integrals in the above equations.

5 Five-Point Results in Different Languages

In this section, we discuss the applicability of the setup of teMZVs to string amplitudes of multiplicities higher than four. The main novelties for maximally supersymmetric amplitudes at $n \geq 5$ points are kinematic poles of the worldsheet integrals and higher-dimensional bases of tensor structures for the external polarizations. The appearance of both of these features is captured by the subsequent discussion of five-point one-loop amplitudes of the open superstring.

We will focus on the α'-expansion of the prototype integrals in Eqs. (20)–(23) which are more conveniently written in terms of the propagators in Eqs. (44)–(46),

$$H^{12}_{12345}(s_{ij}, q) = \int_0^1 \mathrm{d}x_5 \left(\prod_{l=1}^{4} \int_0^{x_{l+1}} \mathrm{d}x_l \right) \delta(x_1)\, f^{(1)}_{12} \, \exp\left(\sum_{i<j}^{5} s_{ij} P(x_{ij}) \right) \tag{56}$$

$$\widehat{H}^{13}_{12345}(s_{ij}, q) = \int_0^1 \mathrm{d}x_5 \left(\prod_{l=1}^{4} \int_0^{x_{l+1}} \mathrm{d}x_l \right) \delta(x_1)\, f^{(1)}_{13} \, \exp\left(\sum_{i<j}^{5} s_{ij} P(x_{ij}) \right) \tag{57}$$

$$\begin{aligned} H^{12}_{123|45}(s_{ij}, q) = q^{\frac{s_{45}}{4}} & \left(\prod_{l=3}^{5} \int_0^1 \mathrm{d}x_l \right) \int_0^{x_3} \mathrm{d}x_2 \int_0^{x_2} \mathrm{d}x_1\, \delta(x_1)\, f^{(1)}_{12} \\ & \times \exp\left(\sum_{i<j}^{3} s_{ij} P(x_{ij}) + s_{45} P(x_{45}) + \sum_{\substack{i=1,2,3 \\ j=4,5}} s_{ij} Q(x_{ij}) \right) \end{aligned} \tag{58}$$

$$\begin{aligned} \widehat{H}^{14}_{123|45}(s_{ij}, q) = q^{\frac{s_{45}}{4}} & \left(\prod_{l=3}^{5} \int_0^1 \mathrm{d}x_l \right) \int_0^{x_3} \mathrm{d}x_2 \int_0^{x_2} \mathrm{d}x_1\, \delta(x_1)\, f^{(1)}_{14} \\ & \times \exp\left(\sum_{i<j}^{3} s_{ij} P(x_{ij}) + s_{45} P(x_{45}) + \sum_{\substack{i=1,2,3 \\ j=4,5}} s_{ij} Q(x_{ij}) \right) . \end{aligned} \tag{59}$$

5.1 Kinematic Poles

When reproducing field-theory amplitudes from the $\alpha' \to 0$ limit of string theories, Feynman propagators arise from the boundaries of the moduli spaces. For instance, the s-channel pole in a four-point open-string tree amplitude arises from the region in the disk integral

$$\int_0^1 \frac{\mathrm{d}z_2}{z_2}\, z_2^{s_{12}}\,(1-z_2)^{s_{23}} = \frac{1}{s_{12}} + \mathscr{O}(\alpha')\,, \tag{60}$$

where the puncture z_2 collides with $z_1 = 0$. Since the emergence of kinematic poles s_{ij}^{-1} is solely dictated by local properties of the worldsheet and the short-distance behavior of the Green function, the pole structure of loop amplitudes can be analyzed by the same methods as their tree-level counterparts.[8]

In contrast to the one-loop four-point integrands, the prototype integrals at five points in Eqs. (56)–(59) exhibit additional factors of $f_{ij}^{(1)}$ with

$$f_{ij}^{(1)} = \frac{1}{z_i - z_j} + \mathscr{O}(|z_i - z_j|) \tag{61}$$

which modify the singularity structure at the boundary of the moduli space. In particular, the worldsheet singularities of $f_{12}^{(1)} \mathrm{e}^{s_{12}P(x_{12})}$ translate into kinematic poles $\sim s_{12}^{-1}$ in the five-point one-loop integrals Eqs. (56)–(58) along the lines of the tree-level mechanism in Eq. (60). As a convenient way of capturing the α'-expansion of such singular integrals, we split the integrand of H_{12345}^{12} in Eq. (56) as

$$\begin{aligned} f_{12}^{(1)}\, \mathrm{e}^{\sum_{i<j}^{5} s_{ij}P(x_{ij})} &= f_{12}^{(1)}\, \mathrm{e}^{s_{12}P(x_2)} \big[\Phi(x_2,x_3,x_4,x_5) - \Phi(0,x_3,x_4,x_5) + \Phi(0,x_3,x_4,x_5)\big] \\ \Phi(x_2,x_3,x_4,x_5) &= \exp\left(\sum_{l=3}^{5} s_{1l}P(x_l) + \sum_{2\leq i<j}^{5} s_{ij}P(x_{ij}) \right)\,, \end{aligned} \tag{62}$$

where we remind the reader that we fixed $x_1 = 0$. Then, for the last term of the first line, the integral over x_2 becomes elementary by recognizing $f_{12}^{(1)}\, \mathrm{e}^{s_{12}P(x_2)} = -\frac{1}{s_{12}} \frac{\partial}{\partial x_2} \mathrm{e}^{s_{12}P(x_2)}$ and leads to the following singular part of H_{12345}^{12}:

$$\begin{aligned} &\int_0^1 \mathrm{d}x_5 \left(\prod_{l=1}^{4} \int_0^{x_{l+1}} \mathrm{d}x_l \right) \delta(x_1)\, f_{12}^{(1)}\, \mathrm{e}^{s_{12}P(x_2)}\, \Phi(0,x_3,x_4,x_5) \\ &= -\frac{1}{s_{12}} \int_0^1 \mathrm{d}x_5 \int_0^{x_5} \mathrm{d}x_4 \int_0^{x_4} \mathrm{d}x_3\, \exp\left(s_{12}P(x_3) + \sum_{l=3}^{5} (s_{1l}+s_{2l})P(x_l) + \sum_{3\leq i<j}^{5} s_{ij}P(x_{ij}) \right)\,. \end{aligned} \tag{63}$$

The right-hand side of the equation above can in turn be identified with the planar four-point integral in Eq. (14) after relabeling the Mandelstam invariants as

[8] See [40, 41] for two related approaches to treat the poles of n-point open-string tree amplitudes.

$$\chi : \begin{cases} s_{12} \to s_{123}\,, & s_{13} \to s_{14}+s_{24}\,, \quad s_{14} \to s_{15}+s_{25} \\ s_{23} \to s_{34}\,, & s_{24} \to s_{35}\,, \quad\quad\quad s_{34} \to s_{45} \end{cases} \tag{64}$$

with $s_{123} = s_{12}+s_{13}+s_{23}$. We have assumed s_{12} to have a positive real part in discarding the boundary term $\mathrm{e}^{s_{12}P(x_2)}\big|_{x_2=0}$ in Eq. (63) which exhibits the same short-distance behavior $x_2^{s_{12}}$ as seen in the tree-level integrand Eq. (60). Hence, the integral Eq. (20) can be split into a pole part and a regular part according to

$$\begin{aligned} H^{12}_{12345} &= H^{12,\mathrm{reg}}_{12345} - \frac{I_{1234}(\chi(s_{ij}), q)}{s_{12}} \\ H^{12,\mathrm{reg}}_{12345} &= \int_0^1 \mathrm{d}x_5 \left(\prod_{l=2}^{4} \int_0^{x_{l+1}} \mathrm{d}x_l \right) f^{(1)}(x_2)\, \mathrm{e}^{s_{12}P(x_2)} \big[\Phi(0, x_3, x_4, x_5) - \Phi(x_2, x_3, x_4, x_5) \big]\,. \end{aligned} \tag{65}$$

In reconstructing the α'-expansion of the polar part from a four-point computation, the Mandelstam invariants of I_{1234} have to be transformed according to Eq. (64) instead of using four-point momentum conservation Eq. (15). This is the reason for obtaining

$$\begin{aligned} I_{1234}(\chi(s_{ij}), q) &= \frac{1}{6} + \omega(0,1,0,0)(s_{12} - 2s_{34} - 2s_{45}) \\ &+ \omega(0,1,1,0,0)(s_{12}^2 - 2s_{12}s_{34} + 2s_{34}^2 + 2s_{45}^2) + \omega(0,1,0,1,0)(s_{12} - 2s_{34})s_{45} + \mathscr{O}(\alpha'^3) \end{aligned} \tag{66}$$

instead of Eq. (48) after using five-point momentum conservation Eq. (25). The non-planar integral $H^{12}_{123|45}$ with a kinematic pole defined in Eq. (58) will be addressed by a similar decomposition of the integrand as in Eq. (62)

$$\begin{aligned} f^{(1)}_{12}\, \mathrm{e}^{\sum_{i<j}^{5} s_{ij}P(x_{ij})} &= f^{(1)}_{12}\, \mathrm{e}^{s_{12}P(x_2)} \big[\Psi(x_2,x_3,x_4,x_5) - \Psi(0,x_3,x_4,x_5) + \Psi(0,x_3,x_4,x_5) \big] \\ \Psi(x_2,x_3,x_4,x_5) &= \exp\left(s_{13}P(x_3) + \sum_{\substack{(i,j)=\\(2,3),(4,5)}} s_{ij}P(x_{ij}) + \sum_{j=4,5} s_{1j}Q(x_j) + \sum_{\substack{i=2,3\\j=4,5}} s_{ij}Q(x_{ij}) \right)\,. \end{aligned} \tag{67}$$

Again, one can find a primitive w.r.t. x_2 for the last term in the first line and arrive at a decomposition analogous to Eq. (65)

$$\begin{aligned} H^{12}_{123|45} &= H^{12,\mathrm{reg}}_{123|45} - \frac{I_{12|34}(\chi(s_{ij}), q)}{s_{12}} \\ H^{12,\mathrm{reg}}_{123|45} &= q^{\frac{s_{45}}{4}} \left(\prod_{l=3}^{5} \int_0^1 \mathrm{d}x_l \right) \int_0^{x_3} \mathrm{d}x_2\, f^{(1)}(x_2)\, \mathrm{e}^{s_{12}P(x_2)} \big[\Psi(0,x_3,x_4,x_5) - \Psi(x_2,x_3,x_4,x_5) \big]\,, \end{aligned} \tag{68}$$

with the same mapping Eq. (64) of the Mandelstam invariants that governed the planar counterpart H^{12}_{12345}. The function $I_{12|34}(\chi(s_{ij}), q)$ of five-particle Mandelstam invariants along with s_{12}^{-1} is still expressible in terms of untwisted eMZVs,

$$I_{12|34}(\chi(s_{ij}),q) = q^{\frac{s_{45}}{4}} \left\{ 1 + s_{45}^2 \left(\omega(0,0,2) + \frac{5\zeta_2}{6} \right) \right. \tag{69}$$
$$\left. + \frac{1}{2}\left[(s_{14}+s_{24})^2 + (s_{15}+s_{25})^2 + s_{34}^2 + s_{35}^2 \right] \left(\omega(0,0,2) + \frac{\zeta_2}{3} \right) + \mathscr{O}(\alpha'^3) \right\},$$

see Eq. (53) for the analogous four-point expansion.

5.2 The Regular Parts

For the regular parts $H_{12345}^{12,\mathrm{reg}}$ and $H_{123|45}^{12,\mathrm{reg}}$ of the five-point integrals over $f_{12}^{(1)}$ defined in Eqs. (65) and (68), the integrands

$$\begin{aligned} \Phi(0,x_3,x_4,x_5) - \Phi(x_2,x_3,x_4,x_5) &= -\sum_{j=3}^{5} s_{2j}\, \Gamma\left(\begin{smallmatrix} 1 \\ x_j \end{smallmatrix}; x_2 \right) + \mathscr{O}(\alpha'^2) \\ \Psi(0,x_3,x_4,x_5) - \Psi(x_2,x_3,x_4,x_5) &= -\, s_{23}\, \Gamma\left(\begin{smallmatrix} 1 \\ x_3 \end{smallmatrix}; x_2 \right) - s_{24}\, \Gamma\left(\begin{smallmatrix} 1 \\ x_4+\tau/2 \end{smallmatrix}; x_2 \right) \\ &\quad - s_{25}\, \Gamma\left(\begin{smallmatrix} 1 \\ x_5+\tau/2 \end{smallmatrix}; x_2 \right) + \mathscr{O}(\alpha'^2) \end{aligned} \tag{70}$$

manifestly vanish as $x_2 \to 0$. Hence, they cancel the singularity of the integrands $f^{(1)}(x_2)$ in Eqs. (65) and (68), and the integrations over x_3, x_4, x_5 yield convergent eMZVs at all orders, starting with[9]

$$H_{12345}^{12,\mathrm{reg}} = (s_{23} - s_{25})\big[\omega(0,1,0,1,0) + 2\,\omega(0,1,1,0,0) \big] + \mathscr{O}(\alpha'^2) \tag{71}$$
$$H_{123|45}^{12,\mathrm{reg}} = \mathscr{O}(\alpha'^2)\,. \tag{72}$$

The leading three orders in the low-energy expansion of the planar integral H_{12345}^{12} can then be assembled by inserting Eqs. (66) and (71) into Eq. (65). Likewise, the non-planar integral $H_{123|45}^{12}$ follows from plugging Eqs. (69) and (72) into Eq. (68).

The kinematic poles of the integrals H_{12345}^{12} and $H_{123|45}^{12}$ only arise because the variables x_1 and x_2 of the worldsheet singularity $f_{12}^{(1)} \sim x_{12}^{-1}$ are neighbors in the integration domain $0 < x_2 < x_3 < x_4 < x_5 < 1$. In contrast, the integrals $\widehat{H}_{12345}^{13}$ and $\widehat{H}_{123|45}^{14}$ in Eqs. (57) and (59), do not acquire any kinematic pole in this way. Accordingly, Taylor expanding the exponentials in the integrand automatically yields convergent eMZVs order by order in α' upon integration over x_2, x_3, x_4, x_5, e.g.

---

[9]The convergent integrals leading to Eq. (72) can be performed via rearrangements such as [4] $\Gamma\left(\begin{smallmatrix} 1 & 1 \\ 0 & z \end{smallmatrix}; z \right) = -2\,\Gamma\left(\begin{smallmatrix} 0 & 2 \\ 0 & 0 \end{smallmatrix}; z \right) - \Gamma\left(\begin{smallmatrix} 2 & 0 \\ 0 & 0 \end{smallmatrix}; z \right) - \zeta_2$, which is yet another example from the class of identities discussed around Eq. (47). Note that the singular integration kernels $f^{(1)}$ manifestly drop out from this identity.

$$\widehat{H}^{13}_{12345} = -\,\omega(0,1,0,0) + (s_{12}+s_{23}+s_{45})\,\omega(0,1,1,0,0) \\ + (s_{12}-s_{15}+s_{23}-s_{34}-s_{45})\,\omega(0,1,0,1,0) + \mathscr{O}(\alpha'^2) \tag{73}$$

$$\widehat{H}^{14}_{123|45} = q^{\frac{s_{45}}{4}}\left\{(s_{24}-s_{34})\left(\omega(0,0,2)+\frac{\zeta_2}{3}\right)+\mathscr{O}(\alpha'^2)\right\}. \tag{74}$$

Note that to the orders considered, the α'-expansions of the five-point integrals can be easily confirmed to preserve the integration-by-parts relations

$$0 = \int_{D(\lambda)} \prod_{j=1}^{5} \mathrm{d}z_j\, \frac{\partial}{\partial z_2}\,\delta(z_1) \prod_{i<j}^{5} \exp\left(\tfrac{s_{ij}}{2}G(z_{ij})\right) \tag{75}$$

$$= \int_{D(\lambda)} \prod_{j=1}^{5} \mathrm{d}z_j\, \delta(z_1)\left[s_{23}f^{(1)}_{23}+s_{24}f^{(1)}_{24}+s_{25}f^{(1)}_{25}-s_{12}f^{(1)}_{12}\right] \prod_{i<j}^{5} \exp\left(\tfrac{s_{ij}}{2}G(z_{ij})\right).$$

Such relations are crucial for manifesting the gauge invariance of the string amplitude. They do not depend on the planar or non-planar ordering λ in the integration region $D(\lambda)$, cf. Eq. (6). Each of the summands in Eq. (75) is expressible as a relabeling of one of the prototype integrals in Eqs. (56)–(59). It does not require much effort to show that non-planar integrals with a domain of the form $D(1,2,3,4|5)$ can be expanded using the same methods.

5.3 Putting Everything Together

Given the low-energy expansion of all the permutation-inequivalent prototype integrals Eqs. (56)–(59), one can expand the five-point cylinder amplitude Eq. (19) at the level of the integrand w.r.t. q: The coefficients $I^{\rho(2,3)}_{\lambda}(s_{ij},q)$ of the independent kinematic factors $A^{\mathrm{tree}}_{\mathrm{SYM}}(1,\rho(2,3),4,5)$ with permutation $\rho \in S_2$ are linear combinations of the H^{ij}_{λ} and $\widehat{H}^{ij}_{\lambda}$ implicitly defined by combining Eqs. (16) and (18) with BCJ relations of the $A^{\mathrm{tree}}_{\mathrm{SYM}}$.

Also the five-point tree amplitudes of the open superstring can be expanded in a BCJ basis of (super-)Yang–Mills amplitudes [42]: When considering the two single-trace orderings $A^{\mathrm{tree}}_{\mathrm{open}}(1,\tau(2,3),4,5)$ of disk amplitudes, the relation to their field-theory counterparts $A^{\mathrm{tree}}_{\mathrm{SYM}}(1,\rho(2,3),4,5)$ is encoded in 2×2 matrices $(P_w)_{\tau}{}^{\rho}$ and $(M_w)_{\tau}{}^{\rho}$ indexed by the permutations $\tau,\rho \in S_2$ [43],

$$A^{\mathrm{tree}}_{\mathrm{open}}(1,\tau(2,3),4,5) = \sum_{\rho\in S_2}(1+\zeta_2 P_2+\zeta_3 M_3+\zeta_2^2 P_4+\mathscr{O}(\alpha'^5))_{\tau}{}^{\rho} \\ \times A^{\mathrm{tree}}_{\mathrm{SYM}}(1,\rho(2,3),4,5). \tag{76}$$

The entries of the 2×2 matrices P_w and M_w are degree-w polynomials in s_{ij} with rational coefficients, e.g.

$$P_2 = \begin{pmatrix} s_{12}s_{34} - s_{34}s_{45} - s_{51}s_{12} & s_{13}s_{24} \\ s_{12}s_{34} & s_{13}s_{24} - s_{24}s_{45} - s_{51}s_{13} \end{pmatrix}, \tag{77}$$

and analogous expressions for matrices at higher order in α' or multiplicity can be downloaded from [44].

The same matrices P_2, M_3, P_4 governing the low-energy expansion of tree amplitudes Eq. (76) can be found in the planar sector at one loop: It is convenient to focus on the two choices $\lambda = 1, 2, 3, 4, 5$ and $\lambda = 1, 3, 2, 4, 5$ of the single-trace ordering which line up with the basis $A^{\text{tree}}_{\text{SYM}}(1, \rho(2, 3), 4, 5)$ of kinematic factors in Eq. (19). Doing so, the α'-expansions of the planar integrals H^{12}_{12345} and $\widehat{H}^{13}_{12345}$ uplift the relation Eq. (76) between open-string and (super-)Yang–Mills tree-level amplitudes to one loop

$$A_{\text{cyl}}(1, \tau(2, 3), 4, 5) = \int_0^1 \frac{\mathrm{d}q}{q} \sum_{\rho \in S_2} I_{1\tau(23)45}{}^{\rho}(s_{ij}, q) A^{\text{tree}}_{\text{SYM}}(1, \rho(2, 3), 4, 5) \tag{78}$$

with the leading low-energy orders [4]

$$\begin{aligned} -I_{1\tau(23)45}{}^{\rho}(s_{ij}, q) &= \frac{1}{6}P_2 + \left(\frac{3\zeta_3}{2\pi^2} - \frac{9\mathscr{E}_0(4, 0, 0; q)}{\pi^2}\right) M_3 \\ &\quad + \left(\frac{\pi^2}{18} - 5\mathscr{E}_0(4, 0; q) + \frac{150}{\pi^2}\mathscr{E}_0(6, 0, 0, 0; q)\right) P_4 \\ &\quad + \left(\frac{3}{2}\mathscr{E}_0(4, 0; q) - \frac{225}{\pi^2}\mathscr{E}_0(6, 0, 0, 0; q)\right) L_4 + \mathscr{O}(\alpha'^5)\,. \end{aligned} \tag{79}$$

At order α'^4, we encounter a new matrix L_4 with entries

$$\begin{aligned} (L_4)_{23}{}^{23} &= s_{12}^2 s_{23}^2 + 2s_{12}^2 s_{23}s_{24} + s_{12}^2 s_{24}^2 + 2s_{12}^2 s_{23}s_{34} + 2s_{12}s_{13}s_{23}s_{34} + 2s_{12}s_{23}^2 s_{34} \\ &\quad + 2s_{12}^2 s_{24}s_{34} + s_{12}s_{13}s_{24}s_{34} + 2s_{12}s_{23}s_{24}s_{34} + s_{12}^2 s_{34}^2 + 2s_{12}s_{13}s_{34}^2 \\ &\quad + s_{13}^2 s_{34}^2 + 2s_{12}s_{23}s_{34}^2 + 2s_{13}s_{23}s_{34}^2 + s_{23}^2 s_{34}^2 \end{aligned} \tag{80}$$

$$\begin{aligned} (L_4)_{23}{}^{32} &= -s_{13}s_{24}(3s_{12}s_{23} + s_{13}s_{23} + s_{23}^2 + 2s_{12}s_{24} + s_{13}s_{24} + s_{23}s_{24} \\ &\quad + 3s_{12}s_{34} + 2s_{13}s_{34} + 3s_{23}s_{34}) \end{aligned} \tag{81}$$

and $(L_4)_{32}{}^{32} = (L_4)_{23}{}^{23}\big|_{2\leftrightarrow 3}$ as well as $(L_4)_{32}{}^{23} = (L_4)_{23}{}^{32}\big|_{2\leftrightarrow 3}$. The q-expansion of its coefficient does not have any zero mode, consistent with the fact that the q^0 order of Eq. (79) has to match the α'-derivative of the tree-level amplitude [37].

Cylinder diagrams as drawn in Fig. 1 can be interpreted not only as a one-loop process involving open strings but also as a tree-level exchange of closed strings [16]. In particular, the non-planar cylinder diagram gives rise to a propagator $\sim s_{12}^{-1}$

of gravitational states upon integration over q. Accordingly, the low-energy limit of double-trace open-string amplitudes at one loop reproduces the corresponding double-trace amplitudes in Einstein–Yang–Mills field theory [45]

$$A^{\text{tree}}_{\text{EYM}}(1,2,3|4,5) = s_{24} A^{\text{tree}}_{\text{SYM}}(1,3,2,4,5) - s_{34} A^{\text{tree}}_{\text{SYM}}(1,3,2,4,5)\,. \tag{82}$$

Indeed, the α'-expansions of the non-planar integrals $H^{12}_{123|45}$ and $\widehat{H}^{14}_{123|45}$ give rise to

$$\begin{aligned} A_{\text{cyl}}(1,2,3|4,5) = -\frac{1}{2}\int_0^1 \frac{\mathrm{d}q}{q}\, q^{\frac{s_{45}}{4}} \Big\{ & s_{45}\, A^{\text{tree}}_{\text{EYM}}(1,2,3|4,5) \\ & + \left(\frac{\zeta_2}{2} - 12\mathscr{E}_0(4,0;q)\right) s_{45}^3\, A^{\text{tree}}_{\text{EYM}}(1,2,3|4,5) \\ & + 12\mathscr{E}_0(4,0;q)\,\big[\, s_{34}(s_{12}s_{23}s_{45}+2s_{12}s_{24}s_{45}+s_{45}s_{34}^2+s_{45}^2s_{34}+3s_{12}s_{24}s_{15}) \\ & \qquad \times A^{\text{tree}}_{\text{SYM}}(1,2,3,4,5) - (2\leftrightarrow 3)\,\big] + \mathscr{O}(\alpha'^5)\Big\} \end{aligned} \tag{83}$$

and match the desired Einstein–Yang–Mills limit Eq. (82) by means of the integral $\int_0^1 \mathrm{d}q\; q^{\frac{s_{45}}{4}-1} = \frac{4}{s_{45}}$ at the leading order. It would be interesting to explore the higher-order structure of the α'-expansion at one loop, in particular, if it exhibits an echo of the tree-level pattern of Refs. [43, 46] under the motivic coaction.

6 Summary

In these proceedings, we investigate the appearance of eMZVs in one-loop amplitudes of the open superstring. In reviewing earlier results on the planar [4] and non-planar cylinder diagram [6], we streamline intermediate steps of the computations provided in the references, thus allowing a more efficient calculation. We extend their results in two directions: First, the treatment of kinematic poles in planar and non-planar five-point integrals is carefully explained. Second, the final expressions for the low-energy expansions at four and five points are cast into the language of iterated Eisenstein integrals.

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Expansions at Cusps and Petersson Products in Pari/GP

Henri Cohen

Abstract We begin by explaining how to compute Fourier expansions at all cusps of any modular form of integral or half-integral weight thanks to a theorem of Borisov–Gunnells and explicit expansions of Eisenstein series at all cusps. Using this, we then give a number of methods for computing arbitrary Petersson products. All this is available in the current release of the `Pari/GP` package.

1 Introduction

In this paper we consider the practical problem of numerically computing Petersson products of two modular forms whenever it is defined. In some cases this can be done using the Rankin–Selberg convolution of the forms, but in general this is not always possible nor practical.

We will describe three methods. The first is applicable when both forms are cusp forms, and is a variant of the well-known formulas of Haberland. The second is a modification of the first, necessary when at least one of the forms is not a cusp form. Both of these methods need the essential condition that the weight k be integral and greater than or equal to 2. The third method is due to P. Nelson and D. Collins [1, 2]. It has the great advantage of being also applicable when $k = 1$ or k half-integral, but the great disadvantage of being much slower when k is integral and greater than or equal to 2.

All of these methods require the possibility of computing the Fourier expansion of $f|_k\gamma$ for an arbitrary γ in the full modular group. The method used in `Pari/GP` [3] is to express any modular form (possibly multiplied by a known Eisenstein or theta series) as a linear combination of products of *two* Eisenstein series, which is always possible thanks to a theorem of Borisov–Gunnells [4, 5], so we will begin by studying this in detail here, so that the formulas can be recorded.

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2 Eisenstein Series

2.1 Introduction

In the sequel, we let χ_1 and χ_2 be two *primitive* characters modulo N_1 and N_2 respectively. For $k \geq 3$ we define

$$G_k(\chi_1, \chi_2)(\tau) = \frac{1}{2} \sum_{N_1 \mid c,\ d}{}' \frac{\overline{\chi_1(d)}\chi_2(c/N_1)}{(c\tau + d)^k},$$

and for $k = 2$ and $k = 1$ we define G_k by analytic continuation to $s = 0$ of the same sum with an extra factor $|c\tau + d|^{-2s}$ (Hecke's trick). We will always assume that $\chi_1\chi_2(-1) = (-1)^k$, otherwise the series is identically zero.

If $k \neq 2$ or $k = 2$ and χ_1 and χ_2 are not both trivial, then $G_k \in M_k(\Gamma_0(N_1N_2), \chi_1\chi_2)$ (if $k = 2$ and χ_1 and χ_2 are both trivial we have a nonanalytic term in $1/\Im(\tau)$). The Fourier expansion at infinity is given by

$$G_k(\chi_1, \chi_2)(\tau) = \left(\frac{-2\pi i}{N_1}\right)^k \frac{\mathfrak{g}(\overline{\chi_1})}{(k-1)!} F_k(\chi_1, \chi_2)(\tau),$$

where $\mathfrak{g}(\overline{\chi})$ is the standard Gauss sum associated to $\overline{\chi}$,

$$F_k(\chi_1, \chi_2)(\tau) = \delta_{N_2,1} \frac{L(\chi_1, 1-k)}{2} + \sum_{n \geq 1} \sigma_{k-1}(\chi_1, \chi_2, n) q^n,$$

where δ is the Kronecker delta, and

$$\sigma_{k-1}(\chi_1, \chi_2, n) = \sum_{d \mid n,\ d>0} d^{k-1} \chi_1(d) \chi_2(n/d)\ .$$

By convention, we will set $F_0 = 1$.

An important theorem of Borisov–Gunnells [4, 5] says that in weight $k \geq 3$, and very often also in weight 2, any modular form $f \in M_k(\Gamma_0(N), \chi)$ is a linear combination of $F_\ell(\chi_1, \chi_2)(e\tau) F_{k-\ell}(\chi_1', \chi_2')(e'\tau)$ for suitable characters χ, ℓ, e and e'.

If we are in the unfavorable case of the theorem (only in weight 2), or in weight 1, we can simply multiply by a known Eisenstein series (of weight 1 or 2) to be in a case where the theorem applies. Similarly, if we are in half-integral weight, we simply multiply by a suitable power of $\theta \in M_{1/2}(\Gamma_0(4))$ to be able to apply the theorem.

For us, the main interest of this theorem is that the Fourier expansion of $F_k|_k\gamma$ as well as that of $\theta|_{1/2}\gamma$ can be explicitly computed for all $\gamma \in \Gamma$, the full modular group, so this allows us to compute $f|_k\gamma$ for any modular form f, and in particular find the Fourier expansions at any cusp.

2.2 Expansion of $F_k|_k\gamma$

As usual we denote by N_1 and N_2 the conductors of χ_1 and χ_2. For simplicity of notation we will set $F_k(\chi_1, \chi_2, e)(\tau) := F_k(\chi_1, \chi_2)(e\tau)$ and $N = N_1N_2e$, so that $F_k(\chi_1, \chi_2, e) \in M_k(\Gamma_0(N), \chi_1\chi_2)$. Note that in the application using the Borisov–Gunnells theorem N will only be a *divisor* of the level.

We now let $\gamma \in \mathrm{GL}_2^+(\mathbb{Q})$ be any matrix with rational coefficients and strictly positive determinant. We want to compute the Fourier expansion at infinity of $F_k(\chi_1, \chi_2, e)|_k\gamma$. For this, we first make three reductions. First, trivially the action of γ is homogeneous, so possibly after multiplying γ by a common denominator we may assume that $\gamma = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right) \in M_2^+(\mathbb{Z})$. Second, by Euclid we can find integers u, v, and g such that $\gcd(A, C) = g = uA + vC$, and we have the matrix identity

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} A/g & -v \\ C/g & u \end{pmatrix} \begin{pmatrix} g & uB + vD \\ 0 & (AD - BC)/g \end{pmatrix} ,$$

where we note that the first matrix is in Γ. Since the second one is upper triangular, its action on a Fourier expansion is trivial to write down, so we are reduced to the case where $\gamma \in \Gamma$.

The third and last reduction is based on the following easy lemma:

Lemma 2.1 *Let $\gamma \in \Gamma$. There exist $\beta \in \Gamma_0(N)$ and $m \in \mathbb{Z}$ such that*

$$\gamma = \beta \begin{pmatrix} A & B \\ C & D \end{pmatrix} T^m$$

with $C \mid N$, $C > 0$, and $N \mid B$.

Since the action of $\beta = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \Gamma_0(N)$ on $M_k(\Gamma_0(N), \chi)$ is simply multiplication by $\chi(d)$, and since once again the action of the translation T^m is trivial to write down on Fourier expansions, this lemma allows us to reduce to $\gamma \in \Gamma$ with the additional conditions $C \mid N$, $C > 0$, and $N \mid B$.

To state the main result we need to introduce an additional function needed to express the constant terms:

Definition 2.2 Let χ be a Dirichlet character modulo M, let f be its conductor, and let χ_f be the primitive character modulo f equivalent to χ. We define

$$S_k(\chi) = (M/f)^k \mathfrak{g}(\chi_f) \frac{\overline{B_k(\chi_f)}}{k} \prod_{p \mid N} \left(1 - \frac{\chi_f(p)}{p}\right) ,$$

where as usual $B_k(\chi_f)$ is the χ_f-Bernoulli number and the product is over the prime divisors of N.

Note that $S_k(\chi) = -(2(k-1)!M^k/(-2\pi i)^k)L(\chi, k)$, but we have preferred to give it in the above form to emphasize the fact that it belongs to a specific cyclotomic field.

We are now ready to state the main result, where we always use the convention $q^x = e^{2\pi i\tau x}$ when $x \in \mathbb{Q}$:

Theorem 2.3 *Set $N = eN_1N_2$, and let $\gamma = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right) \in \Gamma$ be such that $C \mid N$, $C > 0$, and $N \mid B$. Set $g = \gcd(e, C)$, $g_1 = \gcd(N_1 g, C)$, and $g_2 = \gcd(N_2 g, C)$. If $(k, \chi_1, \chi_2) \neq (2, 1, 1)$ we have*

$$F_k(\chi_1, \chi_2, e)|_k\gamma = \frac{1}{z_k(\chi_1, \chi_2, C)} \sum_{n \geq 0} a_\gamma(n) q^{g_1 g_2 n/N} ,$$

where

1.
$$z_k(\chi_1, \chi_2, C) = 2(N_2 e/g_2)^{k-1}(e/g)\mathfrak{g}(\overline{\chi_1})\mathfrak{g}(\overline{\chi_2}) ,$$

2. For $n \geq 1$

$$a_\gamma(n) = \zeta_N^{A^{-1}(g_1 g_2/C)n} \sum_{m \mid n,\ m \in \mathbb{Z}} \operatorname{sign}(m) m^{k-1} c(n, m) , \quad \textit{with}$$

$$\begin{aligned} c(n,m) = & \sum_{\substack{s_1 \bmod C/g \\ (N_1 g/g_1)s_1 \equiv n/m \pmod{C/g_1}}} \overline{\chi_1}((n/m - (N_1 g/g_1)s_1)/(C/g_1)) \cdot \\ & \cdot \sum_{\substack{s_2 \bmod C/g \\ (N_2 g/g_2)s_2 \equiv m \pmod{C/g_2}}} \overline{\chi_2}((m - (N_2 g/g_2)s_2)/(C/g_2)) \zeta_{C/g}^{-(Ae/g)^{-1}s_1 s_2} . \end{aligned}$$

3. Set

$$T_k(\chi_1, \chi_2) = \begin{cases} (-1)^{k-1} \dfrac{\mathfrak{g}(\overline{\chi_2})}{N_2(g_2/g)^{k-1}} \overline{\chi_1}(-Ae/g) S_k(\overline{\chi_1}\chi_2) & \textit{if } C/g = N_1 , \\ 0 & \textit{if } C/g \neq N_1 . \end{cases}$$

We have

$$a_\gamma(0) = \begin{cases} T_k(\chi_1, \chi_2) & \textit{if } k > 1 , \\ T_1(\chi_1, \chi_2) + T_1(\chi_2, \chi_1) & \textit{if } k = 1 . \end{cases}$$

Note that $(k, \chi_1, \chi_2) = (2, 1, 1)$ corresponds to the quasimodular form F_2 (or E_2) which can be easily treated directly thanks to the first matrix identity given above applied to $\gamma = \left(\begin{smallmatrix} eA & eB \\ C & D \end{smallmatrix}\right)$.

2.3 Rationality Questions

To use this theorem in algorithmic practice, we need to make a choice. As can be seen on the expression of $a_\gamma(n)$, the coefficients of the expansion belong to the large cyclotomic field $\mathbb{Q}(\zeta_N, \zeta_{\phi(N)})$, which is in fact also the field which contains Gauss sums of characters modulo N. When N is not tiny, say when N is a prime around 1000, this is a very large number field, so it seems almost impossible to work with exact elements of the field. In our implementation we thus have chosen to work with approximate complex values having hopefully sufficient accuracy (note that this is sufficient in the application to Petersson products). At the end of the computation of $f|_k\gamma$ we may however want to recover the exact algebraic values. This can of course be done using LLL-type algorithms, with an a priori guess of the field of coefficients. But this can be done rigorously by using the following results.

First, assume that $\gcd(N/\gcd(N, C), C) = 1$, or equivalently $(N, C^2) = (N, C)$ (so that the cusp A/C will be regular). We then have the following two results:

Lemma 2.4 *Assume that* $\gcd(N/\gcd(N, C), C) = 1$*, and set* $g = \gcd(N, C)$ *and* $Q = N/g$*. There exist an Atkin–Lehner matrix of the form* $W_Q = \left(\begin{smallmatrix} Qx & y \\ N & Q \end{smallmatrix}\right)$*, a matrix* $\delta = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \Gamma_0(N)$*, and an integer* v*, such that*

$$\gamma = W_Q\delta\begin{pmatrix} 1/Q & v/Q \\ 0 & 1 \end{pmatrix} \; ,$$

and we have $d \equiv Q^{-1}D \pmod{N/Q}$*, where* Q^{-1} *is an inverse of* Q *modulo* C*.*

As usual, since the action of δ on $M_k(\Gamma_0(N), \chi)$ is multiplication by $\chi(d)$ and the action of an upper triangular matrix on Fourier expansions is trivial to write, we are reduced to computing the field of coefficients of $f|_k W_Q$. This is given by a theorem essentially due to Shimura and Ohta, and extended to cover half-integral weight as well. We first define a normalizing constant $C(k, \chi, W_Q)$ as follows. First recall that if $\gcd(Q, N/Q) = 1$, which is the case here, we can write in a unique way $\chi = \chi_Q\chi_{N/Q}$ with χ_Q defined modulo Q and $\chi_{N/Q}$ modulo N/Q.

Definition 2.5 Let $W_Q = \left(\begin{smallmatrix} Qx & y \\ Nz & Qt \end{smallmatrix}\right)$ be a general Atkin–Lehner matrix.

1. We set $s(k, W_Q) = 1$ unless k is a half integer, in which case we set $s(k, W_Q) = i^{(x-1)/2}$ if Q is odd, and $s(k, W_Q) = 1 + (-1)^{k+y/2}i$ if $4 \mid Q$ (note that we cannot have $Q \equiv 2 \pmod 4$).
2. We define $C(k, \chi, W_Q) = s(k, W_Q)/(\mathfrak{g}((\chi_Q)_f)Q^{k/2})$, where $(\chi_Q)_f$ is the primitive character equivalent to χ_Q.

The theorem is as follows:

Theorem 2.6 *Let* $F \in M_k(\Gamma_0(N), \chi)$ *with* k *integral or half integral, set* $K = \mathbb{Q}(F)$*, let* $Q\|N$ *be a primitive divisor of* N*, and let* $W_Q = \left(\begin{smallmatrix} Qx & y \\ Nz & Qt \end{smallmatrix}\right)$ *be a general Atkin–Lehner matrix. We have* $\mathbb{Q}(C(k, \chi, W_Q)F|_k W_Q) \subset K$*.*

In the general case we cannot use Atkin–Lehner involutions, but again using the Borisov–Gunnells theorem F. Brunault and M. Neururer recently proved the following theorem, and we thank them for permission to include it here. Their proof will be given in a separate paper.

Theorem 2.7 *Let $\gamma = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right) \in \Gamma$, denote by $M \mid N$ the conductor of χ, and as in the previous theorem set $K = \mathbb{Q}(F)$. If $F \in M_k(\Gamma_0(N), \chi)$ with k integral the Fourier coefficients of $F|_k\gamma$ belong to the cyclotomic extension $K(\zeta_R)$, where $R =$* $\operatorname{lcm}(N/\gcd(N, CD), M/\gcd(M, BC))$.

2.4 Eisenstein Series Over $\Gamma_1(N)$

Instead of using products of two Eisenstein series over $\Gamma_0(N)$ as above (which corresponds to the present implementation (June 2018) in `Pari/GP`), one can also use products of two Eisenstein series over $\Gamma_1(N)$ instead, and then project on $M_k(\Gamma_0(N), \chi)$. This corresponds in fact to the Eisenstein series used by Borisov–Gunnells, and will probably replace the previous implementation. Once again, we give the precise formulas.

For the level N being understood, for $k \geq 3$ we define

$$G_k(a) = \frac{1}{N} \sideset{}{'}\sum_{N|c,\ d} \frac{\zeta_N^{-ad}}{(c\tau + d)^k}\ ,$$

and for $k = 2$ and $k = 1$ we define G_k by analytic continuation to $s = 0$. This will be holomorphic unless $k = 2$ and $N \mid a$. Otherwise $G_k(a)$ belongs to $M_k(\Gamma_1(N))$, and its Fourier expansion at infinity is given by $G_k(a) = ((-2\pi i/N)^k/(k-1)!)F_k(a)$, with

$$F_k(a) = -N^{k-1}B_k(\{a/N\})/k + \sum_{n\geq 1} q^n \sum_{m|n} m^{k-1}(\delta_{m,a} + (-1)^k\delta_{m,-a})\ ,$$

where $\delta_{m,a} = 1$ if and only if $m \equiv a \pmod{N}$, and 0 otherwise.

For $k = 2$ and $a \equiv 0 \pmod{N}$, we understand $F_k(a)$ as meaning $F_k(a) - 2E_2$ with E_2 the usual quasi-modular form of weight 2 on the full modular group, which will be both holomorphic and in $M_2(\Gamma_1(N))$.

Definition 2.8 Let χ be a Dirichlet character modulo N. We set

$$\phi_\ell(a, b) = \sum_{A\in(\mathbb{Z}/N\mathbb{Z})^\times} \chi(A)F_\ell(Aa)F_{k-\ell}(Ab)\ .$$

It is clear that $\phi_\ell(a, b) \in M_k(\Gamma_0(N), \chi)$. An imprecise reformulation of the Borisov–Gunnells theorem is as follows:

Theorem 2.9 (Borisov–Gunnells) *The $\mathbb{C}$-vector space spanned by the $\phi_\ell(a, b)$ for $1 \leq \ell \leq k/2$, $a \mid N$ and $0 \leq b < N/a$, which is a subspace of $M_k(\Gamma_0(N), \chi)$, contains $S_k(\Gamma_0(N), \chi)$, except possibly for some well-understood exceptions when* $k = 2$.

As mentioned in the introduction, the exceptions do not matter since we can multiply by some known Eisenstein series so as to be in higher weight, and similarly multiply by θ if we are in half-integral weight. Also, to obtain the whole of $M_k(\Gamma_0(N),\chi)$ we must add a number of other completely explicit Eisenstein series, whose behavior under $|_k\gamma$ is also known.

Thus, as in the previous section, we need to give the expansion of $F_k(a)|_k\gamma$. The result is as follows.

Theorem 2.10 *Let $\gamma = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right) \in \Gamma$ and set $g_1 = \gcd(C,N)$ and $w_1 = N/g_1$. For $(k,a) \neq (2, 0 \bmod N)$ (otherwise simply subtract $2E_2$) we have $F_k(a)|_k\gamma = s(0) + \sum_{n\geq 1} s(n)q^{n/w_1}$, where:*

1. *For $n \geq 1$,*

$$s(n) = \frac{1}{w_1} \sum_{\substack{m|n,\ m\in\mathbb{Z} \\ Dm\equiv a \pmod{g_1}}} \operatorname{sign}(m)m^{k-1}\zeta_{w_1}^{((Dm-a)/g_1)(n/m)(C/g_1)^{-1}},$$

where $(C/g_1)^{-1}$ is the inverse modulo $N/g_1 = w_1$.

2. *For $n = 0$,*

$$s(0) = -\frac{g_1^k}{N}\frac{B_k(\{aA/g_1\})}{k} + \frac{\delta_{k,1}\delta(a/g_1)}{w_1}T$$

with

$$T = \begin{cases} -1/(1-\zeta_{w_1}^{(a/g_1)(C/g_1)^{-1}}) \text{ if } N \nmid a\ , \\ -1/2 \text{ if } N \mid a\ . \end{cases}$$

From this theorem we deduce the expansion of $\phi_\ell(a,b)|_k\gamma$ in integral powers of q^{1/w_1}, and it is then immediate to obtain from this an expansion of the form $q^\alpha \sum_{n\geq 0} c(n)q^{n/w_0}$, with $w_0 = N/\gcd(C^2,N)$ and α some rational number in $[0,1[$ with denominator divisible by w_1.

2.5 Expansion of $\theta|_{1/2}\gamma$

For completeness, we also give the expansion of $\theta|_{1/2}\gamma$ which is needed in the half-integral weight case. Thanks to the first two reductions above (the third is not necessary) we may assume that $\gamma = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right) \in \Gamma$. We recall that the *theta multiplier* $v_\theta(\gamma)$ is given by

$$v_\theta(\gamma) = \left(\frac{-4}{D}\right)^{-1/2}\left(\frac{C}{D}\right),$$

where we always choose the principal branch of the square root. The result is then as follows:

Proposition 2.11 *1. If* $4 \mid C$ *we have*

$$\theta|_{1/2}\gamma = v_\theta(\gamma)\theta = v_\theta(\gamma)\left(1 + 2\sum_{n\ge1} q^{n^2}\right) .$$

2. If $C \equiv 2 \pmod 4$, *set* $\alpha = \left(\begin{smallmatrix} A-2B & B \\ C-2D & D \end{smallmatrix}\right)$. *Then*

$$\theta|_{1/2}\gamma = 2v_\theta(\alpha)\sum_{n\ge0} q^{(2n+1)^2/4} .$$

3. If $2 \nmid C$, *let* $\lambda \equiv -D/C \pmod 4$, *and set* $D' = D + \lambda C$, $B' = \lambda A$, *and* $\alpha = \left(\begin{smallmatrix} -B' & A \\ -D' & C \end{smallmatrix}\right)$. *Then*

$$\theta|_{1/2}\gamma = \frac{1-i}{2} v_\theta(\alpha)\left(1 + 2\sum_{n\ge1} i^{-\lambda n^2} q^{n^2/4}\right) .$$

2.6 Fourier Expansion of $f|_k\gamma$

We need to recall some notation relative to the Fourier expansion of $f|_k\gamma$ for $\gamma \in \Gamma$ and $f \in M_k(\Gamma_0(N), \chi)$. It is easy to show that it has the form

$$f|_k\gamma(\tau) = q^{\alpha(\gamma)}\sum_{n\ge0} a_\gamma(n) q^{n/w(\gamma)} ,$$

where $w(\gamma)$ is the *width* of the cusp $\gamma(i\infty)$ and $\alpha(\gamma)$ is a rational number in $[0, 1[$, which by definition is different from 0 if and only if the cusp is *irregular*. For $\gamma = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)$, these quantities are given by the formulas

$$w(\gamma) = \frac{N}{\gcd(N, C^2)} \quad \text{and} \quad e^{2\pi i\alpha(\gamma)} = \chi\left(1 + \frac{ANC}{\gcd(N, C^2)}\right) = \chi(1 + ACw(\gamma)) .$$

In addition, note that the denominator of $\alpha(\gamma)$ divides $\gcd(N, C^2)/\gcd(N, C)$, and that $w(\gamma)$ and $\alpha(\gamma)$ only depend on the representative c of the cusp $\gamma(i\infty) = A/C$, so we will denote them $w(c)$ and $\alpha(c)$.

2.7 Computation of all $f|_k\gamma_j$

In the application to Petersson products we will need to compute *all* the Fourier expansions of $f|_k\gamma_j$ for a system of right coset representatives of $\Gamma_0(N)\backslash\Gamma$, i.e., such that $\Gamma = \bigsqcup_{j=1}^r \Gamma_0(N)\gamma_j$. Although the formulas that we will give are independent of this choice, for efficiency reasons it is essential to do it properly.

Let C be a set of representatives of cusps of $\Gamma_0(N)$ (which is *much* smaller than the set of cosets: for instance if N is prime we have $N+1$ cosets but only 2 cusps), and for each $c \in C$ let $\gamma_c \in \Gamma$ such that $\gamma_c(i\infty) = c$, and as above let $w(c)$ be the width of the cusp c. We claim that the $(\gamma_c T^m)_{c\in C,\ 0\le m<w(c)}$ form a system of right coset representatives of $\Gamma_0(N)\backslash\Gamma$. Indeed, let $\gamma \in \Gamma$, and let c be the representative of the cusp $\gamma(i\infty)$. By definition this means that there exists $\delta \in \Gamma_0(N)$ such that $\gamma(i\infty) = \delta(c) = \delta\gamma_c(i\infty)$, so $\gamma = \delta\gamma_c T^m$ for some integer m, and by definition of the width $\gamma_c T^{w(c)}\gamma_c^{-1} \in \Gamma_0(N)$, so we can always reduce m modulo $w(c)$, proving our claim since $\sum_{c\in C} w(c) = [\Gamma : \Gamma_0(N)]$.

Thus, we simply compute

$$f|_k\gamma_c(\tau) = q^{\alpha(c)}\sum_{n\ge 0} a_{\gamma_c}(n)q^{n/w(c)}\ ,$$

and we deduce that

$$f|_k(\gamma_c T^m)(\tau) = e^{2\pi i m\alpha(c)}q^{\alpha(c)}\sum_{n\ge 0} a_{\gamma_c}(n)\zeta_{w(c)}^{nm}q^{n/w(c)}$$

with $\zeta_{w(c)} = e^{2\pi i/w(c)}$, so we only need to compute $|C|$ expansions and not $[\Gamma : \Gamma_0(N)]$.

3 Petersson Products: Haberland-Type Formulas

Now that we know how to compute the Fourier expansion of $f|_k\gamma$ for any $\gamma \in \Gamma$ (and even $\gamma \in \mathrm{GL}_2^+(\mathbb{Q})$), we apply this to the computation of Petersson products.

3.1 Preliminary Formulas

Although this has been explained in several places, for instance in [6–8], it is necessary to reproduce the statements and proofs, since we will need some important modifications. In this section we always assume that k is an integer such that $k \ge 2$, so that $(X-\tau)^{k-2}$ is a polynomial.

In what follows, f and g will denote two modular forms in the space $M_k(\Gamma_0(N), \chi)$, and as above we denote by $(\gamma_j)_{1\le j\le r}$ a set of right coset representatives of the full modular group Γ modulo $\Gamma_0(N)$, so that $\Gamma = \bigsqcup_{j=1}^r \Gamma_0(N)\gamma_j$. Finally, we set $f_j = f|_k\gamma_j$ and $g_j = g|_k\gamma_j$.

It is clear that for any $\alpha \in \Gamma$ there exist an index which by abuse of notation we will write as $\alpha(j)$, and an element $\delta_j(\alpha) \in \Gamma_0(N)$ such that $\gamma_j\alpha = \delta_j(\alpha)\gamma_{\alpha(j)}$, and the map $j \mapsto \alpha(j)$ is a bijection of $[1, r]$.

Definition 3.1 For any $j \in [1, r]$ and $Z_j \in \overline{\mathfrak{H}}$ we define

$$G_j(Z_j; \tau) = \int_{Z_j}^{\tau} \overline{g_j(\tau_2)}(\tau - \overline{\tau_2})^{k-2} \, d\overline{\tau_2} \,.$$

Note that this function is essentially an *Eichler integral* of g_j, so will have quasi-modularity properties in weight $2 - k$. More precisely:

Proposition 3.2 *Keep the above notation. We have*

$$(G_j(Z_j; \tau)|_{2-k}\alpha)(\tau) = \overline{\chi(\delta_j(\alpha))} \left(G_{\alpha(j)}(Z_{\alpha(j)}; \tau) - P_{\alpha(j)}(\alpha; \tau)\right) \,,$$

where as usual $\chi\left(\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)\right) = \chi(d)$, *and* P_j *is the* polynomial *in* τ

$$P_j(\alpha; \tau) = \int_{Z_j}^{\alpha^{-1}\left(Z_{\alpha^{-1}(j)}\right)} \overline{g_j(\tau_2)}(\tau - \overline{\tau_2})^{k-2} \, d\overline{\tau_2} \,.$$

Corollary 3.3 *Keep the notation of the proposition. For any* A *and* B *in* $\overline{\mathfrak{H}}$ *we have*

$$\left(\int_A^B - \int_{\alpha(A)}^{\alpha(B)}\right) \sum_{1 \le j \le r} f_j(\tau) G_j(Z_j; \tau) \, d\tau = \int_A^B \sum_{1 \le j \le r} f_j(\tau) P_j(\alpha; \tau) \, d\tau \,.$$

The main theorem proved for instance in [7], but which is an immediate consequence of Stokes's theorem, is the following:

Theorem 3.4 *Let* H *be some subgroup of* Γ *of finite index* $s = [\Gamma : H]$, *and let* $D(H)$ *denote a fundamental domain for* H *whose boundary* $\partial(D(H))$ *is a hyperbolic polygon. Then for any choice of the* Z_j *we have*

$$rs(2i)^{k-1} < f, g >_{\Gamma_0(N)} = \int_{\partial(D(H))} \sum_{1 \le j \le r} f_j(\tau) G_j(Z_j; \tau) \, d\tau \,.$$

Note that the subgroup H can be chosen arbitrarily. To simplify, we will choose it so that $\partial(D(H))$ is a hyperbolic quadrilateral (A_1, A_2, A_3, A_4) such that there exist an element $\alpha_1 \in \Gamma$ sending $[A_1, A_2]$ to $[A_3, A_2]$ and $\alpha_2 \in \Gamma$ sending $[A_3, A_4]$ to $[A_1, A_4]$. We thus have

$$\int_{\partial(D(H))} = \left(\int_{A_1}^{A_2} - \int_{\alpha_1(A_1)}^{\alpha_1(A_2)}\right) + \left(\int_{A_3}^{A_4} - \int_{\alpha_2(A_3)}^{\alpha_2(A_4)}\right) \,.$$

Applying the above corollary and the theorem we deduce the following.

Definition 3.5 The forms f and g being implicit, we define

$$G_j(A, B; C, D) = \int_A^B \int_C^D f_j(\tau)\overline{g_j(\tau_2)}(\tau - \overline{\tau_2})^{k-2}\, d\tau\, d\overline{\tau_2}\ .$$

Corollary 3.6 *We have*

$$rs(2i)^{k-1} < f, g >_{\Gamma_0(N)} = \sum_{1\le j\le r} (I_j(f, g) + J_j(f, g))\ ,$$

where

$$I_j(f, g) = G_j\left(A_1, A_2; Z_j, \alpha_1^{-1}\left(Z_{\alpha_1^{-1}(j)}\right)\right)$$
$$J_j(f, g) = G_j\left(A_3, A_4; Z_j, \alpha_2^{-1}\left(Z_{\alpha_2^{-1}(j)}\right)\right)\ .$$

3.2 *The Cuspidal Case*

We now distinguish whether both f and g are cusp forms or otherwise.

Assume first that f and g are both cusp forms. As in [7] we choose $H = \Gamma(2)$, which has index 6 in Γ, and we can take for $D(H)$ the hyperbolic quadrilateral with $A_1 = 1$, $A_2 = i\infty$, $A_3 = -1$, and $A_4 = 0$, so that $\alpha_1 = T^{-2} = \left(\begin{smallmatrix}1 & -2\\ 0 & 1\end{smallmatrix}\right)$ and $\alpha_2 = \left(\begin{smallmatrix}1 & 0\\ 2 & 1\end{smallmatrix}\right)$. We also choose $Z_j = 0$ for all j, so that $\alpha_2^{-1}(\mathbb{Z}_{\alpha_2^{-1}(j)}) = \alpha_2^{-1}(0) = 0$, hence $P_j(\alpha_2; \tau) = 0$, so that $J_j(f, g) = 0$ for all j. On the other hand

$$P_j(\alpha_1; \tau) = \int_0^2 \overline{g_j(\tau_2)}(\tau - \overline{\tau_2})^{k-2}\, d\overline{\tau_2}\ ,$$

so that

$$6r(2i)^{k-1} < f, g >_{\Gamma_0(N)} = \sum_{1\le j\le r} G_j(1, i\infty; 0, 2)\ .$$

Shifting both τ and τ_2 by 1 gives the following:

Corollary 3.7 *Assume that f and g are both cusp forms. We then have*

$$\begin{aligned}6r(2i)^{k-1} < f, g >_{\Gamma_0(N)} &= \sum_{1\le j\le r} G_j(0, i\infty; -1, 1)\\ &= \sum_{1\le j\le r} \int_0^{i\infty}\int_{-1}^1 f_j(\tau)\overline{g_j(\tau_2)}(\tau - \overline{\tau_2})^{k-2}\, d\tau\, d\overline{\tau_2}\\ &= \sum_{1\le j\le r}\ \sum_{0\le n\le k-2} (-1)^n \binom{k-2}{n} I_{k-2-n}(0, i\infty, f_j)\overline{I_n(-1, 1, g_j)}\ ,\end{aligned}$$

where we have set

$$I_n(A,B,f)=\int_A^B \tau^n f(\tau)\,d\tau\ .$$

The essential advantage of this formula is that we have reduced the computation of a Petersson product, which is a double integral, to a small finite number of single integrals, which are essentially the periods associated to f and g; this is in fact exactly the statement of Haberland's theorem.

The main problem is that, even though the Petersson product is defined when only one of f and g is a cusp form, we cannot apply the above formula since the period integrals will diverge for non cusp forms. We thus consider the general case.

3.3 The Noncuspidal But Convergent Case

We now assume that f and g are in $M_k(\Gamma_0(N),\chi)$, not necessarily cusp forms. For the Petersson product to converge it is necessary and sufficient that at each cusp either f or g vanishes. Equivalently, for each $j\in[1,r]$ either f_j or g_j vanishes as $\tau\to i\infty$. We denote by E the subset of $j\in[1,r]$ such that f_j vanishes as $\tau\to i\infty$, so that if $j\notin E$ then g_j vanishes as $\tau\to i\infty$. Consider now $T=\left(\begin{smallmatrix}1&1\\0&1\end{smallmatrix}\right)$ the usual translation by 1. As usual $\gamma_j T=\delta_j(T)\gamma_{T(j)}$ for some bijection $j\mapsto T(j)$ and $\delta_j(T)\in\Gamma_0(N)$. Thus $f_j|_kT=\chi(\delta_j(T))f|_{T(j)}$, and it follows that both E and its complement are stable by the bijection induced by T.

For simplicity, we are going to choose $H=\Gamma$, and as fundamental domain the usual fundamental domain of the modular group, which has the advantage of having a single cusp on its boundary. Thus as above, setting as usual $\rho=e^{2\pi i/3}$, we have $A_1=\rho+1$, $A_2=i\infty$, $A_3=\rho$, and $A_4=i$, with $\alpha_1=T^{-1}$ and $\alpha_2=S=\left(\begin{smallmatrix}0&-1\\1&0\end{smallmatrix}\right)$.

We will choose $Z_j=i$ if $j\in E$ and $Z_j=i\infty$ if $j\notin E$. With the notation of Corollary 3.6 we have

$$I_j(f,g)=\int_{\rho+1}^{i\infty} f_j(\tau)P_j(T^{-1};\tau)\,d\tau\ ,$$

with

$$P_j(T^{-1};\tau)=\int_{Z_j}^{Z_{T(j)}+1}\overline{g_j(\tau_2)}(\tau-\overline{\tau_2})^{k-2}\,d\overline{\tau_2}\ .$$

Note that if $j\in E$ there is no convergence problem since $f_j(\tau)$ tends to 0 exponentially fast. On the other hand, if $j\notin E$ we have chosen $Z_j=i\infty$, and we also have $T(j)\notin E$ by what we said above, so $P_j(T^{-1};\tau)$ vanishes in that case. We thus have

$$\sum_{1\le j\le r} I_j(f,g)=\sum_{j\in E} G_j(\rho+1,i\infty;i,i+1)\ ,$$

and we can again expand this by the binomial theorem as a linear combination of products of two simple integrals, since the integral of $f_j(\tau)$ converges at $i\infty$.

Similarly, we have

$$J_j(f,g)=\int_{\rho}^{i} f_j(\tau)P_j(S;\tau)\,d\tau\ ,$$

with

$$P_j(S;\tau)=\int_{Z_j}^{-1/Z_{S(j)}}\overline{g_j(\tau_2)}(\tau-\overline{\tau_2})^{k-2}\,d\overline{\tau_2}\ .$$

Here we must distinguish four cases.

1. If $j\in E$ and $j\in S(E)$ (or equivalently $S(j)\in E$) then $Z_j=i$ and $Z_{S(j)}=i$ so $-1/Z_{S(j)}=i$, hence $P_j(S;\tau)=0$.
2. If $j\in E$ and $j\notin S(E)$, so that $S(j)\notin E$ we have $Z_j=i$, $Z_{S(j)}=i\infty$, so P_j is an integral from i to 0 hence $J_j(f,g)=G_j(\rho,i;i,0)$. Note that since $S(j)\notin E$ by assumption $g_{S(j)}$ vanishes at $i\infty$, or equivalently g_j vanishes at 0 so the integral makes sense.
3. If $j\notin E$ and $j\in S(E)$, we have $Z_j=i\infty$, $Z_{S(j)}=i$, so $J_j(f,g)=G_j(\rho,i;i\infty,i)=-G_j(\rho,i;i,i\infty)$.
4. If $j\notin E$ and $j\notin S(E)$, we have $Z_j=i\infty$, $Z_{S(j)}=i\infty$, so $J_j(f,g)=G_j(\rho,i;i\infty,0)$.

The changes of variable $\tau\mapsto S(\tau)$ and $\tau_2\mapsto S(\tau_2)$ show that $G_j(\rho,i;i,0)=G_{S(j)}(\rho+1,i;i,i\infty)$. Thus

$$\sum_{j\in E,\ j\notin S(E)} J_j(f,g)=\sum_{j\notin E,\ j\in S(E)} G_j(\rho+1,i;i,i\infty)\ .$$

Combining with (3), it follows by transitivity that

$$\left(\sum_{j\in E,\ j\notin S(E)}+\sum_{j\notin E,\ j\in S(E)}\right)J_j(f,g)=\sum_{j\notin E,\ j\in S(E)} G_j(\rho+1,\rho;i,i\infty)\ .$$

We have thus shown the following:

Theorem 3.8 *We have*

$$r(2i)^{k-1}<f,g>_{\Gamma_0(N)}=S_1+S_2+S_3$$

with

$$S_1=\sum_{j\in E}G_j(\rho+1,i\infty;i,i+1)\ ,$$

$$S_2=\sum_{j\notin E,\ j\in S(E)} G_j(\rho+1,\rho;i,i\infty)\ ,$$

$$S_3 = \sum_{j \notin E,\ j \notin S(E)} G_j(\rho, i; i\infty, 0)\ ,$$

and each G_j can be expressed as a linear combination of products of two convergent *single integrals by using the binomial theorem.*

Note that if f is a cusp form we have $E = [1, r]$ and only S_1 contributes, and if both f and g are cusp forms, we can either use this theorem or the formula given in Corollary 3.7.

3.4 Computation of Partial Periods

In all of the above formulas, using the notation of Corollary 3.7 we need to compute integrals of the form $I_n(a, b, f_j)$ and $I_n(a, b, g_j)$ for specific values of (a, b) in the completed upper half-plane. Putting them together for $0 \le n \le k-2$, this means that we must compute the *partial periods*

$$P(a, b, F)(X) = \int_a^b (X-\tau)^{k-2} F(\tau)\, d\tau$$

for $F = f_j$ and all j. For future reference, note the following important but trivial identity:

Lemma 3.9 *For any $\gamma \in \Gamma$ we have*

$$P(a, b, F|_k\gamma)(X) = P(\gamma(a), \gamma(b), F)|_{2-k}\gamma(X)\ .$$

We also have the following immediate lemma:

Lemma 3.10 *Let $R_{k-2}(X) = \sum_{0 \le n \le k-2} X^n/n!$ be the $(k-2)$nd partial sum of the exponential series. For all $m > 0$ we have*

$$\int_a^{i\infty} (X-\tau)^{k-2} e^{2\pi m i\tau}\, d\tau = -e^{2\pi m i a} \frac{(k-2)!}{(2\pi m i)^{k-1}} R_{k-2}(2\pi m i(X-a))\ .$$

We consider several cases. Keep in mind that in all the formulas that we use for computing Petersson products the endpoints of integration are either cusps or points in $\mathfrak{H}$ with reasonably large imaginary part (at least $\sqrt{3}/2$).

1. If $a \in \mathfrak{H}$ and $b = i\infty$ (or the reverse), we write as usual $f_j(\tau) = \sum_{n \ge 0} a_\gamma(n) q^{\alpha(c)+n/w(c)}$ (where $c = \gamma_j(i\infty)$), so that

$$\int_a^b (X-\tau)^{k-2} f_j(\tau)\, d\tau = \sum_{n \ge 0} a_\gamma(n) \int_a^{i\infty} (X-\tau)^{k-2} e^{2\pi i(\alpha(c)+n/w(c))\tau}\, d\tau\ ,$$

and the inner integral is given by the lemma. The dominant term in the resulting series is $e^{2\pi(\alpha(c)+n/w(c))ia}$, so the convergence will be in $e^{-2\pi\Im(a)n/w(c)}$.

2. If $a \in \mathfrak{H}$ and b is a cusp (or the reverse), we choose $\gamma \in \Gamma$ such that $b = \gamma(i\infty)$, make the change of variable $\tau = \gamma(\tau')$, and we are reduced to (1) with $f_{\gamma(j)}$ instead of f_j.
3. If a and b are in $\mathfrak{H}$ we simply write $\int_a^b = \int_a^{i\infty} - \int_b^{i\infty}$ and use (1).
4. If $a = 0$ and $b = i\infty$ (or the reverse), we write the integral as $\int_0^{it_0} + \int_{it_0}^{i\infty}$. The second integral is treated as in (1), so with convergence in $e^{-2\pi t_0 n/w(c)}$. In the first integral we make the change of variable $\tau \mapsto S(\tau) = -1/\tau$, and we again treat the resulting integral as in (1), with convergence in $e^{-2\pi(1/t_0)n/w(S(c))}$, where $w(S(c))$ is the width of the cusp $S(c) = \gamma_j(S(i\infty))$. To optimize the speed, we thus choose $t_0 = (w(c)/w(S(c)))^{1/2}$, so that the convergence of both integrals will be in $e^{-2\pi n/(w(c)w(S(c)))^{1/2}}$.
5. Finally, if a and b are both cusps, we use the well-known *Manin decomposition* of a modular symbol as a sum of Manin symbols. More precisely, we proceed as follows. Write $a = A/C$ and $b = B/D$ with $\gcd(A, C) = \gcd(B, D) = 1$. Then if $AD - BC = 1$ we set $\gamma = \left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right)$, and using Lemma 3.9 we transform our integral into an integral from 0 to $i\infty$, so we apply (4) (similarly if $AD - BC = -1$). Otherwise, setting $\Delta = AD - BC$ and using u and v such that $uA + vC = 1$, we write
$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} A & -v \\ C & u \end{pmatrix} \begin{pmatrix} 1 & uB + vD \\ 0 & \Delta \end{pmatrix} = \gamma \begin{pmatrix} 1 & B' \\ 0 & \Delta \end{pmatrix}$$
for $B' = uB + vD$, where $\gamma \in \Gamma$. Let $(p_j/q_j)_{-1 \le j \le m}$ be the convergents of the regular continued fraction expansion of B'/Δ with $p_{-1}/q_{-1} = 1/0$ and $p_m/q_m = B'/\Delta$, and let M_j be the matrix
$$M_j = \begin{pmatrix} (-1)^{j-1} p_j & p_{j-1} \\ (-1)^{j-1} q_j & q_{j-1} \end{pmatrix} \in \Gamma \ .$$
It is then immediate to show that
$$P(A/C, B/D, F)(X) = \sum_{0 \le j \le m} P(0, i\infty, F|_k(\gamma M_j))|_{2-k}(\gamma M_j)^{-1}(X) \ ,$$
so once again we can apply (4).

Note that in Theorem 3.8 we need to use (1), (3), and (4), while in Corollary 3.7 we need to use (4) and (5), and in (5) we have $(a, b) = (-1, 1)$ so the Manin decomposition consists here simply in writing $\int_{-1}^{1} = \int_{-1}^{0} + \int_0^1$, both integrals being then sent to integrals from 0 to $i\infty$ by suitable $\gamma \in \Gamma$.

In practice, the computation of these integrals forms only a very small part of the computation time. Almost all of the time is spent in computing the Fourier expansions at infinity of $f|_k\gamma_j$, for instance using products of two Eisenstein series as we do in this package. Note that there is of course no need to *rationalize* the expansions, and to compute all these expansions at once we use the specific choice of the γ_j explained in Sect. 2.7.

4 Petersson Products: The Method of Nelson and Collins

4.1 The Basic Formula

Recall that the completed zeta function $\Lambda(s)$ defined by $\Lambda(s) = \pi^{-s/2}\Gamma(s/2)\zeta(s)$ satisfies $\Lambda(1-s) = \Lambda(s)$. Nelson's method, completed by Collins [1, 2], is based on the following proposition, essentially due to Rankin:

Proposition 4.1 *Let $F(\tau)$ be a bounded measurable function on $\mathfrak{H}$ invariant by the modular group Γ, and such that for some fixed $\alpha > 0$ we have $F(x+iy) = O(y^{-\alpha})$ for almost all $\tau = x+iy$ with $y \geq 1$. Denote by $a(0;F)(y)$ the constant term of the Fourier expansion of $F(\tau)$ and by $\mathscr{M}(a(0;F))(s) = \int_0^\infty y^s a(0,F)(y)dy/y$ its Mellin transform. For any $\delta > 0$ we have*

$$\int_{\Gamma\backslash\mathfrak{H}} F(\tau)\,d\mu = \int_{\Re(s)=1+\delta} (4s-2)\Lambda(2s)\mathscr{M}(a(0;F))(s-1)\,ds\ ,$$

where $d\mu = dxdy/y^2$ is the usual invariant hyperbolic measure.

Proof Recall that the standard nonholomorphic Eisenstein series of weight 0 is defined by $E(s) = \sum_{\gamma\in\Gamma_\infty\backslash\Gamma} \Im(\gamma\tau)^s$, and its completed function $\mathscr{E}(s) = \Lambda(2s)E(s)$ satisfies $\mathscr{E}(1-s) = \mathscr{E}(s)$ and has only two poles, which are simple, at $s=0$ and $s=1$ with residues $-1/2$ and $1/2$ respectively. Standard unfolding shows that

$$\int_{\Gamma\backslash\mathfrak{H}} E(s)(\tau)F(\tau)\,d\mu = \int_0^\infty y^{s-2}\int_0^1 F(x+iy)\,dx\,dy\ .$$

The inner integral is equal to $a(0;F)(y)$ so that

$$\int_{\Gamma\backslash\mathfrak{H}} E(s)(\tau)F(\tau)\,d\mu = \mathscr{M}(a(0;F))(s-1)\ .$$

On the other hand, by the residue theorem if C_δ is the infinite vertical contour whose vertical sides are $\Re(s) = -\delta$ and $\Re(s) = 1+\delta$, by the residue theorem we first have

$$\frac{1}{2\pi i}\int_{C_\delta} s\mathscr{E}(s)\,ds = \mathrm{Res}_{s=0}\, s\mathscr{E}(s) + \mathrm{Res}_{s=1}\, s\mathscr{E}(s) = 1/2\ ,$$

and on the other hand, since $\mathscr{E}$ decreases exponentially when $|\Im(s)| \to \infty$ and $\mathscr{E}(1-s) = \mathscr{E}(s)$, this integral is equal to

$$\frac{1}{2\pi i}\int_{\Re(s)=1+\delta}(2s-1)\mathscr{E}(s)\,ds\;.$$

Multiplying the resulting identity by $2F(\tau)$ and integrating on $\Gamma\backslash\mathfrak{H}$ gives

$$\frac{1}{2\pi i}\int_{\Re(s)=1+\delta}(4s-2)\Lambda(2s)\int_{\Gamma\backslash\mathfrak{H}}E(s)F(\tau)\,ds\,d\mu=\int_{\Gamma\backslash\mathfrak{H}}F(\tau)\,d\mu\;,$$

hence

$$\int_{\Gamma\backslash\mathfrak{H}}F(\tau)\,d\mu=\frac{1}{2\pi i}\int_{\Re(s)=1+\delta}(4s-2)\Lambda(2s)\mathscr{M}(a(0;F))(s-1)\,ds\;,$$

proving the proposition. □

Corollary 4.2 *Let G be a subgroup of finite index of Γ, let $C(G)$ be a system of representatives of the cusps of G, and for each $c\in C(G)$ let $\gamma_c\in\Gamma$ such that $\gamma_c(i\infty)=c$. If $F(\tau)$ is a bounded measurable function invariant by G we have*

$$\int_{G\backslash\mathfrak{H}}F(\tau)\,d\mu=\frac{1}{2\pi i}\int_{\Re(s)=1+\delta}(4s-2)\Lambda(2s)\sum_{c\in C}w(c)\mathscr{M}(a(0;F|\gamma_c))(s-1)ds\;,$$

where $w(c)$ is the width of the cusp c.

Proof Immediate by applying the proposition to $F_1=\sum_{\gamma\in G\backslash\Gamma}F|\gamma$, noting that $\int_{\Gamma\backslash\mathfrak{H}}F_1(\tau)\,d\mu=\int_{G\backslash\mathfrak{H}}F(\tau)\,d\mu$, and that $a(0;F|\gamma_c')=a(0;F|\gamma_c)$ for any γ_c' such that $\gamma_c'(i\infty)=\gamma_c(i\infty)=c$. □

4.2 Collins's Formula

We are of course going to apply the above corollary to the function $F(\tau)=f(\tau)\overline{g(\tau)}y^k$, with $y=\Im(\tau)$. Recall from Sect. 2.6 that we have expansions

$$f|_k\gamma(\tau)=q^{\alpha(c)}\sum_{n\ge0}a_\gamma(n)q^{n/w(c)}\quad\text{and}\quad g|_k\gamma(\tau)=q^{\alpha(c)}\sum_{n\ge0}b_\gamma(n)q^{n/w(c)}$$

with the same $\alpha(c)$ and $w(c)$. It follows that the constant term $a_\gamma(0;F)$ is given by

$$a_\gamma(0,F)=y^k\sum_{n\ge0}a_\gamma(n)\overline{b_\gamma(n)}e^{-4\pi y(\alpha(c)+n/w(c))}\;,$$

so that

$$\mathscr{M}(a_\gamma(0;F))(s)=\frac{\Gamma(s+k)}{(4\pi)^{s+k}}\sum_{n\ge0}\frac{a_\gamma(n)\overline{b_\gamma(n)}}{(\alpha(c)+n/w(c))^{s+k}}\;.$$

We must now be careful about convergence of the Petersson product. When $k \geq 1$, the necessary and sufficient condition is that at every cusp either f or g vanishes, or equivalently that for every γ at least one of the forms $f|_k\gamma$ and $g|_k\gamma$ vanishes at infinity. In these cases, if $\alpha(c) = 0$ we have necessarily $a_\gamma(0)\overline{b_\gamma(0)} = 0$, which means that we omit the term $n = 0$, while if $\alpha(c) \neq 0$ we must keep it.

However the Petersson product also converges without any condition on f and g if $k = 1/2$. In that case, if $\alpha(c) = n = 0$ the contribution to $a_\gamma(0; F)$ is $a_\gamma(0)\overline{b_\gamma(0)}y^{1/2}$, and although the Mellin transform is divergent, we will need to take a limit as we will see below.

We deduce from the above corollary and the explicit expression of $\Lambda(2s)$ the following temporary result:

Proposition 4.3 *Keep the above assumptions and notation. We have*

$$< f, g >_{\Gamma_0(N)} = \frac{1}{[\Gamma : \Gamma_0(N)]} \sum_{c \in C(G)} w(c) \sum_{n \geq 0} \frac{a_{\gamma_c}(n)\overline{b_{\gamma_c}(n)}}{(4\pi(\alpha(c) + n/w(c)))^{k-1}} \cdot$$
$$\cdot \frac{1}{2\pi i} \int_{\Re(s)=1+\delta} (4s-2) \frac{\Gamma(s)\Gamma(k+s-1)\zeta(2s)}{(4\pi^2(\alpha(c) + n/w(c)))^s} \, ds \; .$$

There are now two ways to continue, and we consider both.

First, we write $\zeta(2s) = \sum_{m \geq 1} m^{-2s}$, so that the integral is equal to the sum from $m = 1$ to ∞ of the inverse Mellin transform at $x = 4\pi^2 m^2(\alpha(c) + n/w(c))$ of the function $(4s-2)\Gamma(s)\Gamma(k+s-1)$. Since this inverse Mellin transform is equal to

$$4x^{(k-1)/2}(2x^{1/2}K_{k-2}(2x^{1/2}) - K_{k-1}(2x^{1/2})) \; ,$$

we obtain our final theorem, due to D. Collins, although in a slightly different form:

Theorem 4.4 *Let f and g be in $M_k(\Gamma_0(N), \chi)$ such that either fg vanishes at all cusps or $k = 1/2$, and keep all the above notation. We have*

$$< f, g >_{\Gamma_0(N)} = \frac{4(8\pi)^{-(k-1)}}{[\Gamma : \Gamma_0(N)]} \sum_{c \in C(G)} w(c) \cdot$$
$$\cdot \sum_{n \geq 0} \frac{a_{\gamma_c}(n)\overline{b_{\gamma_c}(n)}}{((\alpha(c) + n/w(c)))^{k-1}} W_k(4\pi(\alpha(c) + n/w(c))^{1/2}) \; ,$$

where $W_k(x) = \sum_{m \geq 1} (mx)^{k-1}(mxK_{k-2}(mx) - K_{k-1}(mx))$. In the special case $k = 1/2$, $\alpha(c) = 0$, and $n = 0$, the term $(n/w(c))^{1/2}W_{1/2}(4\pi(n/w(c))^{1/2}$ is to be interpreted as its limit as $n \to 0$, in other words as $1/(4(2\pi)^{1/2})$.

We will study the function $W_k(x)$ and its implementation below.

But there is another way to continue. Assume for simplicity that $\alpha(c) = 0$ (so that the sum starts at $n = 1$). We can write

$$\zeta(2s)\sum_{n\ge1}\frac{a_{\gamma_c}(n)\overline{b_{\gamma_c}(n)}}{n^{s+k-1}}=\sum_{N\ge1}\frac{A_{\gamma_c}(N)}{N^{s+k-1}}\;,$$

with

$$A_{\gamma_c}(N)=\sum_{m^2\mid N}m^{2(k-1)}a_{\gamma_c}(N/m^2)\overline{b_{\gamma_c}(N/m^2)}\;.$$

Once $a_{\gamma_c}(n)$ and $b_{\gamma_c}(n)$ computed, the computation of $A_{\gamma_c}(N)$ takes negligible time. The advantage is that $\zeta(2s)$ has disappeared, and we now obtain a formula involving only the term $m=1$ in the definition of W_k, i.e., the function $V_k(x)=x^{k-1}(xK_{k-2}(x)-K_{k-1}(x))$.

When $\alpha(c)\neq 0$ a similar but more complicated formula can easily be written. Since anyway as we will see the function $W_k(x)$ can be computed essentially as fast as the function $V_k(x)$, we have not used this other method.

4.3 Computation of the Function $W_k(x)$

First note that $W_k(x)$ is exponentially decreasing at infinity, more precisely thanks to the corresponding result for the K-Bessel function it is immediate to show that as $x\to\infty$ we have

$$W_k(x)\sim\sqrt{\pi/2}x^{k-1/2}e^{-x}\;.$$

To compute $W_k(x)$ we introduce the simpler function $U_k(x)=\sum_{m\ge1}(mx)^k K_k(mx)$, and thanks to the recursions for the K-Bessel functions we have $W_k(x)=U_k(x)-(2k-1)U_{k-1}(x)$, so we must compute $U_k(x)$. We distinguish between k half-integral and k integral. For k half-integral we have the following easy proposition which comes from the fact that K_k is an elementary function:

Proposition 4.5 *Define polynomials $P_k(x)$ by $P_0(x)=1$ and the recursion $P_{k+1}(x)=x((k+1)P_k(x)-(x-1)P_k'(x))$ for $x\ge0$, and set $S_k(x)=P_k(x)/(x-1)^{k+1}$. For all $k\ge0$ integral we have*

$$U_{k+1/2}(x)=\sqrt{\frac{\pi}{2}}\sum_{0\le j\le k}\frac{x^{k-j}(k+j)!}{j!(k-j)!2^j}S_{k-j}(e^x)\;.$$

This makes the computation of $U_{k+1/2}(x)$ essentially trivial.

We now consider the slightly more difficult problem of computing $U_k(x)$ when k is integral. Since $K_k(mx)$ tends exponentially fast to 0 we could of course simply sum $(mx)^kK_k(mx)$ until the terms become negligible with respect to the desired accuracy, using the `Pari/GP` built-in function `besselk` for computing K-Bessel functions. But there is a way which is at least an order of magnitude faster. First note the following lemma, which comes directly from the integral representation of the K-Bessel function:

Lemma 4.6 *We have*

$$U_k(x) = \frac{x^k}{2}\int_{-\infty}^{\infty} S_k(e^{x\cosh(t)})\cosh(kt)\,dt\ ,$$

where the functions S_k are as above.

Note that as $t \to \pm\infty$ the function $e^{x\cosh(t)}$ tends to infinity *doubly exponentially*, and since $S_k(X) = P_k(X)/(X-1)^{k+1}$, the integrand tends to 0 doubly-exponentially. This is exactly the context of *doubly exponential integration*, except that here there is no change of variable to be done. The basic theorem, due to Takahashi and Mori, states that the fastest way to compute this integral is as a Riemann sum $h\sum_{-N\le j\le N} R_k(jh)$, where R_k is the integrand and h and N are chosen appropriately (we do not need the theorem since we compute the errors explicitly, but it is reassuring that we do not have a better way). An easy study both of the speed of doubly-exponential decrease and of the Euler–MacLaurin error made in approximating the integral by Riemann sums gives the following:

Proposition 4.7 *Set $R_k(x) = S_k(e^{x\cosh(t)})\cosh(kt)$, where S_k is given by Proposition 4.5. Let $B > 0$ and set $C = B + k\log(x)/\log(2) + 1$, $D = C\log(2) + 2.06$, $E = 2((C-1)\log(2) + \log(k!))/x$, $T = \log(E)(1 + (2k/x)/E)$, $N = \lceil (T/\pi^2)(D + \log(D/\pi^2))\rceil$, and $h = T/N$. There exists a small (explicit) constant c_k such that*

$$|U_k(x) - x^k h(R_k(0)/2 + \sum_{1\le j\le N} R_k(hj))| < c_k 2^{-B}\ .$$

Note that in practice, since we need both, it is faster to compute $U_k(x)$ and $U_{k-1}(x)$ simultaneously.

4.4 Conclusion: Comparison of the Methods

After explaining how to expand $f|_k\gamma$ using products of two Eisenstein series, we have given two methods to compute Petersson products. The first is limited to integral weight $k \ge 2$, while the second is applicable to any k integral or half-integral. In fact, the second method is applicable to more general modular forms, for instance to modular forms with multiplier system of modulus 1 (such as $\eta(\tau)$ and more generally eta quotients), since the only thing that we need is that $f(\tau)\overline{g(\tau)}y^k$ be invariant by some subgroup of Γ. For instance, this implies formulas such as

$$\sum_{m\ge1,\ m\equiv\pm1 \pmod 6} \frac{m}{e^{2\pi m/\sqrt{6}} - 1} = \frac{1}{12}\ ,$$

which can easily be proved directly.

In both methods we need to compute the Fourier expansions of $(f|_k\gamma_c)_{c\in C}$ for a system of representatives c of cusps, the Fourier expansions of $f|_k\gamma_j$ for a complete system of coset representatives, necessary in the Haberland case, being trivially obtained from those. This will be by far the most time-consuming part of the methods. The computation of the integrals in the Haberland case, or of the infinite series involving the transcendental function $W_k(x)$ in the Nelson–Collins case will in fact require little time in comparison.

The main difference between the methods comes from the speed of convergence. In the Haberland case, we have seen that the convergence is at worse in $e^{-2\pi n/N}$ (when the width of the cusp is equal to N, for instance for the cusp 0), and for this to be less than e^{-E}, say, we need $n > (E/(2\pi))N$, proportional to E. On the other hand, in the Nelson–Collins case the convergence is at worse in $e^{-4\pi(n/N)^{1/2}}$, so here we need $n > (E/(4\pi))^2N$, proportional to E^2. Thus this latter method is considerably slower than the former, especially in high accuracy, hence must be used only when Haberland-type methods are not applicable, in other words in weight 1 and half-integral weight.

As a typical timing example, in level 96, weight 4, computing a Petersson product at 19 decimal digits (using Haberland) requires 1.29 s and at 38 decimal digits 2.27 s. On the other hand, in level 96 weight $5/2$, computing a Petersson product at 19 decimal digits (using Nelson–Collins) requires 3.56 s, but at 38 decimal digits 16.2 s.

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CM Evaluations of the Goswami-Sun Series

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Abstract In recent work, Sun constructed two q-series, and he showed that their limits as $q \to 1$ give new derivations of the Riemann-zeta values $\zeta(2) = \pi^2/6$ and $\zeta(4) = \pi^4/90$. Goswami extended these series to an infinite family of q-series, which he analogously used to obtain new derivations of the evaluations of $\zeta(2k) \in \mathbb{Q} \cdot \pi^{2k}$ for every positive integer k. Since it is well known that $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$, it is natural to seek further specializations of these series which involve special values of the Γ-function. Thanks to the theory of complex multiplication, we show that the values of these series at all CM points τ, where $q := e^{2\pi i \tau}$, are algebraic multiples of specific ratios of Γ-values. In particular, classical formulas of Ramanujan allow us to explicitly evaluate these series as algebraic multiples of powers of $\Gamma\left(\frac{1}{4}\right)^4/\pi^3$ when $q = e^{-\pi}, e^{-2\pi}$.

1 Introduction and Statement of Results

Recently, Sun [10] obtained two q-series identities which allowed him to prove that

$$\lim_{\substack{q\to 1\\ |q|<1}} (1-q)^2 \sum_{n=0}^{\infty} \frac{q^n(1+q^{2n+1})}{(1-q^{2n+1})^2} = \frac{3}{2}\zeta(2) = \frac{\pi^2}{4} \tag{1}$$

and

$$\lim_{\substack{q\to 1\\ |q|<1}} (1-q)^4 \sum_{n=0}^{\infty} \frac{q^{2n}(1+4q^{2n+1}+q^{4n+2})}{(1-q^{2n+1})^4} = \frac{45}{8}\zeta(4) = \frac{\pi^4}{16}. \tag{2}$$

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Sun's formulas lead to the natural question: Are these q-series a glimpse of an infinite family that offers new derivations for the evaluations of $\zeta(2k)$ for all positive integers k? Goswami elegantly answered this problem in [5]; he defined a natural family of identities whose limits as $q \to 1$ with $|q| < 1$ give Euler's formula for the Riemann-zeta values at all even integers.

These results have been described as q-analogues of Euler's identities for $\zeta(2k)$. Here we offer further support of this view. Namely, to be a strong q-analogue, one hopes for further specializations of q which are expressions in related special functions. We address this question by observing that $\zeta(2k) \in \mathbb{Q} \cdot \pi^{2k} = \mathbb{Q} \cdot \Gamma\left(\frac{1}{2}\right)^{4k}$, and we ask if Goswami's series have evaluations involving algebraic multiples of naturally corresponding Γ-values. We show that this is indeed the case, thanks to the theory of complex multiplication and modular forms.

In order to state our results, we first recall the q-series that Goswami assembled which extended Sun's original identities into an infinite family. Throughout, k is a positive integer. If we denote the Stirling numbers of the second kind by $\left\{ {n \atop k} \right\}$, then we define $a_k(m)$ and $b_k(\ell)$ by

$$a_k(m) := \sum_{j=0}^{2k-1} j!(-1)^j \left\{ {2k-1 \atop j} \right\} \binom{j}{m},$$

$$b_k(\ell) := \sum_{m=0}^{2k-1} (-1)^m a_k(m) \binom{2k-m-1}{\ell} \in \mathbb{Z}.$$

Using these quantities, we define the degree $2k-2$ polynomial

$$P^e_{2k-2}(z) := \sum_{\ell=1}^{2k-1} (-1)^\ell b_k(\ell) z^{\ell-1},$$

and the degree $4k-2$ polynomial

$$P^o_{4k-2}(z) := (1+z)^{2k} P^e_{2k-2}(z) - 2^{2k-1} z P^e_{2k-2}\left(z^2\right).$$

For notational convenience, we define Goswami's q-series as follows.

$$\mathcal{G}_{2k}(q) := \begin{cases} \displaystyle\sum_{n=0}^{\infty} \frac{q^{2n+1} P^o_{4k-2}\left(q^{2n+1}\right)}{\left(1-q^{4n+2}\right)^{2k}}, & \text{if } k \text{ is odd.} \\ \displaystyle 2^{2k-1} \sum_{n=0}^{\infty} \frac{q^{4n+2} P^e_{2k-2}\left(q^{4n+2}\right)}{\left(1-q^{4n+2}\right)^{2k}}, & \text{if } k \text{ is even,} \end{cases} \tag{3}$$

Remark. When $k = 1$ and $k = 2$, these are essentially Sun's q-series. A critical feature of the results obtained here is that the $\mathcal{G}_{2k}(q)$ are holomorphic modular forms on $\Gamma_0(4)$ of integer weight $2k$.

As usual, we let $\overline{\mathbb{Q}}$ denote the algebraic closure of the field of rational numbers. Suppose that $D < 0$ is the fundamental discriminant of the imaginary quadratic field $\mathbb{Q}(\sqrt{D})$. Let $h(D)$ denote the class number of $\mathbb{Q}(\sqrt{D})$, and define $h'(D) := 1/3$ (resp. $1/2$) when $D = -3$ (resp. -4), and $h'(D) := h(D)$ when $D < -4$. We then let

$$\omega_D := \frac{1}{\sqrt{\pi}} \left(\prod_{j=1}^{|D|-1} \Gamma\left(\frac{j}{|D|}\right)^{\chi_D(j)} \right)^{\frac{1}{2h'(D)}}, \tag{4}$$

where $\chi_D(\bullet) := \left(\frac{D}{\bullet}\right)$. In terms of this notation, we obtain the following theorem.

Theorem 1.1 *If $D < 0$ is a fundamental discriminant and $\tau \in \mathbb{H} \cap \mathbb{Q}(\sqrt{D})$, then*

$$\mathcal{G}_{2k}\left(e^{2\pi i\tau}\right) \in \overline{\mathbb{Q}} \cdot \omega_D^{2k}.$$

Thanks to classical formulas of Ramanujan [1], it is simple to explicitly evaluate $\mathcal{G}_{2k}\left(e^{-\pi}\right)$ and $\mathcal{G}_{2k}\left(e^{-2\pi}\right)$. To make this precise, we define the rational number[1]

$$\mathcal{Z}(2k) := -\frac{(-16)^k B_{2k}\left(4^k - 1\right)}{8k} = 4^{k-1}\left(4^k - 1\right)(2k)! \cdot \frac{\zeta(2k)}{\pi^{2k}}, \tag{5}$$

where B_{2k} is the index $2k$ Bernoulli number. Furthermore, we let $(a;q)_\infty := \prod_{n\geq 0}(1 - aq^n)$ denote the usual infinite q-Pochhammer symbol. If $k \geq 2$, then define $\alpha_{2k}(1), \ldots, \alpha_{2k}(k-1)$ to be the unique rational numbers satisfying

$$\sum_{j=1}^{k-1} \alpha_{2k}(j) \cdot \frac{q^j \left(q^4;q^4\right)_\infty^{16j} (q;q)_\infty^{8j}}{\left(q^2;q^2\right)_\infty^{24j}} = \left(\mathcal{G}_{2k}(q) - \mathcal{Z}(2k) \cdot \frac{q^k\left(q^4;q^4\right)_\infty^{8k}}{\left(q^2;q^2\right)_\infty^{4k}}\right) \cdot \frac{(q;q)_\infty^{8k}\left(q^4;q^4\right)_\infty^{8k}}{\left(q^2;q^2\right)_\infty^{20k}}.$$

Since the jth summand on the left is of the form $\alpha_{2k}(j)q^j + O\left(q^{j+1}\right)$, the $\alpha_{2k}(j)$ are easily computed by diagonalization. In the case where $k = 1$, there simply are no $\alpha_{2k}(j)$ numbers. In terms of this notation, we obtain the following corollary.

Corollary 1.2 *If k is a positive integer and $a := \sqrt{2} - 1$, then*

$$\mathcal{G}_{2k}\left(e^{-\pi}\right) = \left(\frac{\mathcal{Z}(2k)}{2^{7k}} + \frac{1}{2^{2k}} \sum_{j=1}^{k-1} \frac{\alpha_{2k}(j)}{2^{5j}}\right) \cdot \left(\frac{\Gamma\left(\frac{1}{4}\right)^4}{\pi^3}\right)^k,$$

[1]In [5], Goswami refers to $\mathcal{Z}(2k)$ as d_k. We use $\mathcal{Z}(2k)$ to emphasize that these numbers are simple rational multiples of $\zeta(2k)/\pi^{2k}$.

$$\mathcal{G}_{2k}\left(e^{-2\pi}\right) = \left(\frac{\mathcal{Z}(2k)a^{2k}}{2^{9k}} + \frac{1}{2^{5k}a^{2k}}\sum_{j=1}^{k-1}\frac{\alpha_{2k}(j)a^{4j}}{2^{4j}}\right)\cdot\left(\frac{\Gamma\left(\frac{1}{4}\right)^4}{\pi^3}\right)^k.$$

Examples. Here we illustrate Corollary 1.2 for $k = 3$ and 4. If $k = 3$, then we have that

$$\mathcal{G}_6\left(e^{-\pi}\right) = \left(\frac{\mathcal{Z}(6)}{2^{21}} + \frac{1}{2^{12}}\right)\cdot\left(\frac{\Gamma\left(\frac{1}{4}\right)^4}{\pi^3}\right)^3,$$

$$\mathcal{G}_6\left(e^{-2\pi}\right) = \left(\frac{\mathcal{Z}(6)\left(\sqrt{2}-1\right)^6}{2^{27}} + \frac{1-\left(\sqrt{2}-1\right)^4}{2^{19}\left(\sqrt{2}-1\right)^2}\right)\cdot\left(\frac{\Gamma\left(\frac{1}{4}\right)^4}{\pi^3}\right)^3.$$

If $k = 4$, then we have that

$$\mathcal{G}_8\left(e^{-\pi}\right) = \left(\frac{\mathcal{Z}(8)}{2^{28}} + \frac{1}{2^{12}}\right)\cdot\left(\frac{\Gamma\left(\frac{1}{4}\right)^4}{\pi^3}\right)^4,$$

$$\mathcal{G}_8\left(e^{-2\pi}\right) = \left(\frac{\mathcal{Z}(8)\left(\sqrt{2}-1\right)^8}{2^{36}} + \frac{1-\left(\sqrt{2}-1\right)^4}{2^{21}}\right)\cdot\left(\frac{\Gamma\left(\frac{1}{4}\right)^4}{\pi^3}\right)^4.$$

These examples will be explained further in Sect. 5.

This paper is organized as follows. In Sect. 2, we recall the Goswami-Sun identities and the relation between $\mathcal{G}_{2k}(q)$ and modular forms. In Sect. 3, we recall essential facts about modular forms, and in Sect. 4, we use these results to prove Theorem 1.1 and Corollary 1.2. In Sect. 5, we conclude with a discussion of the examples given above.

2 The Goswami-Sun Identities

We now recall Goswami's work. Let $T_n = n(n+1)/2$ denote the nth triangular number, and define the generating function of T_n to be

$$\psi(q) := \sum_{n\geq 0} q^{T_n}.$$

Then Goswami [5, Theorems 3.1 and 3.2] proves the following theorem.

Theorem 2.1 *For any positive integer k, we have that*

$$T_{2k}(\tau) := \mathcal{G}_{2k}(q) - \mathcal{Z}(2k)\cdot q^k\psi\left(q^2\right)^{4k}$$

is the Fourier expansion of a weight $2k$ *cusp form on* $\Gamma_0(4)$*, where* $q := e^{2\pi i\tau}$ *and* $\tau \in \mathbb{H}$.

In Sect. 3, we apply the theory of modular forms and complex multiplication to study $T_{2k}(\tau)$ and $q^k\psi\left(q^2\right)^{4k}$ at all CM points.

3 Some Facts About Modular Forms

Here we recall some basic facts about modular forms.

3.1 CM Values of Modular Forms

In Goswami's work [5], the limit of the q-series identity in Theorem 2.1 as $q \to 1$ gives the constant term of a weight $2k$ Eisenstein series, which is described in terms of ζ-values. Our work depends on the values of modular forms at CM points.

Classically, the Chowla-Selberg formula [3] was developed in order to evaluate the Dedekind eta-function

$$\eta(\tau) := q^{1/24}\prod_{n=1}^{\infty}\left(1-q^n\right)$$

at CM points whose discriminants are fundamental discriminants. This was refined by van der Poorten and Williams [9, Theorem 9.3], who gave a closed formula for values of $\eta(\tau)$ in which τ is still required to be a CM point whose discriminant is fundamental. More generally, we have the following theorem (for example, see p. 84 of [2]) regarding evaluations of all modular forms at all CM points.

Theorem 3.1 *Suppose that* $D < 0$ *is the fundamental discriminant of the imaginary quadratic field* $\mathbb{Q}(\sqrt{D})$*. Then the number* $\Omega_D \in \mathbb{C}^*$ *defined by*

$$\Omega_D := \frac{1}{\sqrt{2\pi|D|}}\left(\prod_{j=1}^{|D|-1}\Gamma\left(\frac{j}{|D|}\right)^{\chi_D(j)}\right)^{\frac{1}{2h'(D)}}$$

has the property that $f(\tau) \in \overline{\mathbb{Q}}\cdot\Omega_D^k$ *for all* $\tau \in \mathbb{H}\cap\mathbb{Q}(\sqrt{D})$*, all* $k \in \mathbb{Z}$*, and all modular forms* f *of weight* k *with algebraic Fourier coefficients.*

In the special cases of the CM points $\tau \in \{i/2, i, 2i, 4i\}$, Theorem 3.1 can be made explicit using the following formulas of Ramanujan (see p. 326 of [1]),

$$f\left(-e^{-\pi}\right) = \frac{\pi^{\frac{1}{4}}e^{\frac{\pi}{24}}}{2^{\frac{3}{8}}\Gamma\left(\frac{3}{4}\right)},$$

$$f\left(-e^{-2\pi}\right) = \frac{\pi^{\frac{1}{4}} e^{\frac{\pi}{12}}}{2^{\frac{1}{2}} \Gamma\left(\frac{3}{4}\right)},$$

$$f\left(-e^{-4\pi}\right) = \frac{\pi^{\frac{1}{4}} e^{\frac{\pi}{6}}}{2^{\frac{7}{8}} \Gamma\left(\frac{3}{4}\right)},$$

$$f\left(-e^{-8\pi}\right) = \frac{\pi^{\frac{1}{4}} \left(\sqrt{2}-1\right)^{\frac{1}{4}} e^{\frac{\pi}{3}}}{2^{\frac{21}{16}} \Gamma\left(\frac{3}{4}\right)},$$

where $f(-q) := \prod_{n\geq 1}(1-q^n)$. The above formulas can be rewritten in terms of the Dedekind eta-function by noticing that $\eta(\tau) = q^{1/24} f(-q)$. By applying the functional equation of the Γ-function, namely $\Gamma(1-z)\Gamma(z) = \pi/\sin(\pi z)$ for $z \notin \mathbb{Z}$, in terms of

$$\Omega_{-4} = \frac{1}{2\sqrt{2\pi}} \cdot \frac{\Gamma\left(\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)},$$

we obtain

$$\eta(i/2) = 2^{\frac{1}{8}} \cdot \Omega_{-4}^{\frac{1}{2}}, \qquad \eta(i) = \Omega_{-4}^{\frac{1}{2}}, \qquad \eta(2i) = \frac{1}{2^{\frac{3}{8}}} \cdot \Omega_{-4}^{\frac{1}{2}},$$
$$\eta(4i) = \frac{\left(\sqrt{2}-1\right)^{\frac{1}{4}}}{2^{\frac{13}{16}}} \cdot \Omega_{-4}^{\frac{1}{2}}. \tag{6}$$

We shall make use of these formulas to prove Corollary 1.2.

3.2 Modular Forms on $\Gamma_0(4)$

Here we recall standard facts about modular forms on $\Gamma_0(4)$. Recall that the theta function given by

$$\theta(\tau) := \sum_{n=-\infty}^{\infty} q^{n^2}$$

is a weight $\frac{1}{2}$ modular form on $\Gamma_0(4)$, and that the weight 2 Eisenstein series

$$F(\tau) := \sum_{n=0}^{\infty} \sigma_1(2n+1) q^{2n+1}$$

is a modular form on $\Gamma_0(4)$ as well, where $\sigma_1(n)$ denotes the sum of the positive divisors of n. It is known that every modular form on $\mathrm{SL}_2(\mathbb{Z})$ and $\Gamma_0(4)$ can be expressed as a rational function in $\eta(\tau)$, $\eta(2\tau)$, and $\eta(4\tau)$ (see [8, Theorem 1.67] for

$\mathrm{SL}_2(\mathbb{Z})$ and [7] for $\Gamma_0(4)$). In the case of $\Gamma_0(4)$, this fact relies on the observation that $F(\tau)$ and $\theta(\tau)$ are given in terms of Dedekind eta-quotients in the following way:

$$\theta(\tau) = \frac{\eta(2\tau)^5}{\eta(\tau)^2\eta(4\tau)^2}, \qquad F(\tau) = \frac{\eta(4\tau)^8}{\eta(2\tau)^4}. \tag{7}$$

It is also very well known that the two Eisenstein series $E_4(\tau)$ and $E_6(\tau)$ generate the algebra of all modular forms on $\mathrm{SL}_2(\mathbb{Z})$ (for example, see [8, Theorem 1.23]). The analogous statement for modular forms on $\Gamma_0(4)$ involves the forms $F(\tau)$ and $\theta(\tau)$. Namely, the following complete description of the spaces $M_k\left(\Gamma_0(4), \psi_k\right)$ for $k \in \frac{1}{2}\mathbb{N}$ and

$$\psi_k := \begin{cases} \chi_0, & \text{if } k \in 2\mathbb{Z} \text{ or } k \in \frac{1}{2} + \mathbb{Z}, \\ \left(\frac{-4}{\bullet}\right), & \text{if } k \in 1 + 2\mathbb{Z}, \end{cases}$$

where χ_0 is the trivial character, is proved in [4, 6]. As a graded algebra, we have that

$$\bigoplus_{k \in \frac{1}{2}\mathbb{Z}} M_k\left(\Gamma_0(4), \psi_k\right) \cong \mathbb{C}[F, \theta].$$

Moreover, we have the following proposition (see [7, Corollary 3.3]) describing canonical representations of modular forms on $\Gamma_0(4)$ in terms of $F(\tau)$ and $\theta(\tau)$.

Proposition 3.2 *If $k \in \frac{1}{2}\mathbb{N}$, then each $f(\tau) \in M_k\left(\Gamma_0(4), \psi_k\right)$ has a unique expansion in terms of $F(\tau)$ and $\theta(\tau)$ of the form*

$$f(\tau) = \sum_{j=0}^{[k/2]} \alpha_k(j) F(\tau)^j \theta(\tau)^{2k-4j}. \tag{8}$$

Moreover, $f(\tau)$ is a cusp form if and only if the coefficients $\alpha_k(j)$ satisfy:

(i) $\alpha_k(0) = 0$,

(ii) $\alpha_k(k/2) = 0$ *when* $k \in 2\mathbb{Z}$, *and*

(iii) $\sum_{j=0}^{[k/2]} \alpha_k(j) \left(\frac{1}{16}\right)^j = 0.$

Combining the above decomposition in terms of $F(\tau)$ and $\theta(\tau)$ for the cusp form $T_{2k}(\tau)$ with the eta-quotients in (7), we obtain new expressions for the series $\mathcal{G}_{2k}(q)$ in Sect. 4.

4 Proof of Theorem 1.1 and Corollary 1.2

We may write the product on the right hand side of Theorem 2.1 in terms of eta-quotients as follows:

$$\mathcal{Z}(2k) \cdot q^k \psi\left(q^2\right)^{4k} = \mathcal{Z}(2k) \cdot q^k \prod_{n=1}^{\infty} \frac{\left(1-q^{4n}\right)^{4k}}{\left(1-q^{4n-2}\right)^{4k}} = \mathcal{Z}(2k) \cdot \frac{\eta(4\tau)^{8k}}{\eta(2\tau)^{4k}}. \tag{9}$$

Now, by (8)[2] we can express the cusp form $T_{2k}(\tau)$ as

$$T_{2k}(\tau) = \sum_{j=0}^{k} \alpha_{2k}(j) F(\tau)^j \theta(\tau)^{4k-4j}, \tag{10}$$

and by (7) we can write (10) in terms of eta-quotients in the following way:

$$T_{2k}(\tau) = \frac{\eta(2\tau)^{20k}}{\eta(\tau)^{8k}\eta(4\tau)^{8k}} \sum_{j=0}^{k} \alpha_{2k}(j) \cdot \frac{\eta(4\tau)^{16j}\eta(\tau)^{8j}}{\eta(2\tau)^{24j}}.$$

By Proposition 3.2*(i)* and *(ii)*, we may simplify this expression to

$$T_{2k}(\tau) = \frac{\eta(2\tau)^{20k}}{\eta(\tau)^{8k}\eta(4\tau)^{8k}} \sum_{j=1}^{k-1} \alpha_{2k}(j) \cdot \frac{\eta(4\tau)^{16j}\eta(\tau)^{8j}}{\eta(2\tau)^{24j}}. \tag{11}$$

Now, combining (9) with (11), we see that the series $\mathcal{G}_{2k}(q)$ can be expressed as

$$\mathcal{G}_{2k}(q) = \mathcal{Z}(2k) \cdot \frac{\eta(4\tau)^{8k}}{\eta(2\tau)^{4k}} + \frac{\eta(2\tau)^{20k}}{\eta(\tau)^{8k}\eta(4\tau)^{8k}} \sum_{j=1}^{k-1} \alpha_{2k}(j) \cdot \frac{\eta(4\tau)^{16j}\eta(\tau)^{8j}}{\eta(2\tau)^{24j}}. \tag{12}$$

From the above expression for $\mathcal{G}_{2k}(q)$, it is clear that if $k \geq 1$, then the $\alpha_{2k}(j)$ are the unique rational numbers such that

$$\sum_{j=1}^{k-1} \alpha_{2k}(j) \cdot \frac{\eta(4\tau)^{16j}\eta(\tau)^{8j}}{\eta(2\tau)^{24j}} = \left(\mathcal{G}_{2k}(q) - \mathcal{Z}(2k) \cdot \frac{\eta(4\tau)^{8k}}{\eta(2\tau)^{4k}}\right) \cdot \frac{\eta(\tau)^{8k}\eta(4\tau)^{8k}}{\eta(2\tau)^{20k}}.$$

This implies the definition for the $\alpha_{2k}(j)$ in (6).

Theorem 3.1 along with (12) immediately imply that evaluations of the Goswami-Sun series at CM points $\tau \in \mathbb{H} \cap \mathbb{Q}(\sqrt{D})$ give values in $\overline{\mathbb{Q}} \cdot \Omega_D^{2k}$, which proves Theorem 1.1 because

$$\omega_D^{2k} = 2^k |D|^k \cdot \Omega_D^{2k}.$$

$\square$

[2]The weights in Theorem 1.1 are $2k$ as opposed to k in the section above.

Proof (*of Corollary* 1.2) If $D = -4$, then $\mathbb{Q}(\sqrt{D}) = \mathbb{Q}(i)$ and by (4) we have

$$\omega_{-4} = \frac{1}{\sqrt{\pi}} \cdot \frac{\Gamma\left(\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)}.$$

We apply the functional equation of the Γ-function to rewrite ω_{-4} as

$$\omega_{-4} = \frac{\Gamma\left(\frac{1}{4}\right)^2}{\sqrt{2}\pi^{3/2}}.$$

In particular, applying the values of $\eta(\tau)$ in (6) to all of the eta-functions in (12), we evaluate $\mathcal{G}_{2k}\left(e^{2\pi i\tau}\right)$ at $\tau = \frac{i}{2}$ and $\tau = i$ to obtain the values in Corollary 1.2. □

5 Examples

Example 5.1 If $k = 3$, then Theorem 1.1 becomes

$$\mathcal{G}_6(q) = \mathcal{Z}(6) \cdot \frac{\eta(4\tau)^{24}}{\eta(2\tau)^{12}} + \frac{\eta(2\tau)^{60}}{\eta(\tau)^{24}\eta(4\tau)^{24}}\Bigg(\alpha_6(1) \cdot \frac{\eta(4\tau)^{16}\eta(\tau)^8}{\eta(2\tau)^{24}} + \alpha_6(2) \cdot \frac{\eta(4\tau)^{32}\eta(\tau)^{16}}{\eta(2\tau)^{48}}\Bigg),$$

and we calculate that $\alpha_6(1) = 1$ and $\alpha_6(2) = -16$. Then we have that

$$\mathcal{G}_6(q) = \mathcal{Z}(6) \cdot \frac{\eta(4\tau)^{24}}{\eta(2\tau)^{12}} + \frac{\eta(2\tau)^{60}}{\eta(\tau)^{24}\eta(4\tau)^{24}}\left(\frac{\eta(4\tau)^{16}\eta(\tau)^8}{\eta(2\tau)^{24}} - 16 \cdot \frac{\eta(4\tau)^{32}\eta(\tau)^{16}}{\eta(2\tau)^{48}}\right).$$

Corollary 1.2 in this case gives

$$\mathcal{G}_6\left(e^{-\pi}\right) = \left(\frac{\mathcal{Z}(6)}{2^{21}} + \frac{1}{2^{12}}\right) \cdot \left(\frac{\Gamma\left(\frac{1}{4}\right)^4}{\pi^3}\right)^3 = 0.0633804556\ldots$$

and

$$\mathcal{G}_6\left(e^{-2\pi}\right) = \left(\frac{\mathcal{Z}(6)\left(\sqrt{2}-1\right)^6}{2^{27}} + \frac{1-\left(\sqrt{2}-1\right)^4}{2^{19}\left(\sqrt{2}-1\right)^2}\right) \cdot \left(\frac{\Gamma\left(\frac{1}{4}\right)^4}{\pi^3}\right)^3 = 0.0018690318\ldots.$$

Example 5.2 If $k = 4$, then Theorem 1.1 becomes

$$\mathcal{G}_8(q) = \mathcal{Z}(8) \cdot \frac{\eta(4\tau)^{32}}{\eta(2\tau)^{16}} + \frac{\eta(2\tau)^{80}}{\eta(\tau)^{32}\eta(4\tau)^{32}} \left(\alpha_8(1) \cdot \frac{\eta(4\tau)^{16}\eta(\tau)^8}{\eta(2\tau)^{24}} \right.$$
$$\left. + \alpha_8(2) \cdot \frac{\eta(4\tau)^{32}\eta(\tau)^{16}}{\eta(2\tau)^{48}} + \alpha_8(3) \cdot \frac{\eta(4\tau)^{48}\eta(\tau)^{24}}{\eta(2\tau)^{72}} \right),$$

and we calculate that $\alpha_8(1) = 0$, $\alpha_8(2) = 128$, and $\alpha_8(3) = -2048$. Then we have that

$$\mathcal{G}_8(q) = \mathcal{Z}(8) \cdot \frac{\eta(4\tau)^{32}}{\eta(2\tau)^{16}} + \frac{\eta(2\tau)^{80}}{\eta(\tau)^{32}\eta(4\tau)^{32}} \left(128 \cdot \frac{\eta(4\tau)^{32}\eta(\tau)^{16}}{\eta(2\tau)^{48}} \right.$$
$$\left. -2048 \cdot \frac{\eta(4\tau)^{48}\eta(\tau)^{24}}{\eta(2\tau)^{72}} \right).$$

Corollary 1.2 in this case gives

$$\mathcal{G}_8\left(e^{-\pi}\right) = \left(\frac{\mathcal{Z}(8)}{2^{28}} + \frac{1}{2^{12}} \right) \cdot \left(\frac{\Gamma\left(\frac{1}{4}\right)^4}{\pi^3} \right)^4 = 0.2980189122\ldots$$

and

$$\mathcal{G}_8\left(e^{-2\pi}\right) = \left(\frac{\mathcal{Z}(8)\left(\sqrt{2}-1\right)^8}{2^{36}} + \frac{1-\left(\sqrt{2}-1\right)^4}{2^{21}} \right) \cdot \left(\frac{\Gamma\left(\frac{1}{4}\right)^4}{\pi^3} \right)^4$$
$$= 0.0004465790\ldots.$$

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Automatic Proof of Theta-Function Identities

Jie Frye and Frank Garvan

Abstract This is a tutorial for using two new MAPLE packages, `thetaids` and `ramarobinsids`. The `thetaids` package is designed for proving generalized eta-product identities using the valence formula for modular functions. We show how this package can be used to find theta-function identities as well as prove them. As an application, we show how to find and prove Ramanujan's 40 identities for his so called Rogers–Ramanujan functions $G(q)$ and $H(q)$. In his thesis Robins found similar identities for higher level generalized eta-products. Our `ramarobinsids` package is for finding and proving identities for generalizations of Ramanujan's $G(q)$ and $H(q)$ and Robin's extensions. These generalizations are associated with certain real Dirichlet characters. We find a total of over 150 identities.

1 Introduction

The Rogers–Ramanujan functions are

$$G(q) = \sum_{n=0}^{\infty} \frac{q^{n^2}}{(q;q)_n} = \prod_{n=0}^{\infty} \frac{1}{(1-q^{5n+1})(1-q^{5n+4})}, \tag{1.1}$$

$$H(q) = \sum_{n=0}^{\infty} \frac{q^{n(n+1)}}{(q;q)_n} = \prod_{n=0}^{\infty} \frac{1}{(1-q^{5n+2})(1-q^{5n+3})}.$$

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The ratio of these two functions is the famous Rogers–Ramanujan continued fraction [1]

$$\frac{G(q)}{H(q)} = \prod_{n=0}^{\infty} \frac{(1-q^{5n+2})(1-q^{5n+3})}{(1-q^{5n+1})(1-q^{5n+4})}$$
$$= 1 + \cfrac{q}{1+\cfrac{q^2}{1+\cfrac{q^3}{1+\cfrac{q^4}{1+\ddots}}}}.$$

Ramanujan also found

$$H(q)G(q)^{11} - q^2G(q)H(q)^{11} = 1 + 11G(q)^6H(q)^6 \tag{1.2}$$

and

$$H(q)G(q^{11}) - q^2G(q)H(q^{11}) = 1, \tag{1.3}$$

and remarked that "each of these formulae is the simplest of a large class". Here we have used the standard q-notation

$$(a;q)_n := \prod_{j=0}^{n-1}(1-aq^j) \qquad (a;q)_\infty := \prod_{j=0}^{\infty}(1-aq^j).$$

In 1974 Birch [7] published a description of some manuscripts of Ramanujan including a list of forty identities for the Rogers–Ramanujan functions. Biagioli [6] showed how the theory of modular forms could be used to prove identities of this type efficiently. See [2, 5] for recent work. It is instructive to write the Rogers–Ramanujan functions in terms of generalized eta-products.

The Dedekind eta-function is defined by

$$\eta(\tau) = q^{\frac{1}{24}} \prod_{n=1}^{\infty}(1-q^n),$$

where $\tau \in \mathscr{H} := \{\tau \in \mathbb{C} : \operatorname{Im}\tau > 0\}$ and $q := e^{2\pi i\tau}$, and the generalized Dedekind eta function is defined to be

$$\eta_{\delta;g}(\tau) = q^{\frac{\delta}{2}P_2(g/\delta)} \prod_{m\equiv \pm g \pmod{\delta}} (1-q^m), \tag{1.4}$$

where $P_2(t) = \{t\}^2 - \{t\} + \frac{1}{6}$ is the second periodic Bernoulli polynomial, $\{t\} = t - [t]$ is the fractional part of t, $g, \delta, m \in \mathbb{Z}^+$ and $0 < g < \delta$. The function $\eta_{\delta;g}(\tau)$ is a modular function (modular form of weight 0) on $\mathrm{SL}_2(\mathbb{Z})$ with a multiplier system.

Ramanujan's identities (1.2) and (1.3) can be rewritten as

$$\frac{1}{\eta_{5;2}(\tau)\eta_{5;1}(\tau)^{11}} - \frac{1}{\eta_{5;1}(\tau)\eta_{5;2}(\tau)^{11}} = 1 + 11\,\frac{\eta(5\tau)^6}{\eta(\tau)^6} \tag{1.5}$$

and

$$\frac{1}{\eta_{5;2}(\tau)\eta_{5;1}(11\tau)} - \frac{1}{\eta_{5;1}(\tau)\eta_{5;2}(11\tau)} = 1. \tag{1.6}$$

It is natural to consider higher level analogues of Ramanujan's identities (1.2) and (1.3). The following are nice level 13 analogues:

$$\frac{1}{\eta_{13;2,5,6}(\tau)\eta_{13;1,3,4}(\tau)^3} - \frac{1}{\eta_{13;1,3,4}(\tau)\eta_{13;2,5,6}(\tau)^3} = 1 + 3\,\frac{\eta(13\tau)^2}{\eta(\tau)^2} \tag{1.7}$$

and

$$\frac{1}{\eta_{13;2,5,6}(\tau)\eta_{13;1,3,4}(3\tau)} - \frac{1}{\eta_{13;1,3,4}(\tau)\eta_{13;2,5,6}(3\tau)} = 1. \tag{1.8}$$

Here we have used the notation

$$\eta_{\delta;g_1,g_2,\ldots,g_k}(\tau) = \eta_{\delta;g_1}(\tau)\,\eta_{\delta;g_1}(\tau)\,\cdots\,\eta_{\delta;g_k}(\tau).$$

Equation (1.7) was found by Ramanujan [3, Eq. (8.4), p. 373], and Eq. (1.8) is due to Robins [20], who considered more general identities. The following is a level 17 analogue of (1.8) and appears to be new.

$$\frac{1}{\eta_{17;3,5,6,7}(\tau)\eta_{17;1,2,4,8}(2\tau)} - \frac{1}{\eta_{17;1,2,4,8}(\tau)\eta_{17;3,5,6,7}(2\tau)} = 1. \tag{1.9}$$

Motivated by these examples and other work of Robins [20] one is led naturally to consider

$$G(n,N,\chi) = G(n) := \prod_{\substack{\chi(g)=1\\ 0<g<\frac{N}{2}}} \frac{1}{\eta_{N;g}(n\tau)}, \quad H(n,N,\chi) = H(n) := \prod_{\substack{\chi(g)=-1\\ 0<g<\frac{N}{2}}} \frac{1}{\eta_{N;g}(n\tau)}, \tag{1.10}$$

where χ is a non-principal real Dirichlet character mod N satisfying $\chi(-1) = 1$. Ratios of functions of this type were studied by Huber and Schultz [13]. They found the following level 17 identity:

$$(r^2 + 8\,r - 1)^2\, s^2 - 2\,r\,(r^2+1)\,s + r^2 = 0, \tag{1.11}$$

where

$$r = \frac{H\left(1, 17, \left(\frac{\cdot}{17}\right)\right)}{G\left(1, 17, \left(\frac{\cdot}{17}\right)\right)}, \quad s = \frac{\eta(17\tau)^3}{\eta(\tau)^3}.$$

The main goal of the `thetaids` MAPLE package is to automatically prove identities for generalized eta-products using the theory of modular functions. In Sects. 3 and 4 we describe the `ramarobinsids` package, which uses the `thetaids` package to search for and prove identities for general functions $G(n, N, \chi)$ and $H(n, N, \chi)$ that are like the theta-function identities considered by Ramanujan [5] and Robins [20].

We note that Liangjie [22] gave an algorithm for proving relations for certain theta-functions and their derivatives using a different method. We also note that Lovejoy and Osburn [15–18], have used an earlier version of the `thetaids` package to prove theta-functions identities that were needed to establish an number of results for mock-theta functions.

1.1 Installation Instructions

First install the `qseries` package from

http://qseries.org/fgarvan/qmaple/qseries

and follow the directions on that page. Before proceeding it is advisable to become familiar with the functions in the `qseries` package. See [9] for a tutorial. Then go to

http://qseries.org/fgarvan/qmaple/thetaids

to install the `thetaids` package. In Sect. 3 you will need to install the `ramarobinsids` package from

http://qseries.org/fgarvan/qmaple/ramarobinsids

2 Proving Theta-Function Identities

To prove a given theta-function identity one needs to basically do the following.

(i) Rewrite the identity in terms of generalized eta-functions.
(ii) Check that each term in the identity is a modular function on some group $\Gamma_1(N)$.
(iii) Determine the order at each cusp of $\Gamma_1(N)$ of each term in the identity.
(iv) Use the valence formula to determine up to which power of q is needed to verify the identity.
(v) Finally prove the identity by carrying out the verification.

In this section we explain how to carry out each of these steps in MAPLE. Then we show how the whole process of proof can be automated.

2.1 Encoding Theta-Functions, Eta-Functions and Generalized Eta-Functions

We recall Jacobi's triple product for theta-functions:

$$\prod_{n=1}^{\infty}(1 - zq^{n-1})(1 - z^{-1}q^n)(1 - q^n) = \sum_{n=-\infty}^{\infty} (-1)^n z^n q^{n(n-1)/2}, \tag{2.1}$$

so that

$$\prod_{n=1}^{\infty}(1 - q^{\delta n-g})(1 - q^{\delta n+g-\delta})(1 - q^{\delta n}) = \sum_{n=-\infty}^{\infty} (-1)^n q^{\frac{1}{2}n(\delta n-\delta+2g)}. \tag{2.2}$$

In the `qseries` MAPLE package the function on the left side of (2.2) is encoded symbolically as `JAC(g, δ, infinity)`. This is the building block of the functions in our package. In the `qseries` package `JAC(0,δ,infinity)` corresponds symbolically to

$$\prod_{n=1}^{\infty}(1 - q^{\delta n}) = \sum_{n=-\infty}^{\infty} (-1)^n q^{\frac{\delta}{2}n(3n+1)}, \tag{2.3}$$

which is Euler's Pentagonal Number Theorem.

Function	Symbolic MAPLE form
$\prod_{n=1}^{\infty}(1 - q^{\delta n-g})(1 - q^{\delta n+g-\delta})(1 - q^{\delta n})$	`JAC(g, δ, infinity)`
$\prod_{n=1}^{\infty}(1 - q^{\delta n})$	`JAC(0, δ, infinity)`
$\eta_{\delta;g}(\tau)$	`GETA(δ,g)`
$\eta(\delta\tau)$	`EETA(δ)`

We will also consider generalized eta-products. Let N be a fixed positive integer. A generalized Dedekind eta-product of level N has the form

$$f(\tau) = \prod_{\substack{\delta\mid N\\ 0<g<\delta}} \eta_{\delta;g}^{r_{\delta,g}}(\tau), \tag{2.4}$$

where

$$r_{\delta,g} \in \begin{cases} \frac{1}{2}\mathbb{Z} & \text{if } g = \delta/2, \\ \mathbb{Z} & \text{otherwise.} \end{cases} \tag{2.5}$$

In MAPLE we represent the generalized eta-product

$$\eta_{N;g_1}(\tau)^{r_1}\,\eta_{N;g_2}(\tau)^{r_2}\,\cdots\,\eta_{N;g_m}(\tau)^{r_m}$$

symbolically by the list

$$[[N, g_1, r_1], [N, g_2, r_2] \ldots, [N, g_m, r_m]].$$

We call such a list a *geta-list*.

2.2 Symbolic Product Conversion

`jac2eprod` — Converts a quotient of theta-functions in `JAC` notation to a product of generalized eta-functions in `EETA` and `GETA` notation. We illustrate the use of this function using the Rogers–Ramanujan functions $G(q)$, $H(q)$ defined in (1.1). Before applying the `jac2eprod` function we first use the `jacprodmake` function from the `qseries` package to convert $G(q)$, $H(q)$ to `JAC` notation.

EXAMPLE:

```
> with(qseries):
> with(thetaids):
> G:=q->add(q^(n^2)/aqprod(q,q,n),n=0..10):
> H:=q->add(q^(n^2+n)/aqprod(q,q,n),n=0..10):
> JG:=jacprodmake(G(q),q,50);
```

$$\frac{JAC(0,5,\infty)}{JAC(1,5,\infty)}$$

```
> JH:=jacprodmake(H(q),q,50);
```

$$\frac{JAC(0,5,\infty)}{JAC(2,5,\infty)}$$

```
> JP:=jacprodmake(H(q)*G(q)^(11),q,80);
```

$$\frac{(JAC\,(0,5,\infty))^{12}}{(JAC\,(1,5,\infty))^{11}\,JAC\,(2,5,\infty)}$$

```
> GP:=jac2eprod(JP);
```

$$\frac{1}{(GETA\,(5,1))^{11}\,GETA\,(5,2)}$$

In the example above we found that

$$\mathrm{JG} = \frac{JAC(0,5,\infty)}{JAC(1,5,\infty)}, \quad \mathrm{JH} = \frac{JAC(0,5,\infty)}{JAC(2,5,\infty)}, \quad \mathrm{JP} = \frac{(JAC\,(0,5,\infty))^{12}}{(JAC\,(1,5,\infty))^{11}\,JAC\,(2,5,\infty)}.$$

This means that it appears that

$$\begin{aligned}
G(q) &= \prod_{n=0}^{\infty} \frac{(1-q^{5n})}{(1-q^{5n+1})(1-q^{5n+4})(1-q^{5n})} = \prod_{n=0}^{\infty} \frac{1}{(1-q^{5n+1})(1-q^{5n+4})},\\
H(q) &= \prod_{n=0}^{\infty} \frac{(1-q^{5n})}{(1-q^{5n+2})(1-q^{5n+3})(1-q^{5n})} = \prod_{n=0}^{\infty} \frac{1}{(1-q^{5n+2})(1-q^{5n+3})},\\
H(q)\,G(q)^{11} &= \prod_{n=0}^{\infty} \frac{1}{(1-q^{5n+1})^{11}(1-q^{5n+4})^{11}(1-q^{5n+2})(1-q^{5n+3})},
\end{aligned}$$

as expected. The `jac2eprod` function was used to convert this last function to symbolic `GETA` notation.

`jac2getaprod` — Converts a quotient of theta-function in `JAC` notation to a product of generalized eta-functions in standard notation.

EXAMPLE:

```
> jac2getaprod(JP);
```

$$\frac{1}{\eta_{5,1}\,(\tau)^{11}\,\eta_{5,2}\,(\tau)}$$

`GETAP2getalist` — Converts a product of generalized eta-functions into a list as described above.

EXAMPLE:
```
> GETAP2getalist(GP);
```

$$[[5, 1, -11], [5, 2, -1]]$$

The list `[[5, 1, -11], [5, 2, -1]]` simply corresponds to

$$(GETA\,(5, 1))^{-11}\, GETA\,(5, 2)^{-1} = \frac{1}{\eta_{5,1}\,(\tau)^{11}\,\eta_{5,2}\,(\tau)}.$$

2.3 Processing Theta-Functions

There are two main functions in the `thetaids` package for processing combinations of theta-functions.

`mixedjac2jac` — Converts a sum of quotients of theta-functions written in terms of `JAC(a,b,infinity)` to a sum with the same base `b`. The functions `jac2series` and `jacprodmake` from the `qseries` package are used.

EXAMPLE:
```
>Y1:=1+jacprodmake(G(q),q,100)*jacprodmake(H(q^2),q,100);
```

$$1 + \frac{JAC\,(0, 5, \infty)\,JAC\,(0, 10, \infty)}{JAC\,(1, 5, \infty)\,JAC\,(4, 10, \infty)}$$

```
> Y2:=mixedjac2jac(Y1);
```

$$1 + \frac{(JAC\,(0, 10, \infty))^3}{JAC\,(1, 10, \infty)\,(JAC\,(4, 10, \infty))^2}$$

`processjacid` — Processes a theta-function identity written as a rational function of `JAC`-functions using `mixedjac2jac` and renormalizing by dividing by the term with the lowest power of q.

As an example, we consider the well-known identity

$$\theta_3(q)^4 = \theta_2(q)^4 + \theta_4(q)^4. \tag{2.6}$$

EXAMPLE:
```
> with(qseries):
> with(thetaids):
> F1:=theta2(q,100)^4:
> F2:=theta3(q,100)^4:
> F3:=theta4(q,100)^4:
> findhom([F1,F2,F3],q,1,0);
```

$$\{X_1 - X_2 + X_3\}$$

```
> JACID0:=qs2jaccombo(F1-F2+F3,q,100);
```

$$16\,\frac{q\,(JAC\,(0,4,\infty))^6}{(JAC\,(2,4,\infty))^2} - \frac{(JAC\,(0,4,\infty))^6\,(JAC\,(2,4,\infty))^6}{(JAC\,(1,4,\infty))^8} + (JAC\,(1,2,\infty))^4$$

```
> JACID1:=processjacid(JACID0);
```

$$-16\,\frac{q\,(JAC\,(1,4,\infty))^8}{(JAC\,(2,4,\infty))^8} + 1 - \frac{(JAC\,(1,4,\infty))^{16}}{(JAC\,(0,4,\infty))^{12}\,(JAC\,(2,4,\infty))^4}$$

```
> expand(jac2getaprod(JACID1));
```

$$-\frac{\eta_{4;1}(\tau)^{16}}{\eta_{4;2}(\tau)^4} + 1 - 16\,\frac{\eta_{4;1}(\tau)^8}{\eta_{4;2}(\tau)^8}$$

We see that (2.6) is equivalent to the identity

$$\frac{\eta_{4;1}(\tau)^{16}}{\eta_{4;2}(\tau)^4} + 16\,\frac{\eta_{4;1}(\tau)^8}{\eta_{4;2}(\tau)^8} = 1. \tag{2.7}$$

2.4 Checking Modularity

Robins [21] has found sufficient conditions under which a generalized eta-product is a modular function on $\Gamma_1(N)$.

Theorem 2.1 ([21] Theorem 3) *The function $f(\tau)$, defined in (2.4), is a modular function on $\Gamma_1(N)$ if* *(i)* $\sum_{\substack{\delta|N\\g}} \delta P_2(\frac{g}{\delta}) r_{\delta,g} \equiv 0 \pmod 2$, *and*

(ii) $\sum_{\substack{\delta|N\\g}} \frac{N}{\delta} P_2(0) r_{\delta,g} \equiv 0 \pmod 2$.

The functions on the left side of (i), (ii) above are computed using the MAPLE functions `vinf` and `v0` respectively. Suppose $f(\tau)$ is given as in (2.4) and this generalized eta-product is encoded as the geta-list L. Recall that each item in the list L has the form $[\delta, g, r_{\delta,g}]$. The syntax is `vinf(L,N)` and `v0(L,N)`. As an example we consider the two generalized eta-products in (2.7).

EXAMPLE:
```
> L1:=[[4,1,16],[4,2,-4]];
```

$$[[4, 1, 16], [4, 2, -4]]$$

```
> vinf(L1,4),v0(L1,4);
```

$$0, 2$$

```
> L2:=[[4,1,8],[4,2,-8]];
```

$$[[4, 1, 8], [4, 2, -8]]$$

```
> vinf(L2,4),v0(L2,4);
```

$$2, 0$$

The numbers 0, 2 are even and we see that both generalized eta-products in (2.7) are modular functions on $\Gamma_1(4)$ by Theorem 2.1.

`Gamma1ModFunc(L,N)` — Checks whether a given generalized eta-product is a modular function on $\Gamma_1(N)$. Here the generalized eta-product is encoded as the geta-list L. The function first checks whether each δ is a divisor of N and checks whether both `vinf(L,N)` and `v0(L,N)` are even. It returns 1 if it is a modular function on $\Gamma_1(N)$ otherwise it returns 0. If the global variable `xprint` is set to *true* then more detailed information is printed. Thus here and throughout `xprint` can be used for debugging purposes.

EXAMPLE:
```
> Gamma1ModFunc(L1,4);
```

$$1$$

```
> xprint := true:
> Gamma1ModFunc(L1,4);
* starting Gamma1ModFunc with L=[[4, 1, 16], [4, 2,
-4]] and N=4
All n are divisors of 4
val0=2
which is even.
valinf=0
which is even.
It IS a modfunc on Gamma1(4)
```

$$1$$

2.5 Cusps

Cho, Koo and Park [8] have found a set of inequivalent cusps for $\Gamma_1(N) \cap \Gamma_0(mN)$. The group $\Gamma_1(N)$ corresponds to the case $m = 1$.

Theorem 2.2 ([8] Corollary 4, p. 930) *Let a, c, a', $c \in \mathbb{Z}$ with $(a, c) = (a', c') = 1$.*

(i) The cusps $\frac{a}{c}$ and $\frac{a'}{c'}$ are equivalent mod $\Gamma_1(N)$ if and only if

$$\begin{pmatrix} a' \\ c' \end{pmatrix} \equiv \pm \begin{pmatrix} a + nc \\ c \end{pmatrix} \pmod{N}$$

for some integer n.

(ii) The following is a complete set of inequivalent cusps mod $\Gamma_1(N)$.

$$\begin{aligned} \mathscr{S} = \Bigg\{ \frac{y_{c,j}}{x_{c,i}} &: 0 < c \mid N,\ 0 < s_{c,i},\ a_{c,j} \le N,\ (s_{c,i}, N) = (a_{c,j}, N) = 1, \\ & s_{c,i} = s_{c,i'} \iff s_{c,1} \equiv \pm s_{c',i'} \pmod{\tfrac{N}{c}}, \\ & a_{c,j} = a_{c,j'} \iff \begin{cases} a_{c,j} \equiv \pm a_{c,j'} \pmod{c}, & \text{if } c = \frac{N}{2} \text{ or } N, \\ a_{c,j} \equiv a_{c,j'} \pmod{c}, & \text{otherwise}, \end{cases} \\ & x_{c,i}, y_{c,j} \in \mathbb{Z} \text{ chosen s.th. } x_{c,i} \equiv c s_{c,i},\ y_{c,j} \equiv a_{c,j} \pmod{N},\ (x_{c,i}, y_{c,j}) = 1 \Bigg\}, \end{aligned}$$

(iii) and the fan width of the cusp $\frac{a}{c}$ *is given by*

$$\kappa(\tfrac{a}{c}, \Gamma_1(N)) = \begin{cases} 1, & \text{if } N = 4 \text{ and } (c,4) = 2, \\ \frac{N}{(c,N)}, & \text{otherwise.} \end{cases}$$

In this theorem, it is understood as usual that the fraction $\frac{\pm 1}{0}$ corresponds to ∞.

`cuspequiv1`(a_1, c_1, a_2, c_2, N) — determines whether the cusps a_1/c_1 and a_2/c_2 are $\Gamma_1(N)$-equivalent using Theorem 2.2(i).

EXAMPLE:

```
> cuspequiv1(1,3,1,9,40);
```

$$false$$

```
> cuspequiv1(1,9,2,9,40);
```

$$true$$

We see that modulo $\Gamma_1(40)$ the cusps $\frac{1}{3}$ and $\frac{1}{9}$ are inequivalent and the cusps $\frac{1}{9}$ and $\frac{2}{9}$ are equivalent.

`Acmake(c,N)` — returns the set $\{a_{c,j}\}$ where c is a positive divisor of N.

`Scmake(c,N)` — returns the set $\{s_{c,i}\}$ where c is a positive divisor of N.

`newxy(x,y,N)` — returns $[x_1, y_1]$ for given $(x, y, N) = 1$ such that $x_1 \equiv x \pmod{N}$ and $y_1 \equiv y \pmod{N}$.

`cuspmake1(N)` — returns a set of inequivalent cusps for $\Gamma_1(N)$ using Theorem 2.2. Each cusp a/c in the list is represented by $[a, c]$, so that ∞ is represented by $[1, 0]$. This MAPLE procedure uses the functions `Acmake`, `Scmake` and `newxy`.

`cuspwid1(a,c,N)` — returns the width of the cusp a/c for the group $\Gamma_1(N)$ using Theorem 2.2(iii).

EXAMPLE:

```
> C10:=cuspmake1(10);
```

$$\{[0,1],[1,0],[1,2],[1,3],[1,4],[1,5],[2,5],[3,10]\}$$

```
> for L in C10 do lprint(L,cuspwid1(L[1],L[2],10));od;
    [0, 1], 10
    [1, 0], 1
```

```
    [1, 2], 5
    [1, 3], 10
    [1, 4], 5
    [1, 5], 2
    [2, 5], 2
    [3, 10], 1
```

We have the following table of cusps for $\Gamma_1(10)$.

cusp	cusp-width
0	10
∞	1
$\frac{1}{2}$	5
$\frac{1}{3}$	10
$\frac{1}{4}$	5
$\frac{1}{5}$	2
$\frac{2}{5}$	2
$\frac{3}{10}$	1

`CUSPSANDWIDMAKE(N)` — returns a set of inequivalent cusps for $\Gamma_1(N)$, and corresponding widths. Output has the form `[CUSPLIST,WIDTHLIST]`.

EXAMPLE:

```
> CUSPSANDWIDMAKE1(10);
```

$$\left[\left[oo, 0, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{5}, \frac{2}{5}, \frac{3}{10}\right], [1, 10, 5, 10, 5, 2, 2, 1]\right]$$

2.6 Orders at Cusps

We will use Biagioli's [6] results for theta-functions to calculate orders at cusps of generalized eta-products. We define the theta-function

$$\theta_{\delta;g}(\tau) = q^{(\delta-2g)^2/(8\delta)} \prod_{m=1}^{\infty} (1 - q^{m\delta-g})(1 - q^{m\delta-(\delta-g)})(1 - q^{m\delta}), \tag{2.8}$$

for $0 < g < \delta$. This corresponds to Biagioli's function $f_{\delta,g}$ [6, p. 277]. The classical Dedekind eta-function can be written as

$$\eta(\tau) = \theta_{3;1}(\tau), \tag{2.9}$$

and the generalized Dedekind eta-function can be written as

$$\eta_{\delta;g}(\tau) = \frac{\theta_{\delta;g}(\tau)}{\eta(\delta\tau)} = \frac{\theta_{\delta;g}(\tau)}{\theta_{3\delta;\delta}(\tau)}. \tag{2.10}$$

Biagioli [6] has calculated the invariant order of $\theta_{\delta;g}(\tau)$ at any cusp. Using (2.10) this gives a method for calculating the invariant order at any cusp of a generalized eta-product.

Theorem 2.3 ([6] Lemma 3.2, p. 285) *The order at the cusp $s = \frac{b}{c}$ (assuming $(b,c) = 1$) of the theta function $\theta_{g;\delta}(\tau)$ (defined above and assuming $\delta \nmid g$) is*

$$ord\,(\theta_{g;\delta}(\tau), s) = \frac{e^2}{2\delta}\left(\frac{bg}{e} - \left[\frac{bg}{e}\right] - \frac{1}{2}\right)^2, \tag{2.11}$$

where $e = (\delta, c)$ and $[\ \ ]$ is the greatest integer function.

`Bord`(δ, g, a, c) — returns the order of $\theta_{\delta;g}(\tau)$ at the cusp a/c, assuming $(a,c) = 1$ and $\delta \nmid g$.

`getacuspord`(δ, g, a, c) — returns the order of the generalized eta-function $\eta_{\delta,g}(\tau)$ at the cusp a/c, assuming $(a,c) = 1$ and $\delta \nmid g$.

EXAMPLE:

```
> getacuspord(50,1,4,29);
```

$$\frac{1}{600}$$

We see that

$$\text{ord}\left(\eta_{50;1}(\tau), \frac{4}{29}\right) = \frac{1}{600}.$$

Let G be a generalized eta-product corresponding to the getalist L. The following MAPLE procedure calculates the invariant order ord (G, ζ) for any cusp ζ.

`getaprodcuspord(L,cusp)` — returns of the generalized eta-product corresponding to the geta-list L at the given cusp. The cusp is either a rational or `oo` (infinity).

EXAMPLE:
```
> GL:=[[4,1,16],[4,2,-4]];
```
$$[[4, 1, 16], [4, 2, -4]]$$
```
> getaprodcuspord(GL,1/2);
```
$$-1$$

We see that
$$\text{ord}\left(\frac{\eta_{4;1}(\tau)^{16}}{\eta_{4;2}(\tau)^{4}}, \frac{1}{2}\right) = -1.$$

Following [6, p. 275], [19, p. 91] we consider the order of a function f with respect to a congruence subgroup Γ at the cusp $\zeta \in \mathbb{Q} \cup \{\infty\}$ and denote this by

$$\text{ORD}\,(f, \zeta, \Gamma) = \kappa(\zeta, \Gamma)\,\text{ord}\,(f, \zeta). \tag{2.12}$$

`getaprodcuspORDS`(L, S, W) — returns a list of orders ORD $(G, \zeta, \Gamma_1(N))$ where G is the generalized eta-product corresponding to the getalist L, $\zeta \in S$ (list of inequivalent cusps of $\Gamma_1(N)$) and W is a list of corresponding fan-widths.

EXAMPLE:
```
> CW4:=CUSPSANDWIDMAKE1(4);
```
$$\left[\left[\infty, 0, \frac{1}{2}\right], [1, 4, 1]\right]$$
```
> GL:=[[4,1,16],[4,2,-4]];
```
$$[[4, 1, 16], [4, 2, -4]]$$
```
> getaprodcuspORDS(GL,CW4[1],CW4[2]);
```
$$[0, 1, -1]$$

We know that the generalized eta-product

$$f(\tau) = \frac{\eta_{4;1}(\tau)^{16}}{\eta_{4;2}(\tau)^4}$$

is a modular function on $\Gamma_1(4)$. We calculated ORD $(f, \zeta, \Gamma_1(4))$ at each cusp ζ of $\Gamma_1(4)$.

ζ	ORD $(f, \zeta, \Gamma_1(4)$
∞	0
0	1
$\frac{1}{2}$	-1

Observe that the total order of f with respect to $\Gamma_1(4)$ is 0:

$$\text{ORD}\,(f, \Gamma_1(4)) = \sum_{\zeta \in \mathscr{S}} \text{ORD}\,(f, \zeta, \Gamma_1(4)) = 0 + 1 - 1 = 0,$$

in agreement with the valence formula. See Theorem 2.4 below. Here $\mathscr{S}$ is the set of inequivalent cusps of $\Gamma_1(4)$.

2.7 Proving Theta-Function Identities

Our method for proving theta-function or generalized eta-product identities depends on

Theorem 2.4 (The Valence Formula [19] (p. 98)) *Let $f \neq 0$ be a modular form of weight k with respect to a subgroup Γ of finite index in $\Gamma(1) = SL_2(\mathbb{Z})$. Then*

$$ORD\,(f, \Gamma) = \frac{1}{12}\mu\, k, \tag{2.13}$$

where μ is the index of $\widehat{\Gamma}$ in $\widehat{\Gamma(1)}$,

$$ORD\,(f, \Gamma) := \sum_{\zeta \in R^*} ORD\,(f, \zeta, \Gamma),$$

R^* is a fundamental region for Γ, and $ORD\,(f, \zeta, \Gamma)$ is given in Eq. (2.12).

Remark 2.1 For $\zeta \in \mathfrak{h}$, ORD (f, ζ, Γ) is defined in terms of the invariant order ord (f, ζ), which is interpreted in the usual sense. See [19, p. 91] for details of this and the notation used.

Since any generalized eta-product has weight $k = 0$ and has no zeros and no poles on the upper-half plane we have

Corollary 2.5 *Let $f_1(\tau)$, $f_2(\tau), \ldots, f_n(\tau)$ be generalized eta-products that are modular functions on $\Gamma_1(N)$. Let $\mathcal{S}_N$ be a set of inequivalent cusps for $\Gamma_1(N)$. Define the constant*

$$B = \sum_{\substack{s \in \mathcal{S}_N \\ s \neq \infty}} min\left(\left\{ORD\,(f_j, s, \Gamma_1(N)) \,:\, 1 \leq j \leq n\right\} \cup \{0\}\right), \tag{2.14}$$

and consider

$$g(\tau) := \alpha_1 f_1(\tau) + \alpha_2 f_2(\tau) + \cdots + \alpha_n f_n(\tau) + 1, \tag{2.15}$$

where each $\alpha_j \in \mathbb{C}$. Then

$$g(\tau) \equiv 0$$

if and only if

$$ORD\,(g(\tau), \infty, \Gamma_1(N)) > -B. \tag{2.16}$$

To prove an alleged theta-function identity, we first rewrite it in the form

$$\alpha_1 f_1(\tau) + \alpha_2 f_2(\tau) + \cdots + \alpha_n f_n(\tau) + 1 = 0, \tag{2.17}$$

where each $\alpha_i \in \mathbb{C}$ and each $f_i(\tau)$ is a generalized eta-product of level N. We use the following algorithm:

STEP 1. Use Theorem 2.1 to check that $f_j(\tau)$ is a generalized eta-product on $\Gamma_1(N)$ for each $1 \leq j \leq n$.

STEP 2. Use Theorem 2.2 to find a set $\mathcal{S}_N$ of inequivalent cusps for $\Gamma_1(N)$ and the fan width of each cusp.

STEP 3. Use Theorem 2.3 to calculate the invariant order of each generalized eta-product $f_j(\tau)$ at each cusp of $\Gamma_1(N)$.

STEP 4. Calculate

$$B = \sum_{\substack{s \in \mathcal{S}_N \\ s \neq \infty}} \min\left(\left\{\mathrm{ORD}\,(f_j, s, \Gamma_1(N)) \,:\, 1 \leq j \leq n\right\} \cup \{0\}\right).$$

STEP 5. Show that

$$\mathrm{ORD}\,(g(\tau), \infty, \Gamma_1(N)) > -B$$

where

$$g(\tau) = \alpha_1 f_1(\tau) + \alpha_2 f_2(\tau) + \cdots + \alpha_n f_n(\tau) + 1.$$

Corollary 2.5 then implies that $g(\tau) \equiv 0$ and hence the theta-function identity (2.17).

To calculate the constant B in (2.14) and STEP 4 we use

`mintotORDS(L,n)` — returns the constant B in Eq. (2.14) where L is an array of ORDS:

$$L := [\mathrm{ORD}\,(f_1), \mathrm{ORD}\,(f_2), \ldots, \mathrm{ORD}\,(f_n)],$$

where

$$\mathrm{ORD}\,(f) = [\mathrm{ORD}\,(f, \zeta_1, \Gamma_1(N)), \mathrm{ORD}\,(f, \zeta_2, \Gamma_1(N)), \ldots, \mathrm{ORD}\,(f, \zeta_m, \Gamma_1(N))]$$

and $\zeta_1, \zeta_2, \ldots, \zeta_m$ are the inequivalent cusps of $\Gamma_1(N)$. Each ORD (f) is computed using `getaprodcuspORDS`.

EXAMPLE: As an example we prove Ramanujan's well-known identity

$$\prod_{n=1}^{\infty} \frac{(1-q^n)}{(1-q^{25n})} = R(q^5) - q - \frac{q^2}{R(q^5)}, \tag{2.18}$$

where

$$R(q) = \prod_{n=1}^{\infty} \frac{(1-q^{5n-2})(1-q^{5n-3})}{(1-q^{5n-1})(1-q^{5n-4})}.$$

We rewrite this identity as

$$\frac{\eta(\tau)}{\eta(25\tau)} = \frac{\eta_{25;10}(\tau)}{\eta_{25;5}(\tau)} - 1 - \frac{\eta_{25;5}(\tau)}{\eta_{25;10}(\tau)}. \tag{2.19}$$

Let

$$g(\tau) = f_1(\tau) - f_2(\tau) + f_3(\tau) + 1, \tag{2.20}$$

where

$$f_1(\tau) = \frac{\eta(\tau)}{\eta(25\tau)} = \prod_{j=1}^{12} \eta_{25,j}(\tau), \quad f_2(\tau) = \frac{\eta_{25;10}(\tau)}{\eta_{25;5}(\tau)}, \quad f_3(\tau) = \frac{1}{f_2(\tau)} = \frac{\eta_{25;5}(\tau)}{\eta_{25;10}(\tau)}.$$

STEP 1. We check that each function is a modular function on $\Gamma_1(25)$.

```
> f1:=mul(GETA(25,j), j=1..12):
> f2:=GETA(25,10)/GETA(25,5):
> f3:=1/f2:
```

```
> GP1:=GETAP2getalist(f1):
> GP2:=GETAP2getalist(f2):
> GP3:=GETAP2getalist(f3):
> Gamma1ModFunc(GP1,25),Gamma1ModFunc(GP2,25),
      Gamma1ModFunc(GP3,25);
```

$$1, 1, 1$$

STEP 2. We find a set of inequivalent cusps for $\Gamma_1(25)$ and their fan widths.

```
> CW25:=CUSPSANDWIDMAKE1(25):
> cusps25:=CW25[1];
```

$$[oo, 0, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \frac{1}{5}, \frac{1}{6}, \frac{1}{7}, \frac{1}{8}, \frac{1}{9}, \frac{1}{10}, \frac{1}{11}, \frac{1}{12}, \frac{2}{5}, \frac{2}{25}, \frac{3}{5}, \frac{3}{10}, \frac{3}{25}, \frac{4}{5}, \frac{4}{25}, \frac{6}{25}, \frac{7}{10}, \frac{7}{25}, \frac{8}{25}, \frac{9}{10}, \frac{9}{25}, \frac{11}{25}, \frac{12}{25}]$$

```
> widths25:=CW25[2];
```

$$[1, 25, 25, 25, 25, 5, 25, 25, 25, 25, 5, 25, 25, 5, 1, 5, 5, 1, 5, 1, 1, 5, 1, 1, 5, 1, 1, 1]$$

STEP 3. We compute ORD $(f_j, \zeta, \Gamma_1(25))$ for each j and each cusp ζ of $\Gamma_1(25)$.

```
> ORDS1:=getaprodcuspORDS(GP1,cusps25,widths25);
```

$$[-1, 1, 1, 1, 1, 0, 1, 1, 1, 1, 0, 1, 1, 0, -1, 0, 0, -1, 0, -1, -1, 0, -1, -1, 0, -1, -1, -1]$$

```
> ORDS2:=getaprodcuspORDS(GP2,cusps25,widths25);
```

$$[-1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, -1, -1, 0, 1, 1, 0, -1, -1, 1]$$

```
> ORDS3:=getaprodcuspORDS(GP3,cusps25,widths25);
```

$$[1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1, 0, 0, -1, 0, 1, 1, 0, -1, -1, 0, 1, 1, -1]$$

STEP 4. We calculate the constant B in (2.14).

```
> mintotORDS([ORDS1,ORDS2,ORDS3],3);
```

$$-9$$

STEP 5. To prove the identity (2.18) we need to verify that

$$\mathrm{ORD}\,(g(\tau), \infty, \Gamma_1(25)) > 9.$$

```
> JACL:=map(getalist2jacprod,[GP1,GP2,GP3]):
> JACID:=JACL[1]-JACL[2]+JACL[3]+1:
> QJ:=jac2series(JACID,100):
> series(QJ,q,100);
```

$$\mathrm{O}\left(q^{99}\right)$$

This completes the proof of the identity (2.18). We only had to show that the coefficient of q^j was zero in the q-expansion of $g(\tau)$ for $j \le 10$. We actually did it for $j \le 98$ as a check.

STEPS 1–5 may be automated using

`provemodfuncid(JACID,N)` — returns the constant B in Eq. (2.14) and prints details of the verification and proof of the identity corresponding to `JACID`, which is a linear combination of symbolic `JAC`-functions, and N is the level. If `xprint=true` then more details of the verification are printed. When this function is called there is a query asking whether to verify the identity. Enter `yes` to carry out the verification.

EXAMPLE:

```
> provemodfuncid(JACID,25);
"TERM ", 1, "of ", 4, " *****************"
"TERM ", 2, "of ", 4, " *****************"
"TERM ", 3, "of ", 4, " *****************"
"TERM ", 4, "of ", 4, " *****************"
"mintotord = ", -9
"TO PROVE the identity we need to show that
v[oo](ID) > ", 9
*** There were NO errors.
```

```
*** o Each term was modular function on
Gamma1(25).
*** o We also checked that the total order of
each term was zero.
*** o We also checked that the power of q was
correct in
each term.
"*** WARNING: some terms were constants. ***"
"See array CONTERMS."
To prove the identity we will need to verify if up
to
q^(9).
Do you want to prove the identity? (yes/no)
You entered yes.
We verify the identity to O(q^(59)).
RESULT: The identity holds to O(q^(59)).
CONCLUSION: This proves the identity since we had
only
to show that v[oo](ID) > 9.
```

9

`provemodfuncidBATCH(JACID,N)` — is a version of `provemodfuncid` that prints less detail and does not query.

EXAMPLE:

```
> provemodfuncidBATCH(JACID,25);
*** There were NO errors. Each term was modular
function on
Gamma1(25). Also -mintotord=9. To prove the identity
we need to check up to O(q^(11)).
To be on the safe side we check up to O(q^(59)).
*** The identity is PROVED!
```

`printJACIDORDStable()` — prints an ORDs table for the f_j and lower bound for g after `provemodfuncid` is run. Formatted output from our example is given below in Table 1. By summing the last column we see that $B = -9$, which confirms an earlier calculation using `mintotORDS`.

Table 1 Orders at the cusps of $\Gamma_1(25)$ of the functions f_1, f_2, f_3 and g in (2.20) needed in the proof of Ramanujan's identity (2.19). This table was produced by `printJACIDORDStable()`

ζ	ORD (f_1, ζ)	ORD (f_2, ζ)	ORD (f_3, ζ)	Lower bound for ORD (g, ζ)
$\frac{1}{2}$	1	0	0	0
$\frac{1}{3}$	1	0	0	0
$\frac{1}{4}$	1	0	0	0
$\frac{1}{5}$	0	0	0	0
$\frac{1}{6}$	1	0	0	0
$\frac{1}{7}$	1	0	0	0
$\frac{1}{8}$	1	0	0	0
$\frac{1}{9}$	1	0	0	0
$\frac{1}{10}$	0	0	0	0
$\frac{1}{11}$	1	0	0	0
$\frac{1}{12}$	1	0	0	0
$\frac{2}{5}$	0	0	0	0
$\frac{2}{25}$	-1	1	-1	-1
$\frac{3}{5}$	0	0	0	0
$\frac{3}{10}$	0	0	0	0
$\frac{3}{25}$	-1	1	-1	-1
$\frac{4}{5}$	0	0	0	0
$\frac{4}{25}$	-1	-1	1	-1
$\frac{6}{25}$	-1	-1	1	-1
$\frac{7}{10}$	0	0	0	0
$\frac{7}{25}$	-1	1	-1	-1
$\frac{8}{25}$	-1	1	-1	-1
$\frac{9}{10}$	0	0	0	0
$\frac{9}{25}$	-1	-1	1	-1
$\frac{11}{25}$	-1	-1	1	-1
$\frac{12}{25}$	-1	1	-1	-1

3 Generalized Ramanujan–Robins Identities

As an application of our `thetaids` package we show how to find and prove generalized eta-product identities due to Ramanujan and Robins, and some natural extensions. In Sect. 1 we defined the functions $G(n, N, \chi)$ and $H(n, N, \chi)$, where χ is a non-principal real Dirichlet character mod N satisfying $\chi(-1) = 1$. Robins [20] proved the following striking analogue of Ramanujan's identity (1.3) (or (1.6)):

$$G(3)\,H(1) - G(1)\,H(3) = 1, \tag{3.1}$$

where

$$G(n) = \frac{1}{\eta_{13;1,3,4}(n\tau)}, \quad H(n) = \frac{1}{\eta_{13;2,5,6}(n\tau)}.$$

Equation (3.1) is a restatement of (1.8). In this case $N = 13$ and $\chi = \left(\frac{\cdot}{13}\right)$ is the Legendre symbol.

We will also consider

$$G^*(n, N, \chi) = G^*(n) := \prod_{\substack{\chi(g)=1\\ 0<g<\frac{N}{2}}} \frac{1}{\eta^*_{N;g}(n\tau)}, \quad H^*(n, N, \chi) = H^*(n) := \prod_{\substack{\chi(g)=-1\\ 0<g<\frac{N}{2}}} \frac{1}{\eta^*_{N;g}(n\tau)}, \tag{3.2}$$

where

$$\eta^*_{\delta;g}(\tau) = q^{\frac{\delta}{2}P_2(g/\delta)} \prod_{m\equiv\pm g \pmod{\delta}} (1 - (-q)^m). \tag{3.3}$$

We note that

$$\eta^*_{\delta;g}(\tau) = \omega_{\delta;g}\eta_{\delta;g}(\tau + \pi i),$$

where $\omega_{\delta;g}$ is a root of unity. Using the notation (1.10) (with $N = 5$ and $\chi(\cdot) = \left(\frac{\cdot}{5}\right)$, the Legendre symbol) we may rewrite Ramanujan's identities (1.2), (1.3) as

$$\begin{aligned} &G(1)^{11}H(1) - G(1)H(1)^{11} = 1 + 11G(1)^6H(1)^6,\\ &H(1)G(11) - G(1)H(11) = 1, \end{aligned}$$

respectively.

We have written a number of specialized functions for the purpose of finding and proving identities for these more general G- and H-functions. We have collected these functions into the new `ramarobinsids` package. Go to

http://qseries.org/fgarvan/qmaple/ramarobinsids

and follow the directions on that page. This package requires both the `qseries` and `thetaids` packages.

3.1 Some MAPLE Functions

`Geta(g,d,n)` — returns the generalized eta-function $\eta_{d;g}(n\tau)$ in symbolic `JAC`-form.

`GetaB(g,d,n)` — returns `Geta(g,d,n)` without the the $q^{\frac{d}{2}P_2(g/d)}$ factor.

`GetaL(L,d,n)` — returns the generalized eta-product corresponding to the geta-list in `JAC`-form with τ replaced by $n\tau$.

`GetaBL(L,d,n)` — returns the generalized eta-product `GetaL(g,d,n)` without the q-factor.

`GetaEXP(g,d,n)` — returns lowest power of q in $\eta_{d;g}(n\tau)$.

`GetaLEXP(L,d,n)` — returns lowest power of q for the generalized eta-product corresponding to `GetaL(L,d,n)`.

`MGeta(g,d,n)` — η^* analogue of `Geta(g,d,n)`

`MGetaL(L,d,n)` — η^* analogue of `GetaL(L,d,n)`

`Eeta(n)` — returns Dedekind eta-function $\eta(n\tau)$ in `JAC`-form.

EXAMPLE:

```
> with(ramarobinsids):
> Geta(1,5,2);
```

$$\frac{q^{1/30}JAC(2,10,\infty)}{JAC(0,10,\infty)}$$

```
> GetaB(1,5,2);
```

$$\frac{JAC(2,10,\infty)}{JAC(0,10,\infty)}$$

```
> GetaEXP(1,5,2);
```

$$\frac{1}{30}$$

```
> GetaL([1,3,4],13,1);
```

$$\frac{q^{1/4}}{JAC(0,13,\infty)^3}JAC(1,13,\infty)JAC(3,13,\infty)JAC(4,13,\infty)$$

```
> GetaLB([1,3,4],13,1);
```

$$\frac{JAC(1,13,\infty)JAC(3,13,\infty)JAC(4,13,\infty)}{JAC(0,13,\infty)^3}$$

```
> GetaLEXP([1,3,4],13,1);
```

$$\frac{1}{4}$$

```
> MGeta(1,5,2);
```

$$\frac{q^{1/30} JAC(2,10,\infty)\, JAC(4,40,\infty)\, (JAC(0,20,\infty))^2}{JAC(0,10,\infty)\, JAC(0,40,\infty)\, (JAC(2,20,\infty))^2}$$

```
> MGetaL([1,3,4],13,1);
```

$$\frac{\sqrt[4]{q} JAC(1,13,\infty)\, JAC(2,52,\infty)\, JAC(0,26,\infty)\, JAC(3,13,\infty)\, JAC(6,52,\infty)}{JAC(0,13,\infty)\, JAC(0,52,\infty)\, (JAC(1,26,\infty))^2\, (JAC(3,26,\infty))^2}$$
$$\frac{(JAC(4,26,\infty))^2\, JAC(8,26,\infty)}{JAC(4,13,\infty)\, JAC(8,52,\infty)}$$

```
> Eeta(3);
```

$$q^{1/8} JAC(0,3,\infty)$$

`CHECKRAMIDF(SYMF,ACC,T)` — checks whether a certain symbolic expression of G- and H-functions is an eta-product. This assumes that $G(n)$, $H(n)$, $GM(n)$, $HM(n)$ have already been defined. GM and HM are the η^* analogues of G, H. The `SYMF` symbolic form is written in terms of $\_G$, $\_H$, $\_GM$, $\_HM$. `ACC` is an upperbound on the absolute value of exponents allowed in the formal product, `T` is highest power of q considered. This procedure returns a list of exponents in the formal product if it is a likely eta-product otherwise it returns `NULL`. A number of global variables are also assigned. The main ones are

- `_JFUNC`: `JAC`-expression of `SYMF`.
- `LQD`: lowest power of q.
- `RID`: the conjectured eta-product.
- `ebase`: base of the conjectured eta-product.
- `SYMID`: symbolic form of the identity

EXAMPLE:

```
> with(qseries):
> with(thetaids):
> with(ramarobinsids):
> G:=j->1/GetaL([1,3,4],13,j): H:=j->1/GetaL([2,5,6],13,j):
> GM:=j->1/MGetaL([1,3,4],13,j): HM:=j->1/MGetaL([2,5,6],13,j):
> GE:=j->-GetaLEXP([1,3,4],13,j):HE:=j->-GetaLEXP([2,5,6],13,j):
> GHID:=(_G(1)*_G(2)+_H(1)*_H(2))/(_G(2)*_H(1)-_G(1)*_H(2));
```

$$GHID := \frac{\_G(1)\,\_G(2) + \_H(1)\,\_H(2)}{\_G(2)\,\_H(1) - \_G(1)\,\_H(2)}$$

```
> CHECKRAMIDF(GHID,10,50);
```

$$[-2, 0, -2, 0, -2, 0, -2, 0, -2, 0, -2, 0, 0, 0, -2, 0, -2, 0, \\ -2, 0, -2, 0, -2, 0, -2, 0, -2, 0, -2, 0, -2, 0, -2, 0, -2, 0, -2, 0, 0]$$

```
> ebase;
```

$$26$$

```
> _JFUNC;
```

$$(-q^3 JAC(1,13,\infty)\, JAC(3,13,\infty)\, JAC(4,13,\infty)\, JAC(2,26,\infty)\, JAC(6,26,\infty)\, JAC(8,26,\infty) \\ - JAC(2,13,\infty)\, JAC(5,13,\infty)\, JAC(6,13,\infty)\, JAC(4,26,\infty)\, JAC(10,26,\infty)\, JAC(12,26,\infty)) \\ /q\,(q JAC(2,26,\infty)\, JAC(6,26,\infty)\, JAC(8,26,\infty)\, JAC(2,13,\infty)\, JAC(5,13,\infty)\, JAC(6,13,\infty) \\ - JAC(1,13,\infty)\, JAC(3,13,\infty)\, JAC(4,13,\infty)\, JAC(4,26,\infty)\, JAC(10,26,\infty)\, JAC(12,26,\infty))$$

```
> LDQ;
```

$$-1$$

```
> RID;
```

$$\frac{(\eta(13\tau))^2 (\eta(2\tau))^2}{(\eta(26\tau))^2 (\eta(\tau))^2}$$

```
> SYMID;
```

$$\frac{\_G(1)\_G(2) + \_H(1)\_H(2)}{\_G(2)\_H(1) - \_G(1)\_H(2)} = \frac{(\eta(13\tau))^2 (\eta(2\tau))^2}{(\eta(26\tau))^2 (\eta(\tau))^2}$$

```
> etamake(jac2series(_JFUNC,1001),q,1001);
```

$$\frac{\eta(13\tau)^2 \eta(2\tau)^2}{\eta(26\tau)^2 \eta(\tau)^2}$$

It seems that

$$\frac{G(1)G(2) + H(1)H(2)}{G(2)H(1) - G(1)H(2)} = \frac{\eta(13\tau)^2 \eta(2\tau)^2}{\eta(26\tau)^2 \eta(\tau)^2} \tag{3.4}$$

when $N = 13$ and $\chi(\cdot) = \left(\frac{\cdot}{13}\right)$, at least up to q^{1000}.

EXAMPLE:

```
> RRID1:=_JFUNC-Eeta(13)^2*Eeta(2)^2/E8888eta(26)^2/Eeta(1)^2:
> JRID1:=processjacid(RRID1):
> jmxperiod;
```

$$26$$

```
> provemodfuncidBATCH(JRID1,26);
*** There were NO errors. Each term was modular
function on
Gamma1(26). Also -mintotord=18. To prove the
identity
we need to check up to O(q^(20)).
To be on the safe side we check up to O(q^(70)).
*** The identity is PROVED!
```

Thus identity (3.4) is proved.

The search for and proof of such identities may be automated.

3.2 Ten Types of Identities for Ramanujan's Functions $G(q)$ and $H(q)$

We consider ten types of identities. We write a MAPLE function to search for and prove identities of each type. Here we assume $N = 5$ and $\chi(\cdot) = \left(\frac{\cdot}{5}\right)$. We continue to use the notation (1.10).

In this section

$$G(1) = G(1, 5, \left(\frac{\cdot}{5}\right)) = \frac{1}{\eta_{5;1}(\tau)} = \frac{q^{-1/60}}{(q, q^4; q^5)_\infty}, \quad \text{and}$$
$$H(1) = H(1, 5, \left(\frac{\cdot}{5}\right)) = \frac{1}{\eta_{5;2}(\tau)} = \frac{q^{11/60}}{(q^2, q^3; q^5)_\infty}.$$

EXAMPLE:
```
> with(qseries):
> with(thetaids):
> with(ramarobinsids):
> G:=j->1/GetaL([1],5,j): H:=j->1/GetaL([2],5,j):
> GM:=j->1/MGetaL([1],5,j): HM:=j->1/MGetaL([2],5,j):
> GE:=j->-GetaLEXP([1],5,j): HE:=j->-GetaLEXP([2],5,j):
```

3.2.1 Type 1

We consider identities of the form

$$G(a)\,H(b) \pm G(b)\,H(a) = f(\tau),$$

where $f(\tau)$ is an eta-product and a, b are positive relatively prime integers.

`findtype1(T)` — cycles through symbolic expressions

$$\_G(a)\,\_H(b) + c\,\_G(b)\,\_H(a)$$

where $2 \le n \le T$, $ab = n$, $(a, b) = 1$, $b < a$, $c \in \{-1, 1\}$, and

$$\mathtt{GE}(a) + \mathtt{HE}(b) - (\mathtt{GE}(b) + \mathtt{HE}(a)) = \frac{1}{5}(b - a) \in \mathbb{Z}, \tag{3.5}$$

using `CHECKRAMIDF` to check whether the expression corresponds to a likely eta-product, and if so uses `provemodfuncidBATCH` to prove it. Condition (3.5) eliminates the case of fractional powers of q, which in our case means $a \equiv b \mod 5$. The procedure also returns a list of `[a,b,c]` which give identities.

EXAMPLE:

```
> proveit:=true:
> findtype1(11);
*** There were NO errors. Each term was modular
function on
Gamma1(30). Also -mintotord=8. To prove the identity
we need to check up to O(q^(10)).
To be on the safe side we check up to O(q^(68)).
*** The identity below is PROVED!
[6, 1, -1]
```

$$\_G(6)\_H(1) - \_G(1)\_H(6) = \frac{\eta(6\tau)\eta(\tau)}{\eta(3\tau)\eta(2\tau)}$$

```
*** There were NO errors. Each term was modular
function on
Gamma1(55). Also -mintotord=40. To prove the
identity
we need to check up to O(q^(42)).
To be on the safe side we check up to O(q^(150)).
*** The identity below is PROVED!
[11, 1, -1]
```

$$\_G(11)\_H(1) - \_G(1)\_H(11) = 1$$

$$[[6, 1, -1], [11, 1, -1]]$$

```
> myramtype1 :=findtype1(36);
```

$myramtype1 := [[6, 1, -1], [11, 1, -1], [7, 2, -1], [16, 1, -1], [8, 3, -1], [9, 4, -1], [36, 1, -1]]$

This also produced the following identities with proofs (some output omitted):

$$G(6)\,H(1) - G(1)\,H(6) = \frac{\eta(\tau)\eta(6\tau)}{\eta(2\tau)\eta(3\tau)}, \qquad \Gamma_1(30), \qquad -B = 8, \tag{3.6}$$

$$G(11)\,H(1) - G(1)\,H(11) = 1, \qquad \Gamma_1(55), \qquad -B = 40, \tag{3.7}$$

$$G(7)\,H(2) - G(2)\,H(7) = \frac{\eta(\tau)\eta(14\tau)}{\eta(2\tau)\eta(7\tau)}, \qquad \Gamma_1(70), \qquad -B = 48, \tag{3.8}$$

$$G(16)\,H(1) - G(1)\,H(16) = \frac{\eta(4\tau)^2}{\eta(2\tau)\eta(8\tau)}, \qquad \Gamma_1(80), \qquad -B = 64, \tag{3.9}$$

$$G(8)\,H(3) - G(3)\,H(8) = \frac{\eta(\tau)\eta(4\tau)\eta(6\tau)\eta(24\tau)}{\eta(2\tau)\eta(3\tau)\eta(8\tau)\eta(12\tau)}, \qquad \Gamma_1(120), \qquad -B = 128, \tag{3.10}$$

$$G(9)\,H(4) - G(4)\,H(9) = \frac{\eta(\tau)\eta(6\tau)^2\eta(36\tau)}{\eta(2\tau)\eta(3\tau)\eta(12\tau)\eta(18\tau)}, \qquad \Gamma_1(180), \qquad -B = 288, \tag{3.11}$$

$$G(36)\,H(1) - G(1)\,H(36) = \frac{\eta(4\tau)\eta(6\tau)^2\eta(9\tau)}{\eta(2\tau)\eta(3\tau)\eta(12\tau)\eta(18\tau)}, \qquad \Gamma_1(180), \qquad -B = 288. \tag{3.12}$$

We have included the relevant groups $\Gamma_1(N)$ and values of B (see (2.14) and (2.16)). These identities are known and are Eqs. (3.9), (3.5), (3.10), (3.6), (3.12), (3.14), and (3.15) in [5] respectively.

3.2.2 Type 2

We consider identities of the form

$$G(a)\,G(b) \pm H(a)\,H(b) = f(\tau),$$

where $f(\tau)$ is an eta-product and a, b are positive relatively prime integers.

`findtype2(T)` — cycles through symbolic expressions

$$\_G(a)\,\_G(b) + c\,\_H(a)\,\_H(b)$$

where $2 \leq n \leq T$, $ab = n$, $(a, b) = 1$, $a \leq b$, $c \in \{-1, 1\}$, and

$$\mathtt{GE}(a) + \mathtt{GE}(b) - (\mathtt{HE}(a) + \mathtt{HE}(b)) = -\frac{1}{5}\,(a + b) \in \mathbb{Z}, \tag{3.13}$$

using `CHECKRAMIDF` to check whether the expression corresponds to a likely eta-product, and if so uses `provemodfuncidBATCH` to prove it. Condition (3.13) eliminates the case of fractional powers of q, which in our case means $a \equiv -b \bmod 5$. The procedure also returns a list of `[a,b,c]` which give identities.

```
> findtype2(24);
```

$$[[1, 4, -1], [1, 4, 1], [2, 3, 1], [1, 9, 1], [1, 14, 1], [1, 24, 1]]$$

This also produces the following identities with proofs:

$$G(1)\,G(4) - H(1)\,H(4) = \frac{\eta(10\tau)^5}{\eta(2\tau)\eta(5\tau)^2\eta(20\tau)^2}, \qquad \Gamma_1(20), \qquad -B = 4, \tag{3.14}$$

$$G(1)\,G(4) + H(1)\,H(4) = \frac{\eta(2\tau)^4}{\eta(\tau)^2\eta(4\tau)^2}, \qquad \Gamma_1(20), \qquad -B = 4, \tag{3.15}$$

$$G(2)\,G(3) + H(2)\,H(3) = \frac{\eta(2\tau)\eta(3\tau)}{\eta(\tau)\eta(6\tau)}, \qquad \Gamma_1(30), \qquad -B = 8, \tag{3.16}$$

$$G(1)\,G(9) + H(1)\,H(9) = \frac{\eta(3\tau)^2}{\eta(\tau)\eta(9\tau)}, \qquad \Gamma_1(45), \qquad -B = 24, \tag{3.17}$$

$$G(1)\,G(14) + H(1)\,H(14) = \frac{\eta(2\tau)\eta(7\tau)}{\eta(\tau)\eta(14\tau)}, \qquad \Gamma_1(70), \qquad -B = 48, \tag{3.18}$$

$$G(1)\,G(24) + H(1)\,H(24) = \frac{\eta(2\tau)\eta(3\tau)\eta(8\tau)\eta(12\tau)}{\eta(\tau)\eta(4\tau)\eta(6\tau)\eta(24\tau)}, \qquad \Gamma_1(120), \qquad -B = 128, \tag{3.19}$$

These identities are known and are Eqs. (3.4), (3.3), (3.8), (3.7), (3.11), and (3.13) in [5] respectively.

3.2.3 Type 3

We consider identities of the form

$$\frac{G(a_1)\,G(b_1) \pm H(a_1)\,H(b_1)}{G(a_2)\,H(b_2) \pm H(a_2)\,G(b_2)} = f(\tau),$$

which are not a quotient of Type 1 and 2 identities, and where $f(\tau)$ is an eta-product, a_1, b_1, a_2, b_2 are positive relatively prime integers, and $a_1 b_1 = a_2 b_2$.

`findtype3(T)` — cycles through symbolic expressions

$$\frac{\_G(a_1)\,\_G(b_1) + c_1\,\_H(a_1)\,\_H(b_1)}{\_G(a_2)\,\_H(b_2) + c_2\,\_H(a_2)\,\_G(b_2)}$$

where $2 \le n \le T$, $a_1 b_1 = a_2 b_2 = n$, $(a_1, b_1, a_2, b_2) = 1$, $a_1 \le b_1$, $b_2 < a_2$, $c_1, c_2 \in \{-1, 1\}$, and

$$\mathtt{GE}(a_1) + \mathtt{GE}(b_1) - (\mathtt{HE}(a_1) + \mathtt{HE}(b_1)), \quad \mathtt{GE}(a_2) + \mathtt{HE}(b_2) - (\mathtt{HE}(a_2) + \mathtt{GE}(b_2) \in \mathbb{Z}, \tag{3.20}$$

and $[a_2, b_2, c_2]$ is not an element of the list `myramtype1` (found earlier by `findtype1`), using `CHECKRAMIDF` to check whether the expression corresponds to a likely eta-product, and if so uses `provemodfuncidBATCH` to prove it. The procedure also returns lists $[a_1, b_1, c_1, a_2, b_2, c_2]$ which correspond to identities.

```
> findtype3(126);
```

$$[[3, 7, 1, 21, 1, -1], [2, 13, 1, 26, 1, -1], [1, 34, 1, 17, 2, -1], [1, 39, 1, 13, 3, -1],$$
$$[1, 54, 1, 27, 2, -1], [7, 8, 1, 56, 1, -1], [3, 22, 1, 11, 6, -1], [2, 33, 1, 66, 1, -1],$$
$$[4, 21, 1, 12, 7, -1], [1, 84, 1, 28, 3, -1], [3, 32, 1, 96, 1, -1], [7, 18, 1, 14, 9, -1],$$
$$[2, 63, 1, 126, 1, -1]]$$

This also produces the following identities with proofs:

$$\frac{G(3)\,G(7) + H(3)\,H(7)}{G(21)\,H(1) - H(21)\,G(1)} = 1, \qquad \Gamma_1(105), \qquad -B = 192, \tag{3.21}$$

$$\frac{G(2)\,G(13) + H(2)\,H(13)}{G(26)\,H(1) - H(26)\,G(1)} = 1, \qquad \Gamma_1(130), \qquad -B = 240, \tag{3.22}$$

$$\frac{G(1)\,G(34) + H(1)\,H(34)}{G(17)\,H(2) - H(17)\,G(2)} = \frac{\eta(2\tau)\eta(17\tau)}{\eta(\tau)\eta(34\tau)}, \qquad \Gamma_1(170), \qquad -B = 448, \tag{3.23}$$

$$\frac{G(1)\,G(39)+H(1)\,H(39)}{G(13)\,H(3)-H(13)\,G(3)}=\frac{\eta(3\tau)\eta(13\tau)}{\eta(\tau)\eta(39\tau)},\qquad \Gamma_1(195),\qquad -B=768, \tag{3.24}$$

$$\frac{G(1)\,G(54)+H(1)\,H(54)}{G(27)\,H(2)-H(27)\,G(2)}=\frac{\eta(2\tau)\eta(3\tau)\eta(18\tau)\eta(27\tau)}{\eta(\tau)\eta(6\tau)\eta(9\tau)\eta(54\tau)},\quad \Gamma_1(270),\quad -B=1008, \tag{3.25}$$

$$\star\quad \frac{G(7)\,G(8)+H(7)\,H(8)}{G(56)\,H(1)-H(56)\,G(1)}=\frac{\eta(2\tau)\eta(28\tau)}{\eta(4\tau)\eta(14\tau)},\qquad \Gamma_1(280),\qquad -B=1152, \tag{3.26}$$

$$\frac{G(3)\,G(22)+H(3)\,H(22)}{G(11)\,H(6)-H(11)\,G(6)}=\frac{\eta(2\tau)\eta(33\tau)}{\eta(\tau)\eta(66\tau)},\qquad \Gamma_1(330),\qquad -B=1600, \tag{3.27}$$

$$\frac{G(2)\,G(33)+H(2)\,H(33)}{G(66)\,H(1)-H(66)\,G(1)}=\frac{\eta(3\tau)\eta(22\tau)}{\eta(6\tau)\eta(11\tau)},\qquad \Gamma_1(330),\qquad -B=1600, \tag{3.28}$$

$$\star\quad \frac{G4)\,G(21)+H(4)\,H(21)}{G(12)\,H(7)-H(12)\,G(7)}=\frac{\eta(2\tau)\eta(3\tau)\eta(7\tau)\eta(12\tau)\eta(28\tau)\eta(42\tau)}{\eta(\tau)\eta(4\tau)\eta(6\tau)\eta(14\tau)\eta(21\tau)\eta(84\tau)},\quad \Gamma_1(420),\quad -B=2688, \tag{3.29}$$

$$\star\quad \frac{G(1)\,G(84)+H(1)\,H(84)}{G(28)\,H(3)-H(28)\,G(3)}=\frac{\eta(2\tau)\eta(3\tau)\eta(7\tau)\eta(12\tau)\eta(28\tau)\eta(42\tau)}{\eta(\tau)\eta(4\tau)\eta(6\tau)\eta(14\tau)\eta(21\tau)\eta(84\tau)},\quad \Gamma_1(420),\quad -B=2688, \tag{3.30}$$

$$\star\quad \frac{G(3)\,G(32)+H(3)\,H(32)}{G(96)\,H(1)-H(96)\,G(1)}=\frac{\eta(2\tau)\eta(8\tau)\eta(12\tau)\eta(48\tau)}{\eta(4\tau)\eta(6\tau)\eta(16\tau)\eta(24\tau)},\quad \Gamma_1(480),\quad -B=3072, \tag{3.31}$$

$$\star\quad \frac{G(7)\,G(18)+H(7)\,H(18)}{G(14)\,H(9)-H(14)\,G(9)}=\frac{\eta(2\tau)\eta(3\tau)\eta(42\tau)\eta(63\tau)}{\eta(\tau)\eta(6\tau)\eta(21\tau)\eta(126\tau)},\quad \Gamma_1(630),\quad -B=5760, \tag{3.32}$$

$$\frac{G(2)\,G(63)+H(2)\,H(63)}{G(126)\,H(1)-H(126)\,G(1)}=\frac{\eta(3\tau)\eta(7\tau)\eta(18\tau)\eta(42\tau)}{\eta(6\tau)\eta(9\tau)\eta(14\tau)\eta(21\tau)},$$
$$\Gamma_1(630),\quad -B=5760. \tag{3.33}$$

The equations marked ⋆ appear to be new. The other equations correspond to (3.16), (3.18), (3.35), (3.22), (3.41), (3.40) and (3.39) in [5], and (1.24) in [20] respectively. We have corrected the statement of equation [20, (1.24)].

3.2.4 Type 4

We consider identities of the form

$$G^*(a)\,H^*(b)\pm G^*(b)\,H^*(a)=f(\tau),$$

where $f(\tau)$ is an eta-product, a, b are positive relatively prime integers, and at least one of a, b is even.

`findtype4(T)` — cycles through symbolic expressions

$$\_GM(a)\,\_HM(b)+c\,\_GM(b)\,\_HM(a)$$

where $2\le n\le T$, $ab=n$, $(a,b)=1$, $b<a$, $c\in\{-1,1\}$,

$$\mathtt{GE}(a)+\mathtt{HE}(b)-(\mathtt{GE}(b)+\mathtt{HE}(a))\in\mathbb{Z}, \tag{3.34}$$

and at least one of a, b is even, using `CHECKRAMIDF` to check whether the expression corresponds to a likely eta-product, and if so uses `provemodfuncidBATCH` to prove it. The procedure also returns a list of `[a,b,c]` which give identities.

```
> findtype4(24);
```
$$[[6,1,-1]]$$

This also produces the following identity with proof:

$$G^*(6)\,H^*(1)-G^*(1)\,H^*(6)=\frac{\eta(\tau)\eta(4\tau)^3\eta(6\tau)^3\eta(24\tau)}{\eta(2\tau)^3\eta(3\tau)\eta(8\tau)\eta(12\tau)^3},\quad \Gamma_1(120),\quad -B=128. \tag{3.35}$$

This corresponds to Eq. (3.28) in [5].

3.2.5 Type 5

We consider identities of the form

$$G^*(a)\,G^*(b) \pm H^*(a)\,H^*(b) = f(\tau),$$

where $f(\tau)$ is an eta-product, a, b are positive relatively prime integers, and at least one of a, b is even.

`findtype5(T)` — cycles through symbolic expressions

$$\_GM(a)\,\_GM(b) + c\,\_HM(a)\,\_HM(b)$$

where $2 \le n \le T$, $ab = n$, $(a, b) = 1$, $a \le b$, $c \in \{-1, 1\}$,

$$\mathtt{GE}(a) + \mathtt{GE}(b) - (\mathtt{HE}(a) + \mathtt{HE}(b)) \in \mathbb{Z}, \tag{3.36}$$

and at least one of a, b is even, using `CHECKRAMIDF` to check whether the expression corresponds to a likely eta-product, and if so uses `provemodfuncidBATCH` to prove it. The procedure also returns a list of `[a,b,c]` which give identities.

```
> findtype5(24);
```

$$[[1, 4, 1], [2, 3, 1]]$$

This also produces the following identities with proof:

$$G^*(1)\,G^*(4) + H^*(1)\,H^*(4) = \frac{\eta(4\tau)^2}{\eta(2\tau)\eta(8\tau)}, \quad \Gamma_1(80), \quad -B = 64, \tag{3.37}$$

$$G^*(2)\,G^*(3) + H^*(2)\,H^*(3) = \frac{\eta(2\tau)^3\eta(3\tau)\eta(8\tau)\eta(12\tau)^3}{\eta(\tau)\eta(4\tau)^3\eta(6\tau)^3\eta(24\tau)}, \quad \Gamma_1(120), \quad -B = 128. \tag{3.38}$$

These correspond to Eqs. (3.26) and (3.27) in [5].

3.2.6 Type 6

We consider identities of the form

$$G(a)\,H^*(b) \pm G^*(a)\,H(b) = f(\tau),$$

where $f(\tau)$ is an eta-product, and a, b are positive relatively prime integers.

`findtype6(T)` — cycles through symbolic expressions

$$\_G(a)\,\_HM(b) + c\,\_GM(a)\,\_H(b)$$

where $2 \le n \le T$, $ab = n$, $(a, b) = 1$, $a \ge b$, $c \in \{-1, 1\}$, using `CHECKRAMIDF` to check whether the expression corresponds to a likely eta-product, and if so uses `provemodfuncidBATCH` to prove it. The procedure also returns a list of `[a,b,c]` which give identities.

```
> findtype6(24);
```

$$[[1, 1, -1], [1, 1, 1]]$$

This also produces the following identities with proof:

$$G(1)\,H^*(1) - G^*(1)\,H(1) = 2\,\frac{\eta(20\tau)^2}{\eta(2\tau)\eta(10\tau)}, \qquad \Gamma_1(20), \qquad -B = 4, \tag{3.39}$$

$$G(1)\,H^*(1) + G^*(1)\,H(1) = 2\,\frac{\eta(4\tau)^2}{\eta(2\tau)^2}, \qquad \Gamma_1(20), \qquad -B = 4. \tag{3.40}$$

These are equivalent to Eqs. (3.25) and (3.24) in [5].

3.2.7 Type 7

We consider identities of the form

$$G^*(a)\,G(b) \pm H^*(a)\,H(b) = f(\tau),$$

where $f(\tau)$ is an eta-product, and a, b are positive relatively prime integers.

`findtype7(T)` — cycles through symbolic expressions

$$\_GM(a)\,\_G(b) + c\,\_HM(a)\,\_H(b)$$

where $2 \le n \le T$, $ab = n$, $(a, b) = 1$, $a \le b$, $c \in \{-1, 1\}$, and both a, b are odd, using `CHECKRAMIDF` to check whether the expression corresponds to a likely eta-product, and if so uses `provemodfuncidBATCH` to prove it. The procedure also returns a list of `[a,b,c]` which give identities.

```
> findtype7(24);
```

$$[[1, 9, -1]]$$

This also produces the following identity with proof:

$$G^*(1)\,G(9) - H^*(1)\,H(9) = \frac{\eta(\tau)\eta(12\tau)\eta(18\tau)^2}{\eta(2\tau)\eta(6\tau)\eta(9\tau)\eta(36\tau)}, \quad \Gamma_1(180), \quad -B = 288. \tag{3.41}$$

This corresponds to (3.29) in [5].

3.2.8 Type 8

We consider identities of the form

$$G(1)^a\,H(a) \pm H(1)^a\,G(a) = f(\tau),$$

where $f(\tau)$ is an eta-product, and $a > 1$ is an integer.

`findtype8(T)` — cycles through symbolic expressions

$$\_G(1)^a\,\_H(a) + c\,\_H(1)^a\,\_G(a)$$

where $2 \le a \le T$, and $c \in \{-1, 1\}$, using `CHECKRAMIDF` to check whether the expression corresponds to a likely eta-product, and if so uses `provemodfuncidBATCH` to prove it. The procedure also returns a list of `[a,c]` which give identities.

```
> findtype8(24);
```

$$[[3, -1]]$$

This also produces the following identity with proof:

$$G(1)^3\,H(3) - H(1)^3\,G(3) = 3\,\frac{\eta(15\tau)^3}{\eta(\tau)\eta(3\tau)\eta(5\tau)}, \quad \Gamma_1(15), \quad -B = 4. \tag{3.42}$$

This is equivalent to Eq. (1.27) in Robin's thesis [20].

3.2.9 Type 9

We consider identities of the form

$$G(1)^a\,H(1)^b - H(1)^a\,G(1)^b + x = f(\tau),$$

where $f(\tau)$ is an eta-product, and a, b are positive integers, and $x = 0$ or $x = -1$.

`findtype9()` — determines whether

$$\_G(1)^a\,\_H(1)^b - \_H(1)^a\,\_G(1)^b + x$$

is a likely eta-product for $x = 0$ or $x = -1$ with a, b smallest such positive integers, using `CHECKRAMIDF` to check whether the expression corresponds to a likely eta-product, and if so uses `provemodfuncidBATCH` to prove it. The procedure also returns a list of `[a,b,x]` which give identities.

```
> findtype9();
                              [[11, 1, 1]]
```

This also produces the following identity with proof:

$$G(1)^{11}\,H(1)^1 - H(1)^{11}\,G(1)^1 - 1 = 11\,\frac{\eta(5\tau)^6}{\eta(\tau)^6}, \quad \Gamma_1(5), \quad -B = 2. \tag{3.43}$$

This is Eq. (3.1) in [5].

3.2.10 Type 10

We consider identities of the form

$$\frac{G(a_1)\,H(b_1) \pm\, H(a_1)\,G(b_1)}{G(a_2)\,H^*(b_2) \pm\, H(a_2)\,G^*(b_2)} = f(\tau),$$

in which the numerator is not a Type 1 identity, and where $f(\tau)$ is an eta-product, a_1, b_1, a_2, b_2 are positive relatively prime integers, and $a_1b_1 = a_2b_2$.

`findtype10(T)` — cycles through symbolic expressions

$$\frac{\_G(a_1)\,\_H(b_1) + c_1\,\_H(a_1)\,\_G(b_1)}{\_G(a_2)\,\_HM(b_2) + c_2\,\_H(a_2)\,\_GM(b_2)}$$

where $2 \le n \le T$, $a_1b_1 = a_2b_2 = n$, $(a_1, b_1, a_2, b_2) = 1$, $a_1 > b_1$, $b_2 < a_2$, $c_1, c_2 \in \{-1, 1\}$, and

$$\mathtt{GE}(a_1) + \mathtt{HE}(b_1) - (\mathtt{HE}(a_1) + \mathtt{GE}(b_1)), \quad \mathtt{GE}(a_2) + \mathtt{HE}(b_2) - (\mathtt{HE}(a_2) + \mathtt{GE}(b_2)) \in \mathbb{Z}, \tag{3.44}$$

and $[a_1, b_1, c_1]$ is not an element of the list `myramtype1` (found earlier by `findtype1`), using `CHECKRAMIDF` to check whether the expression corresponds to a likely eta-product, and if so uses `provemodfuncidBATCH` to prove it. The procedure also returns a list of $[a_1, b_1, c_1, a_2, b_2, c_2]$ which give identities.

```
> qthreshold:=3000:
> findtype10(120);
```

$$[[19, 4, -1, 76, 1, 1], [28, 3, -1, 12, 7, 1], [12, 7, -1, 28, 3, 1]]$$

This also produces the following identities with proof:

$$\frac{G(19)\,H(4) - H(19)\,G(4)}{G(76)\,H^*(1) + H(76)\,G^*(1)} = \frac{\eta(2\tau)\eta(76\tau)}{\eta(4\tau)\eta(38\tau)}, \quad \Gamma_1(380), \quad -B = 2160,$$

$$\star \quad \frac{G(28)\,H(3) - H(28)\,G(3)}{G(12)\,H^*(7) + H(12)\,G^*(7)} = \frac{\eta(\tau)\eta(4\tau)\eta(6\tau)\eta(14\tau)^2\eta(21\tau)}{\eta(2\tau)^2\eta(3\tau)\eta(7\tau)\eta(28\tau)\eta(42\tau)},$$
$$\Gamma_1(420), \quad -B = 2400, \tag{3.45}$$

$$\star \quad \frac{G(12)\,H(7) - H(12)\,G(7)}{G(28)\,H^*(3) + H(28)\,G^*(3)} = \frac{\eta(\tau)\eta(6\tau)^2\eta(14\tau)\eta(21\tau)\eta(84\tau)}{\eta(2\tau)\eta(3\tau)\eta(7\tau)\eta(12\tau)\eta(42\tau)^2},$$
$$\Gamma_1(420), \quad -B = 2400. \tag{3.46}$$

Equation (3.45) is (3.38) in [5]. The other type 10 identities appear to be new.

4 More Generalized Ramanujan–Robins Identities

We consider generalized Ramanujan–Robins identities associated with non-principal real Dirichlet characters χ mod N for $N \le 60$, that satisfy $\chi(-1) = 1$. We found David Ireland's *Dirichlet Character Table Generator* [14] useful. See the website

http://www.di-mgt.com.au/dirichlet-character-generator.html

4.1 Mod 8

There is only one non-principal character mod 8 that satisfies $\chi(-1) = 1$, namely $\chi(\cdot) = \left(\frac{8}{\cdot}\right)$. Here $\left(\frac{8}{\cdot}\right)$ is the Kronecker symbol. In this section

$$G(1) = G\left(1, 8, \left(\frac{8}{\cdot}\right)\right) = \frac{1}{\eta_{8;1}(\tau)} = \frac{q^{-11/48}}{(q, q^7; q^8)_\infty}, \quad \text{and}$$
$$H(1) = H\left(1, 8, \left(\frac{8}{\cdot}\right)\right) = \frac{1}{\eta_{8;3}(\tau)} = \frac{q^{13/48}}{(q^3, q^5; q^8)_\infty}.$$

These functions were considered by Robins [20, pp. 16–17]. They are also related to the Göllnitz–Gordon functions [10, 11]:

$$S(q) = \sum_{n=0}^{\infty} \frac{(-q; q^2)_n}{(q^2; q^2)_n} q^{n^2} = \frac{1}{(q, q^4, q^7; q^8)_\infty},$$
$$T(q) = \sum_{n=0}^{\infty} \frac{(-q; q^2)_n}{(q^2; q^2)_n} q^{n^2+2n} = \frac{1}{(q^3, q^4, q^5; q^8)_\infty}.$$

The ratio of these two functions is the famous Ramanujan–Göllnitz–Gordon continued fraction [4, Eq. (9.3)]

$$\frac{S(q)}{T(q)} = \prod_{n=0}^{\infty} \frac{(1 - q^{8n+3})(1 - q^{8n+5})}{(1 - q^{8n+1})(1 - q^{8n+7})}$$
$$= 1 + \cfrac{q + q^2}{1 + \cfrac{q^4}{1 + \cfrac{q^3 + q^6}{1 + \cfrac{q^8}{1 + \ddots}}}}.$$

Some of the identities given in this section are due Robins [20], and many are due to Huang [12]. Any identities that appear to be new are marked $\star$.

4.1.1 Type 1

$$G(3)\,H(1) - G(1)\,H(3) = \frac{\eta(\tau)\eta(12\tau)^2}{\eta(3\tau)\eta(8\tau)\eta(24\tau)}, \qquad \Gamma_1(24), \qquad -B = 6, \tag{4.1}$$

$$G(3)\,H(1)+G(1)\,H(3)=\frac{\eta(2\tau)\eta(4\tau)^2\eta(6\tau)^2}{\eta(\tau)\eta(3\tau)\eta(8\tau)^2\eta(12\tau)},\qquad \Gamma_1(24),\qquad -B=6, \tag{4.2}$$

$$G(5)\,H(1)-G(1)\,H(5)=\frac{\eta(2\tau)\eta(10\tau)\eta(20\tau)}{\eta(5\tau)\eta(8\tau)\eta(40\tau)},\qquad \Gamma_1(40),\qquad -B=20, \tag{4.3}$$

$$G(7)\,H(1)-G(1)\,H(7)=\frac{\eta(4\tau)\eta(28\tau)}{\eta(8\tau)\eta(56\tau)},\qquad \Gamma_1(56),\qquad -B=36, \tag{4.4}$$

$$G(9)\,H(1)-G(1)\,H(9)=\frac{\eta(4\tau)\eta(6\tau)^2\eta(36\tau)}{\eta(3\tau)\eta(8\tau)\eta(12\tau)\eta(72\tau)},\qquad \Gamma_1(72),\qquad -B=60, \tag{4.5}$$

$$G(5)\,H(3)-G(3)\,H(5)=\frac{\eta(\tau)\eta(4\tau)\eta(6\tau)\eta(10\tau)\eta(15\tau)\eta(60\tau)}{\eta(2\tau)\eta(3\tau)\eta(5\tau)\eta(24\tau)\eta(30\tau)\eta(40\tau)},\quad \Gamma_1(120),\quad -B=144. \tag{4.6}$$

4.1.2 Type 2

$$G(1)\,G(1)-H(1)\,H(1)=\frac{\eta(4\tau)^6}{\eta(\tau)\eta(2\tau)\eta(8\tau)^4},\qquad \Gamma_1(8),\qquad -B=1, \tag{4.7}$$

$$G(1)\,G(1)+H(1)\,H(1)=\frac{\eta(2\tau)^6}{\eta(\tau)^3\eta(4\tau)\eta(8\tau)^2},\qquad \Gamma_1(8),\qquad -B=1, \tag{4.8}$$

$$G(1)\,G(3)-H(1)\,H(3)=\frac{\eta(2\tau)^2\eta(6\tau)\eta(12\tau)^2}{\eta(\tau)\eta(3\tau)\eta(4\tau)\eta(24\tau)^2},\qquad \Gamma_1(24),\qquad -B=6, \tag{4.9}$$

$$G(1)\,G(3)+H(1)\,H(3)=\frac{\eta(3\tau)\eta(4\tau)^2}{\eta(\tau)\eta(8\tau)\eta(24\tau)},\qquad \Gamma_1(24),\qquad -B=6, \tag{4.10}$$

$$G(1)\,G(5)+H(1)\,H(5)=\frac{\eta(2\tau)\eta(4\tau)\eta(10\tau)}{\eta(\tau)\eta(8\tau)\eta(40\tau)},\qquad \Gamma_1(40),\qquad -B=20, \tag{4.11}$$

$$G(1)\,G(9)+H(1)\,H(9)=\frac{\eta(2\tau)\eta(3\tau)\eta(12\tau)\eta(18\tau)}{\eta(\tau)\eta(8\tau)\eta(9\tau)\eta(72\tau)},\qquad \Gamma_1(72),\qquad -B=60, \tag{4.12}$$

$$G(1)\,G(15)+H(1)\,H(15)=\frac{\eta(2\tau)\eta(3\tau)\eta(5\tau)\eta(12\tau)\eta(20\tau)\eta(30\tau)}{\eta(\tau)\eta(6\tau)\eta(8\tau)\eta(10\tau)\eta(15\tau)\eta(120\tau)},$$
$$\Gamma_1(120),\quad -B=144. \tag{4.13}$$

4.1.3 Type 3

$$\star\quad \frac{G(3)\,G(5)-H(3)\,H(5)}{G(15)\,H(1)+H(15)\,G(1)}=\frac{\eta(4\tau)\eta(60\tau)}{\eta(12\tau)\eta(20\tau)},\qquad \Gamma_1(120),\qquad -B=256, \tag{4.14}$$

$$\frac{G(3)\,G(5)+H(3)\,H(5)}{G(15)\,H(1)-H(15)\,G(1)}=\frac{\eta(8\tau)\eta(12\tau)\eta(20\tau)\eta(120\tau)}{\eta(4\tau)\eta(24\tau)\eta(40\tau)\eta(60\tau)},$$
$$\Gamma_1(120),\quad -B=224, \tag{4.15}$$

$$\star\quad \frac{G(1)\,G(15)-H(1)\,H(15)}{G(5)\,H(3)+H(5)\,G(3)}=\frac{\eta(4\tau)^2\eta(6\tau)\eta(10\tau)\eta(24\tau)^2\eta(40\tau)^2\eta(60\tau)^2}{\eta(2\tau)\eta(8\tau)^2\eta(12\tau)^2\eta(20\tau)^2\eta(30\tau)\eta(120\tau)^2},$$
$$\Gamma_1(120),\quad -B=192, \tag{4.16}$$

$$\star\quad \frac{G(3)\,G(7)+H(3)\,H(7)}{G(21)\,H(1)-H(21)\,G(1)}=\frac{\eta(8\tau)\eta(21\tau)\eta(28\tau)\eta(168\tau)}{\eta(7\tau)\eta(24\tau)\eta(56\tau)\eta(84\tau)},$$
$$\Gamma_1(168),\quad -B=528, \tag{4.17}$$

$$\star\quad \frac{G(1)\,G(21)+H(1)\,H(21)}{G(7)\,H(3)-H(7)\,G(3)}=\frac{\eta(3\tau)\eta(4\tau)\eta(24\tau)\eta(56\tau)}{\eta(\tau)\eta(8\tau)\eta(12\tau)\eta(168\tau)},$$
$$\Gamma_1(168),\quad -B=528, \tag{4.18}$$

$$\frac{G(1)\,G(39)+H(1)\,H(39)}{G(13)\,H(3)-H(13)\,G(3)}=\frac{\eta(2\tau)\eta(3\tau)\eta(13\tau)\eta(24\tau)\eta(78\tau)\eta(104\tau)}{\eta(\tau)\eta(6\tau)\eta(8\tau)\eta(26\tau)\eta(39\tau)\eta(312\tau)},$$
$$\Gamma_1(312),\quad -B=1632, \tag{4.19}$$

$$\frac{G(1)\,G(55)+H(1)\,H(55)}{G(11)\,H(5)-H(11)\,G(5)}=\frac{\eta(2\tau)\eta(5\tau)\eta(11\tau)\eta(40\tau)\eta(88\tau)\eta(110\tau)}{\eta(\tau)\eta(8\tau)\eta(10\tau)\eta(22\tau)\eta(55\tau)\eta(440\tau)},$$
$$\Gamma_1(440),\quad -B=3680. \tag{4.20}$$

4.1.4 Type 8

$$\star\quad G(1)^3\,H(3)-H(1)^3\,G(3)=3\,\frac{\eta(2\tau)^3\eta(4\tau)\eta(6\tau)\eta(24\tau)^2}{\eta(\tau)^2\eta(3\tau)\eta(8\tau)^4},$$
$$\Gamma_1(24),\quad -B=10. \tag{4.21}$$

4.2 Mod 10

There is only one real non-principal character mod 10 that satisfies $\chi(-1) = 1$, namely the character χ_{10} induced by the Legendre symbol mod 5. In this section

$$G(1) = G(1, 10, \chi_{10}) = \frac{1}{\eta_{10;1}(\tau)} = \frac{q^{-23/60}}{(q, q^9; q^{10})_\infty}, \quad \text{and}$$
$$H(1) = H(1, 10, \chi_{10}) = \frac{1}{\eta_{10;3}(\tau)} = \frac{q^{13/60}}{(q^3, q^7; q^{10})_\infty}.$$

All the identities in this section appear to be new.

4.2.1 Type 1

$$G(6)\,H(1) - G(1)\,H(6) = \frac{\eta(4\tau)\eta(5\tau)\eta(12\tau)\eta(30\tau)^3}{\eta(6\tau)\eta(10\tau)^2\eta(15\tau)\eta(60\tau)^2}, \qquad \Gamma_1(60), \qquad -B = 40. \tag{4.22}$$

4.2.2 Type 2

$$G(2)\,G(3) - H(2)\,H(3) = \frac{\eta(4\tau)\eta(10\tau)^3\eta(12\tau)\eta(15\tau)}{\eta(2\tau)\eta(5\tau)\eta(20\tau)^2\eta(30\tau)^2}, \qquad \Gamma_1(60), \qquad -B = 40, \tag{4.23}$$

$$G(1)\,G(9) - H(1)\,H(9) = \frac{\eta(2\tau)\eta(3\tau)\eta(5\tau)\eta(18\tau)\eta(30\tau)^2\eta(45\tau)}{\eta(\tau)\eta(9\tau)\eta(10\tau)^2\eta(15\tau)\eta(90\tau)^2}, \quad \Gamma_1(90), \quad -B = 96. \tag{4.24}$$

4.2.3 Type 5

$$G^*(1)\,G^*(4) - H^*(1)\,H^*(4) = \frac{\eta(\tau)\eta(4\tau)^3\eta(10\tau)\eta(16\tau)\eta(40\tau)}{\eta(2\tau)^2\eta(5\tau)\eta(8\tau)^2\eta(20\tau)\eta(80\tau)}, \quad \Gamma_1(80), \quad -B = 64. \tag{4.25}$$

4.2.4 Type 6

$$G(1)\,H^*(1) - G^*(1)\,H(1) = 2\,\frac{\eta(20\tau)^2}{\eta(10\tau)^2}, \qquad \Gamma_1(20), \qquad -B = 4, \quad (4.26)$$

$$G(1)\,H^*(1) + G^*(1)\,H(1) = 2\,\frac{\eta(4\tau)^2}{\eta(2\tau)\eta(10\tau)}, \qquad \Gamma_1(20), \qquad -B = 4. \quad (4.27)$$

4.2.5 Type 8

$$G(1)^2\,H(2) - H(1)^2\,G(2) = 2\,\frac{\eta(2\tau)\eta(5\tau)\eta(20\tau)^2}{\eta(\tau)\eta(10\tau)^3}, \quad \Gamma_1(20), \quad -B = 4, \quad (4.28)$$

$$G(1)^2\,H(2) + H(1)^2\,G(2) = 2\,\frac{\eta(4\tau)^2\eta(5\tau)}{\eta(\tau)\eta(10\tau)^2}, \quad \Gamma_1(20), \quad -B = 4, \quad (4.29)$$

$$G(1)^3\,H(3) - H(1)^3\,G(3) = 3\,\frac{\eta(2\tau)^3\eta(5\tau)^2\eta(6\tau)\eta(15\tau)\eta(30\tau)}{\eta(\tau)^2\eta(3\tau)\eta(10\tau)^5}, \quad \Gamma_1(30), \quad -B = 16. \quad (4.30)$$

4.3 *Mod* 12

There is only one non-principal character mod 12 that satisfies $\chi(-1) = 1$, namely $\chi(\cdot) = \left(\frac{12}{\cdot}\right)$. In this section

$$G(1) = G\left(1, 12, \left(\frac{12}{\cdot}\right)\right) = \frac{1}{\eta_{12;1}(\tau)} = \frac{q^{-13/24}}{(q, q^{11}; q^{12})_\infty}, \quad \text{and}$$
$$H(1) = H\left(1, 12, \left(\frac{12}{\cdot}\right)\right) = \frac{1}{\eta_{12;5}(\tau)} = \frac{q^{11/24}}{(q^5, q^7; q^{12})_\infty}.$$

These functions were considered by Robins [20, p17], who found (4.33), (4.34), (4.39), (4.40). The remaining identities appear to be new and are marked ⋆.

4.3.1 Type 1

$$\star \quad G(2)\,H(1) - G(1)\,H(2) = \frac{\eta(\tau)\eta(4\tau)\eta(6\tau)}{\eta(2\tau)\eta(12\tau)^2}, \qquad \Gamma_1(24), \qquad -B = 4, \tag{4.31}$$

$$\star \quad G(2)\,H(1) + G(1)\,H(2) = \frac{\eta(3\tau)^2\eta(4\tau)}{\eta(\tau)\eta(12\tau)^2}, \qquad \Gamma_1(24), \qquad -B = 4, \tag{4.32}$$

$$G(3)\,H(1) - G(1)\,H(3) = \frac{\eta(2\tau)\eta(18\tau)}{\eta(12\tau)\eta(36\tau)}, \qquad \Gamma_1(36), \qquad -B = 12, \tag{4.33}$$

$$G(3)\,H(1) + G(1)\,H(3) = \frac{\eta(4\tau)\eta(6\tau)^5\eta(9\tau)^2}{\eta(2\tau)\eta(3\tau)^2\eta(12\tau)^3\eta(18\tau)^2}, \quad \Gamma_1(36), \quad -B = 12, \tag{4.34}$$

$$\star \quad G(4)\,H(1) - G(1)\,H(4) = \frac{\eta(3\tau)\eta(16\tau)}{\eta(12\tau)\eta(48\tau)}, \qquad \Gamma_1(48), \qquad -B = 24, \tag{4.35}$$

$$\star \quad G(5)\,H(1) - G(1)\,H(5) = \frac{\eta(4\tau)\eta(6\tau)\eta(10\tau)\eta(15\tau)}{\eta(5\tau)\eta(12\tau)^2\eta(60\tau)}, \quad \Gamma_1(60), \quad -B = 40, \tag{4.36}$$

$$\star \quad G(3)\,H(2) - G(2)\,H(3) = \frac{\eta(\tau)\eta(6\tau)\eta(8\tau)\eta(9\tau)\eta(12\tau)\eta(72\tau)}{\eta(2\tau)\eta(3\tau)\eta(24\tau)^2\eta(36\tau)^2}, \quad \Gamma_1(72), \quad -B = 48, \tag{4.37}$$

$$\star \quad G(6)\,H(1) - G(1)\,H(6) = \frac{\eta(8\tau)\eta(9\tau)}{\eta(12\tau)\eta(72\tau)}, \qquad \Gamma_1(72), \qquad -B = 60. \tag{4.38}$$

4.3.2 Type 2

$$G(1)^2 - H(1)^2 = \frac{\eta(2\tau)^3\eta(6\tau)^3}{\eta(\tau)^2\eta(12\tau)^4}, \qquad \Gamma_1(12), \qquad -B = 2, \tag{4.39}$$

$$G(1)^2 + H(1)^2 = \frac{\eta(2\tau)\eta(3\tau)^4\eta(4\tau)}{\eta(\tau)^2\eta(6\tau)\eta(12\tau)^3}, \qquad \Gamma_1(12), \qquad -B = 2, \tag{4.40}$$

$$\star \quad G(1)\,G(2) - H(1)\,H(2) = \frac{\eta(3\tau)^2\eta(8\tau)^2}{\eta(\tau)\eta(12\tau)\eta(24\tau)^2}, \qquad \Gamma_1(24), \qquad -B = 8, \tag{4.41}$$

$$\star \quad G(1)\,G(3) - H(1)\,H(3) = \frac{\eta(2\tau)\eta(4\tau)\eta(9\tau)\eta(18\tau)}{\eta(\tau)\eta(12\tau)\eta(36\tau)^2}, \qquad \Gamma_1(36), \qquad -B = 18, \tag{4.42}$$

$$\star \quad G(1)\,G(5) - H(1)\,H(5) = \frac{\eta(2\tau)\eta(3\tau)\eta(20\tau)\eta(30\tau)}{\eta(\tau)\eta(12\tau)\eta(60\tau)^2}, \qquad \Gamma_1(60), \qquad -B = 40. \tag{4.43}$$

4.3.3 Type 3

$$\frac{G(1)\,G(10) - H(1)\,H(10)}{G(5)\,H(2) - H(5)\,G(2)} = \frac{\eta(2\tau)\eta(5\tau)\eta(24\tau)^2\eta(60\tau)^2}{\eta(\tau)\eta(10\tau)\eta(12\tau)^2\eta(120\tau)^2}, \quad \Gamma_1(120), \quad -B = 256, \tag{4.44}$$

$$\frac{G(5)\,G(7) - H(5)\,H(7)}{G(35)\,H(1) - H(35)\,G(1)} = \frac{\eta(12\tau)\eta(420\tau)}{\eta(60\tau)\eta(84\tau)}, \qquad \Gamma_1(420), \qquad -B = 3648, \tag{4.45}$$

$$\begin{aligned}&\frac{G(1)\,G(35) - H(1)\,H(35)}{G(7)\,H(5) - H(7)\,G(5)} \\ &= \frac{\eta(3\tau)\eta(4\tau)\eta(5\tau)\eta(7\tau)\eta(60\tau)^2\eta(84\tau)^2\eta(105\tau)\eta(140\tau)}{\eta(\tau)\eta(12\tau)^2\eta(15\tau)\eta(20\tau)\eta(21\tau)\eta(28\tau)\eta(35\tau)\eta(420\tau)^2}, \\ &\Gamma_1(420), \quad -B = 2880.\end{aligned} \tag{4.46}$$

4.3.4 Type 4

$$\star \quad G^*(2)\,H^*(1) - G^*(1)\,H^*(2) = \frac{\eta(\tau)\eta(6\tau)\eta(8\tau)^3\eta(48\tau)}{\eta(2\tau)\eta(4\tau)\eta(16\tau)\eta(24\tau)^3}, \quad \Gamma_1(48), \quad -B = 24. \tag{4.47}$$

4.3.5 Type 5

$$\star \quad G^*(1)\, G^*(2) - H^*(1)\, H^*(2) = \frac{\eta(\tau)\eta(6\tau)\eta(16\tau)}{\eta(2\tau)\eta(12\tau)\eta(48\tau)}, \quad \Gamma_1(48), \quad -B = 24. \tag{4.48}$$

4.3.6 Type 6

$$\star \quad G(1)\, H^*(1) - G^*(1)\, H(1) = 2\, \frac{\eta(4\tau)^2\eta(6\tau)^2\eta(24\tau)^3}{\eta(2\tau)\eta(8\tau)\eta(12\tau)^5}, \qquad \Gamma_1(24), \qquad -B = 4, \tag{4.49}$$

$$\star \quad G(1)\, H^*(1) + G^*(1)\, H(1) = 2\, \frac{\eta(4\tau)\eta(6\tau)^2\eta(8\tau)\eta(24\tau)}{\eta(2\tau)\eta(12\tau)^4}, \qquad \Gamma_1(24), \qquad -B = 4. \tag{4.50}$$

4.3.7 Type 7

$$\star \quad G^*(1)\, G(1) - H^*(1)\, H(1) = \frac{\eta(8\tau)\eta(12\tau)^4}{\eta(4\tau)\eta(6\tau)\eta(24\tau)^3}, \quad \Gamma_1(24), \quad -B = 4, \tag{4.51}$$

$$\star \quad G^*(1)\, G(1) + H^*(1)\, H(1) = \frac{\eta(4\tau)^4\eta(6\tau)}{\eta(2\tau)^2\eta(8\tau)\eta(12\tau)\eta(24\tau)}, \quad \Gamma_1(24), \quad -B = 4. \tag{4.52}$$

4.3.8 Type 8

$$\star \quad G(1)^2\, H(2) - H(1)^2\, G(2) = 2\, \frac{\eta(3\tau)\eta(4\tau)^2\eta(6\tau)\eta(24\tau)^3}{\eta(\tau)\eta(8\tau)\eta(12\tau)^5}, \quad \Gamma_1(24), \quad -B = 4, \tag{4.53}$$

$$\star \quad G(1)^2\, H(2) + H(1)^2\, G(2) = 2\, \frac{\eta(3\tau)\eta(4\tau)\eta(6\tau)\eta(8\tau)\eta(24\tau)}{\eta(\tau)\eta(12\tau)^4}, \quad \Gamma_1(24), \quad -B = 4, \tag{4.54}$$

$$\star \quad G(1)^3\, H(3) - H(1)^3\, G(3) = 3\,\frac{\eta(2\tau)^2\eta(3\tau)\eta(4\tau)\eta(6\tau)\eta(9\tau)\eta(36\tau)^2}{\eta(\tau)^2\eta(12\tau)^5\eta(18\tau)},$$
$$\Gamma_1(36), \quad -B = 18. \tag{4.55}$$

4.4 *Mod* 13

There is only one non-principal character mod 13 that satisfies $\chi(-1) = 1$, namely $\chi(\cdot) = \left(\frac{\cdot}{13}\right)$. In this section

$$G(1) = G\left(1, 13, \left(\frac{\cdot}{13}\right)\right) = \frac{1}{\eta_{13;1,3,4}(\tau)} = \frac{q^{-1/4}}{(q, q^3, q^4, q^9, q^{10}, q^{12}; q^{13})_\infty}, \quad \text{and}$$
$$H(1) = H\left(1, 13, \left(\frac{\cdot}{13}\right)\right) = \frac{1}{\eta_{13;2,5,6}(\tau)} = \frac{q^{3/4}}{(q^2, q^5, q^6, q^7, q^8, q^{11}; q^{13})_\infty}.$$

These functions were considered by Robins [20, p. 18], who found the one identity (4.56). The remaining four identities appear to be new and are marked $\star$.

4.4.1 Type 1

$$G(3)\, H(1) - G(1)\, H(3) = 1, \qquad \Gamma_1(39), \qquad -B = 24. \tag{4.56}$$

4.4.2 Type 3

$$\star \quad \frac{G(1)\, G(2) + H(1)\, H(2)}{G(2)\, H(1) - H(2)\, G(1)} = \frac{\eta(2\tau)^2\eta(13\tau)^2}{\eta(\tau)^2\eta(26\tau)^2}, \qquad \Gamma_1(26), \qquad -B = 18, \tag{4.57}$$

$$\star \quad \frac{G(2)\, G(5) + H(2)\, H(5)}{G(10)\, H(1) - H(10)\, G(1)} = 1, \qquad \Gamma_1(130), \qquad -B = 432, \tag{4.58}$$

$$\star \quad \frac{G(1)\,G(14)+H(1)\,H(14)}{G(7)\,H(2)-H(7)\,G(2)} = \frac{\eta(2\tau)\eta(7\tau)\eta(26\tau)\eta(91\tau)}{\eta(\tau)\eta(13\tau)\eta(14\tau)\eta(182\tau)}, \quad \Gamma_1(182), \quad -B = 864. \tag{4.59}$$

4.4.3 Type 9

$$\star \quad G(1)^3\,H(1) - H(1)^3\,G(1) - 1 = 3\,\frac{\eta(13\tau)^2}{\eta(\tau)^2}, \quad \Gamma_1(13), \quad -B = 6. \tag{4.60}$$

4.5 *Mod* 15

There is only one real non-principal character mod 15 that satisfies $\chi(-1) = 1$, namely the one induced by the Legendre symbol mod 5:

$$\chi_{15}(n) = \begin{cases} 1, & n \equiv \pm 1, 4 \pmod{15}, \\ -1, & n \equiv \pm 2, 7 \pmod{15}, \\ 0, & \text{otherwise.} \end{cases}$$

Thus in this section

$$G(1) = G(1, 15, \chi_{15}) = \frac{1}{\eta_{15;1,4}(\tau)} = \frac{q^{-17/30}}{(q, q^4, q^{11}, q^{14}; q^{15})_\infty}, \quad \text{and}$$
$$H(1) = H(1, 15, \chi_{15}) = \frac{1}{\eta_{15;2,7}(\tau)} = \frac{q^{7/30}}{(q^2, q^7, q^8, q^{13}; q^{15})_\infty}.$$

All the identities in this section appear to be new.

4.5.1 Type 2

$$G(1)\,G(4) - H(1)\,H(4) = \frac{\eta(2\tau)\eta(3\tau)\eta(10\tau)\eta(12\tau)\eta(30\tau)^2}{\eta(\tau)\eta(4\tau)\eta(15\tau)^2\eta(60\tau)^2}, \quad \Gamma_1(60), \quad -B = 48. \tag{4.61}$$

4.5.2 Type 3

$$\frac{G(2)\,G(3)-H(2)\,H(3)}{G(6)\,H(1)-H(6)\,G(1)}=\frac{\eta(6\tau)\eta(10\tau)\eta(15\tau)^3\eta(90\tau)}{\eta(3\tau)\eta(5\tau)\eta(30\tau)^3\eta(45\tau)},\qquad \Gamma_1(90),\qquad -B=120. \tag{4.62}$$

4.5.3 Type 6

$$G(1)\,H^*(1)-G^*(1)\,H(1)=2\,\frac{\eta(4\tau)\eta(6\tau)^3\eta(10\tau)\eta(60\tau)^2}{\eta(2\tau)^2\eta(12\tau)\eta(30\tau)^4},\quad \Gamma_1(60),\quad -B=48. \tag{4.63}$$

4.5.4 Type 8

$$G(1)^2\,H(2)+H(1)^2\,G(2)=2\,\frac{\eta(3\tau)^2\eta(6\tau)\eta(10\tau)^2}{\eta(\tau)\eta(2\tau)\eta(15\tau)^3},\quad \Gamma_1(30),\quad -B=12. \tag{4.64}$$

4.6 Mod 17

There is only one non-principal character mod 17 that satisfies $\chi(-1)=1$, namely $\chi(\cdot)=\left(\frac{\cdot}{17}\right)$. In this section

$$\begin{aligned} G(1)=G\left(1,17,\left(\frac{\cdot}{17}\right)\right)&=\frac{1}{\eta_{17;1,2,4,8}(\tau)}\\ &=\frac{q^{-2/3}}{(q,q^2,q^4,q^8,q^9,q^{13},q^{15},q^{16};q^{17})_\infty},\quad \text{and} \end{aligned}$$

$$\begin{aligned} H(1)=H\left(1,17,\left(\frac{\cdot}{17}\right)\right)&=\frac{1}{\eta_{17;3,5,6,7}(\tau)}\\ &=\frac{q^{4/3}}{(q^3,q^5,q^6,q^7,q^{10},q^{11},q^{12},q^{14};q^{17})_\infty}. \end{aligned}$$

These functions were not considered by Robins [20]. Nonetheless we find one identity.

4.6.1 Type 1

$$G(2)\,H(1) - G(1)\,H(2) = 1, \qquad \Gamma_1(34), \qquad -B = 16. \tag{4.65}$$

4.7 *Mod* 21

There is only one non-principal character mod 21 that satisfies $\chi(-1) = 1$, namely $\chi(\cdot) = \left(\frac{21}{\cdot}\right)$. In this section

$$G(1) = G\left(1, 21, \left(\frac{21}{\cdot}\right)\right) = \frac{1}{\eta_{21;1,4,5}(\tau)} = \frac{q^{-5/4}}{(q, q^4, q^5, q^{16}, q^{17}, q^{20}; q^{21})_\infty}, \quad \text{and}$$

$$H(1) = H\left(1, 21, \left(\frac{21}{\cdot}\right)\right) = \frac{1}{\eta_{21;2,8,10}(\tau)} = \frac{q^{3/4}}{(q^2, q^8, q^{10}, q^{11}, q^{13}, q^{19}; q^{21})_\infty}.$$

4.7.1 Type 1

$$G(2)\,H(1) - G(1)\,H(2) = \frac{\eta(3\tau)\eta(6\tau)\eta(7\tau)^2}{\eta(2\tau)\eta(21\tau)^3}, \qquad \Gamma_1(42), \qquad -B = 24, \tag{4.66}$$

$$G(4)\,H(1) - G(1)\,H(4) = \frac{\eta(6\tau)^2\eta(7\tau)\eta(28\tau)}{\eta(2\tau)\eta(21\tau)\eta(42\tau)\eta(84\tau)}, \qquad \Gamma_1(84), \qquad -B = 96. \tag{4.67}$$

4.7.2 Type 2

$$G(1)\,G(2) - H(1)\,H(2) = \frac{\eta(3\tau)\eta(6\tau)\eta(14\tau)^2}{\eta(\tau)\eta(42\tau)^3}, \qquad \Gamma_1(42), \qquad -B = 24. \tag{4.68}$$

4.7.3 Type 7

$$G^*(1)\,G(1) - H^*(1)\,H(1) = \frac{\eta(6\tau)^2\eta(14\tau)^3\eta(84\tau)}{\eta(2\tau)\eta(28\tau)\eta(42\tau)^4}, \quad \Gamma_1(84), \quad -B = 96. \tag{4.69}$$

4.8 *Mod* 24

There are three real non-principal characters mod 24 that satisfy $\chi(-1) = 1$.

(i) The character $\chi_{24,1}(\cdot)$ induced by $\left(\frac{8}{\cdot}\right)$.
(ii) The character $\chi_{24,2}(\cdot) = \left(\frac{12}{\cdot}\right)$ covered previously in Sect. 4.3.
(iii) The character $\chi_{24,3}(\cdot) = \left(\frac{24}{\cdot}\right)$.

4.8.1 $\chi_{24,1}$

We have

$$G(1) = G(1, 24, \chi_{24,1}) = \frac{1}{\eta_{24;1,7}(\tau)} = \frac{q^{-25/24}}{(q, q^7, q^{17}, q^{23}; q^{24})_\infty}, \quad \text{and}$$
$$H(1) = H(1, 24, \chi_{24,1}) = \frac{1}{\eta_{24;5,11}(\tau)} = \frac{q^{23/24}}{(q^5, q^{11}, q^{13}, q^{19}; q^{24})_\infty}.$$

Type 1

$$G(2)\,H(1) - G(1)\,H(2) = \frac{\eta(3\tau)\eta(12\tau)^2}{\eta(6\tau)\eta(24\tau)^2}, \qquad \Gamma_1(48), \qquad -B = 24, \tag{4.70}$$

$$G(2)\,H(1) + G(1)\,H(2) = \frac{\eta(4\tau)^3\eta(6\tau)^4}{\eta(2\tau)^2\eta(3\tau)\eta(8\tau)\eta(12\tau)^2\eta(24\tau)}, \quad \Gamma_1(48), \quad -B = 24, \tag{4.71}$$

$$G(3)\,H(1) - G(1)\,H(3) = \frac{\eta(4\tau)\eta(6\tau)^2\eta(9\tau)\eta(36\tau)}{\eta(3\tau)\eta(8\tau)\eta(12\tau)\eta(18\tau)\eta(72\tau)}, \quad \Gamma_1(72), \quad -B = 60. \tag{4.72}$$

Type 2

$$G(1)\,G(1) - H(1)\,H(1) = \frac{\eta(2\tau)^2\eta(3\tau)^2\eta(4\tau)\eta(12\tau)^2}{\eta(\tau)^2\eta(6\tau)\eta(8\tau)\eta(24\tau)^3}, \qquad \Gamma_1(24), \qquad -B = 12. \tag{4.73}$$

Type 6

$$G(1)\,H^*(1) - G^*(1)\,H(1) = 2\,\frac{\eta(4\tau)^2\eta(12\tau)^2\eta(48\tau)^2}{\eta(2\tau)\eta(8\tau)\eta(24\tau)^4}, \qquad \Gamma_1(48), \qquad -B = 24, \tag{4.74}$$

$$G(1)\,H^*(1) + G^*(1)\,H(1) = 2\,\frac{\eta(4\tau)\eta(6\tau)^2\eta(16\tau)\eta(48\tau)}{\eta(2\tau)\eta(8\tau)\eta(24\tau)^3}, \qquad \Gamma_1(48), \qquad -B = 24. \tag{4.75}$$

Type 7

$$G^*(1)\,G(1) - H^*(1)\,H(1) = \frac{\eta(4\tau)^2\eta(24\tau)^2}{\eta(2\tau)\eta(8\tau)\eta(48\tau)^2}, \quad \Gamma_1(48), \quad -B = 24, \tag{4.76}$$

$$G^*(1)\,G(1) + H^*(1)\,H(1) = \frac{\eta(6\tau)^2\eta(8\tau)^2}{\eta(2\tau)\eta(12\tau)\eta(16\tau)\eta(48\tau)}, \quad \Gamma_1(48), \quad -B = 24. \tag{4.77}$$

Type 8

$$G(1)^2\,H(2) - H(1)^2\,G(2) = 2\,\frac{\eta(3\tau)\eta(4\tau)^2\eta(12\tau)^2\eta(48\tau)^2}{\eta(\tau)\eta(6\tau)\eta(8\tau)\eta(24\tau)^4}, \quad \Gamma_1(48), \quad -B = 24, \tag{4.78}$$

$$G(1)^2\,H(2) + H(1)^2\,G(2) = 2\,\frac{\eta(3\tau)\eta(4\tau)\eta(6\tau)\eta(16\tau)\eta(48\tau)}{\eta(\tau)\eta(8\tau)\eta(24\tau)^3}, \quad \Gamma_1(48), \quad -B = 24. \tag{4.79}$$

Type 10

$$\frac{G(3)\,H(2) + H(3)\,G(2)}{G(6)\,H^*(1) - H(6)\,G^*(1)} = \frac{\eta(4\tau)\eta(6\tau)^3\eta(9\tau)\eta(24\tau)^2\eta(36\tau)\eta(144\tau)^2}{\eta(2\tau)\eta(3\tau)\eta(12\tau)^2\eta(18\tau)^2\eta(48\tau)^2\eta(72\tau)^2}, \quad \Gamma_1(144), \quad -B = 360. \tag{4.80}$$

4.8.2 $\chi_{24,3}$

We have

$$G(1) = G(1, 24, \chi_{24,3}) = \frac{1}{\eta_{24;1,5}(\tau)} = \frac{q^{-37/24}}{(q, q^5, q^{19}, q^{23}; q^{24})_\infty}, \quad \text{and}$$
$$H(1) = H(1, 24, \chi_{24,3}) = \frac{1}{\eta_{24;7,11}(\tau)} = \frac{q^{35/24}}{(q^7, q^{11}, q^{13}, q^{17}; q^{24})_\infty}.$$

Type 1

$$G(2)\,H(1) - G(1)\,H(2) = \frac{\eta(3\tau)\eta(4\tau)^2}{\eta(2\tau)\eta(24\tau)^2}, \qquad \Gamma_1(48), \qquad -B = 24, \tag{4.81}$$

$$G(2)\,H(1) + G(1)\,H(2) = \frac{\eta(6\tau)^3\eta(8\tau)\eta(12\tau)}{\eta(2\tau)\eta(3\tau)\eta(24\tau)^3}, \qquad \Gamma_1(48), \qquad -B = 24, \tag{4.82}$$

$$G(3)\,H(1) - G(1)\,H(3) = \frac{\eta(6\tau)^2\eta(8\tau)\eta(9\tau)\eta(36\tau)}{\eta(3\tau)\eta(18\tau)\eta(24\tau)^2\eta(72\tau)}, \qquad \Gamma_1(72), \qquad -B = 72. \tag{4.83}$$

Type 2

$$G(1)\,G(1) - H(1)\,H(1) = \frac{\eta(2\tau)^2\eta(3\tau)^2\eta(8\tau)\eta(12\tau)^3}{\eta(\tau)^2\eta(6\tau)\eta(24\tau)^5}, \qquad \Gamma_1(24), \qquad -B = 12. \tag{4.84}$$

Type 6

$$G(1)\,H^*(1) - G^*(1)\,H(1) = 2\,\frac{\eta(6\tau)^2\eta(8\tau)^2\eta(12\tau)\eta(48\tau)^3}{\eta(2\tau)\eta(16\tau)\eta(24\tau)^6}, \qquad \Gamma_1(48), \qquad -B = 24, \tag{4.85}$$

$$G(1)\,H^*(1) + G^*(1)\,H(1) = 2\,\frac{\eta(4\tau)\eta(8\tau)\eta(12\tau)^3\eta(48\tau)^2}{\eta(2\tau)\eta(24\tau)^6}, \qquad \Gamma_1(48), \qquad -B = 24. \tag{4.86}$$

Type 7

$$G^*(1)\,G(1) - H^*(1)\,H(1) = \frac{\eta(4\tau)\eta(6\tau)^2\eta(16\tau)\eta(24\tau)^3}{\eta(2\tau)\eta(8\tau)\eta(12\tau)^2\eta(48\tau)^3}, \quad \Gamma_1(48), \quad -B = 24, \tag{4.87}$$

$$G^*(1)\,G(1) + H^*(1)\,H(1) = \frac{\eta(4\tau)\eta(8\tau)\eta(12\tau)}{\eta(2\tau)\eta(48\tau)^2}, \quad \Gamma_1(48), \quad -B = 24. \tag{4.88}$$

Type 8

$$G(1)^2\,H(2) - H(1)^2\,G(2) = 2\,\frac{\eta(3\tau)\eta(6\tau)\eta(8\tau)^2\eta(12\tau)\eta(48\tau)^3}{\eta(\tau)\eta(16\tau)\eta(24\tau)^6}, \quad \Gamma_1(48), \quad -B = 24, \tag{4.89}$$

$$G(1)^2\,H(2) + H(1)^2\,G(2) = 2\,\frac{\eta(3\tau)\eta(4\tau)\eta(8\tau)\eta(12\tau)^3\eta(48\tau)^2}{\eta(\tau)\eta(6\tau)\eta(24\tau)^6}, \quad \Gamma_1(48), \quad -B = 24. \tag{4.90}$$

4.9 Mod 26

There is only one non-principal character mod 26 that satisfies $\chi(-1) = 1$, namely the character χ_{26} induced by $\left(\frac{\cdot}{13}\right)$. In this section

$$G(1) = G(1, 26, \chi_{26}) = \frac{1}{\eta_{26;1,3,9}(\tau)} = \frac{q^{-7/4}}{(q, q^3, q^9, q^{17}, q^{23}, q^{25}; q^{26})_\infty}, \quad \text{and}$$
$$H(1) = H(1, 26, \chi_{26}) = \frac{1}{\eta_{26;5,7,11}(\tau)} = \frac{q^{5/4}}{(q^5, q^7, q^{11}, q^{15}, q^{19}, q^{21}; q^{26})_\infty}.$$

We find only one identity.

4.9.1 Type 10

$$\frac{G(3)\,H(2) - H(3)\,G(2)}{G(6)\,H^*(1) + H(6)\,G^*(1)} = \frac{\eta(26\tau)^3\eta(156\tau)^3}{\eta(52\tau)^3\eta(78\tau)^3}, \quad \Gamma_1(156), \quad -B = 576. \tag{4.91}$$

4.10 Mod 28

There is only one non-principal character mod 28 that satisfies $\chi(-1) = 1$, namely the character $\chi(\cdot) = \left(\frac{28}{\cdot}\right)$. In this section

$$G(1) = G\left(1, 28, \left(\frac{28}{\cdot}\right)\right) = \frac{1}{\eta_{28;1,3,9}(\tau)} = \frac{q^{-17/8}}{(q, q^3, q^9, q^{19}, q^{25}, q^{27}; q^{28})_\infty}, \quad \text{and}$$
$$H(1) = H\left(1, 28, \left(\frac{28}{\cdot}\right)\right) = \frac{1}{\eta_{28;5,11,13}(\tau)} = \frac{q^{15/8}}{(q^5, q^{11}, q^{13}, q^{15}, q^{17}, q^{23}; q^{28})_\infty}.$$

4.10.1 Type 1

$$G(2)\, H(1) - G(1)\, H(2) = \frac{\eta(4\tau)^2\eta(7\tau)\eta(14\tau)}{\eta(2\tau)\eta(28\tau)^3}, \qquad \Gamma_1(56), \qquad -B = 48. \tag{4.92}$$

4.10.2 Type 6

$$G(1)\, H^*(1) - G^*(1)\, H(1) = 2\, \frac{\eta(4\tau)^4\eta(14\tau)^3\eta(56\tau)^3}{\eta(2\tau)^2\eta(8\tau)\eta(28\tau)^7}, \quad \Gamma_1(56), \quad -B = 48. \tag{4.93}$$

4.10.3 Type 7

$$G^*(1)\, G(1) - H^*(1)\, H(1) = \frac{\eta(4\tau)\eta(8\tau)\eta(28\tau)^2}{\eta(2\tau)\eta(56\tau)^3}, \quad \Gamma_1(56), \quad -B = 48. \tag{4.94}$$

4.10.4 Type 8

$$G(1)^2\, H(2) - H(1)^2\, G(2) = 2\, \frac{\eta(4\tau)^4\eta(7\tau)\eta(14\tau)^2\eta(56\tau)^3}{\eta(\tau)\eta(2\tau)\eta(8\tau)\eta(28\tau)^7}, \quad \Gamma_1(56), \quad -B = 48. \tag{4.95}$$

4.11 Mod 30

There is only one real non-principal character mod 30 that satisfies $\chi(-1) = 1$, namely the character χ_{30} induced by the Legendre symbol mod 5. Thus in this section

$$G(1) = G(1, 30, \chi_{30}) = \frac{1}{\eta_{30;1,11}(\tau)} = \frac{q^{-31/30}}{(q, q^{11}, q^{19}, q^{29}; q^{30})_\infty}, \quad \text{and}$$
$$H(1) = H(1, 30, \chi_{30}) = \frac{1}{\eta_{30;7,13}(\tau)} = \frac{q^{41/30}}{(q^7, q^{13}, q^{17}, q^{23}; q^{30})_\infty}.$$

4.11.1 Type 6

$$G(1)\, H^*(1) - G^*(1)\, H(1) = 2\,\frac{\eta(4\tau)\eta(6\tau)^2\eta(60\tau)^2}{\eta(2\tau)\eta(12\tau)\eta(30\tau)^3}, \quad \Gamma_1(60), \quad -B = 48. \tag{4.96}$$

4.11.2 Type 8

$$G(1)^2\, H(2) - H(1)^2\, G(2) = 2\,\frac{\eta(3\tau)\eta(4\tau)\eta(5\tau)\eta(6\tau)\eta(60\tau)^2}{\eta(\tau)\eta(10\tau)\eta(12\tau)\eta(15\tau)\eta(30\tau)^2}, \quad \Gamma_1(60), \quad -B = 48. \tag{4.97}$$

4.12 Mod 34

There is only one real non-principal character mod 34 that satisfies $\chi(-1) = 1$, namely the character χ_{34} induced by the Legendre symbol mod 17.

$$\begin{aligned} G(1) = G(1, 34, \chi_{34}) &= \frac{1}{\eta_{34;1,9,13,15}(\tau)} \\ &= \frac{q^{2/3}}{(q, q^9, q^{13}, q^{15}, q^{19}, q^{21}, q^{25}, q^{33}; q^{34})_\infty}, \quad \text{and} \end{aligned}$$

$$\begin{aligned} H(1) = H(1, 34, \chi_{34}) &= \frac{1}{\eta_{34;3,5,7,11}(\tau)} \\ &= \frac{q^{-4/3}}{(q^3, q^5, q^7, q^{11}, q^{23}, q^{27}, q^{29}, q^{31}; q^{34})_\infty}. \end{aligned}$$

4.12.1 Type 1

$$G(2)\,H(1) - G(1)\,H(2) = -\frac{\eta(2\tau)^2\eta(17\tau)}{\eta(\tau)\eta(34\tau)^2}, \qquad \Gamma_1(68), \qquad -B = 64. \quad (4.98)$$

4.12.2 Type 7

$$G^*(1)\,G(1) - H^*(1)\,H(1) = -\frac{\eta(4\tau)}{\eta(68\tau)}, \quad \Gamma_1(68), \quad -B = 64. \qquad (4.99)$$

4.12.3 Type 9

$$G(1)^2\,H(1) - H(1)^2\,G(1) = -\frac{\eta(2\tau)^2\eta(17\tau)}{\eta(\tau)\eta(34\tau)^2}, \quad \Gamma_1(34), \quad -B = 16. \quad (4.100)$$

4.13 Mod 40

There are three real non-principal characters mod 40 that satisfy $\chi(-1) = 1$.

(i) The character $\chi_{40,1}(\cdot)$ induced by $\left(\frac{\cdot}{5}\right)$. This is actually a character mod 10. See Sect. 4.2.
(ii) The character $\chi_{40,2}(\cdot)$ induced by $\left(\frac{8}{\cdot}\right)$.
(iii) The character $\chi_{40,3}(\cdot) = \left(\frac{40}{\cdot}\right)$.

4.13.1 $\chi_{40,2}$

$$\begin{aligned} G(1) = G(1, 40, \chi_{40,2}) &= \frac{1}{\eta_{40;1,7,9,17}(\tau)} \\ &= \frac{q^{-19/12}}{(q, q^7, q^9, q^{17}, q^{23}, q^{31}, q^{33}, q^{39}; q^{40})_\infty}, \quad \text{and} \end{aligned}$$

$$H(1) = H(1, 40, \chi_{40,2}) = \frac{1}{\eta_{40;3,11,13,19}(\tau)}$$
$$= \frac{q^{17/12}}{(q^3, q^{11}, q^{13}, q^{19}, q^{21}, q^{27}, q^{29}, q^{37}; q^{40})_\infty}.$$

Type 1

$$G(2)\,H(1) - G(1)\,H(2) = \frac{\eta(4\tau)^2\eta(10\tau)^2}{\eta(2\tau)\eta(8\tau)\eta(20\tau)\eta(40\tau)}, \qquad \Gamma_1(80), \qquad -B = 80. \tag{4.101}$$

Type 6

$$G(1)\,H^*(1) + G^*(1)\,H(1) = 2\,\frac{\eta(8\tau)^3\eta(10\tau)\eta(20\tau)^3\eta(80\tau)^3}{\eta(2\tau)\eta(16\tau)\eta(40\tau)^8}, \quad \Gamma_1(80), \quad -B = 112. \tag{4.102}$$

Type 7

$$G^*(1)\,G(1) + H^*(1)\,H(1) = \frac{\eta(4\tau)\eta(8\tau)\eta(10\tau)}{\eta(2\tau)\eta(16\tau)\eta(80\tau)}, \quad \Gamma_1(80), \quad -B = 80. \tag{4.103}$$

Type 8

$$G(1)^2\,H(2) + H(1)^2\,G(2) = 2\,\frac{\eta(4\tau)^2\eta(5\tau)\eta(16\tau)\eta(20\tau)\eta(80\tau)}{\eta(\tau)\eta(8\tau)^2\eta(40\tau)^3}, \quad \Gamma_1(80), \quad -B = 80. \tag{4.104}$$

4.13.2 $\chi_{40,3}$

$$G(1) = G(1, 40, \chi_{40,3}) = \frac{1}{\eta_{40;1,3,9,13}(\tau)},$$
$$= \frac{q^{-43/12}}{(q, q^3, q^9, q^{13}, q^{27}, q^{31}, q^{37}, q^{39}; q^{40})_\infty}, \quad \text{and}$$

$$H(1) = H(1, 40, \chi_{40,3}) = \frac{1}{\eta_{40;7,11,17,19}(\tau)}$$
$$= \frac{q^{41/12}}{(q^7, q^{11}, q^{17}, q^{19}, q^{21}, q^{23}, q^{29}, q^{33}; q^{40})_\infty}.$$

Type 1

$$G(2)\,H(1) - G(1)\,H(2) = \frac{\eta(4\tau)\eta(8\tau)\eta(10\tau)^2}{\eta(2\tau)\eta(40\tau)^3}, \qquad \Gamma_1(80), \qquad -B = 112. \tag{4.105}$$

Type 6

$$G(1)\,H^*(1) + G^*(1)\,H(1) = 2\,\frac{\eta(8\tau)^3\eta(10\tau)\eta(20\tau)^3\eta(80\tau)^3}{\eta(2\tau)\eta(16\tau)\eta(40\tau)^8}, \quad \Gamma_1(80), \quad -B = 112. \tag{4.106}$$

Type 7

$$G^*(1)\,G(1) + H^*(1)\,H(1) = \frac{\eta(4\tau)\eta(10\tau)\eta(16\tau)\eta(40\tau)}{\eta(2\tau)\eta(80\tau)^3}, \quad \Gamma_1(80), \quad -B = 112. \tag{4.107}$$

Type 8

$$G(1)^2\,H(2) + H(1)^2\,G(2) = 2\,\frac{\eta(5\tau)\eta(8\tau)^3\eta(20\tau)^3\eta(80\tau)^3}{\eta(\tau)\eta(16\tau)\eta(40\tau)^8}, \quad \Gamma_1(80), \quad -B = 112. \tag{4.108}$$

4.14 *Mod* 42

There is only one real non-principal character mod 42 that satisfies $\chi(-1) = 1$, namely the one induced by the mod 21 character $\chi_{42}(\cdot) = \left(\frac{\cdot}{3}\right)\left(\frac{\cdot}{7}\right)$.

In this section

$$G(1) = G(1, 42, \chi_{42}) = \frac{1}{\eta_{42;1,5,17}(\tau)} = \frac{q^{-11/4}}{(q, q^5, q^{17}, q^{25}, q^{37}, q^{41}; q^{42})_\infty}, \quad \text{and}$$

$$H(1) = H(1, 42, \chi_{42}) = \frac{1}{\eta_{42;11,13,19}(\tau)} = \frac{q^{13/4}}{(q^{11}, q^{13}, q^{19}, q^{23}, q^{29}, q^{31}; q^{42})_\infty}.$$

4.14.1 Type 1

$$G(2)\,H(1) - G(1)\,H(2) = \frac{\eta(4\tau)\eta(6\tau)^2\eta(7\tau)}{\eta(2\tau)\eta(12\tau)\eta(21\tau)\eta(42\tau)}, \qquad \Gamma_1(84), \qquad -B = 96. \tag{4.109}$$

4.14.2 Type 7

$$G^*(1)\,G(1) - H^*(1)\,H(1) = \frac{\eta(4\tau)\eta(6\tau)\eta(28\tau)}{\eta(2\tau)\eta(84\tau)^2}, \quad \Gamma_1(84), \quad -B = 96. \tag{4.110}$$

4.15 Mod 56

There are three real non-principal characters mod 56 that satisfy $\chi(-1) = 1$.

(i) The character $\left(\frac{56}{\cdot}\right)$.
(ii) The character induced by the mod 28 character $\left(\frac{28}{\cdot}\right)$. See Sect. 4.10.
(iii) The character induced by the mod 8 character $\left(\frac{8}{\cdot}\right)$.

Only the third character led to new identities. In this section we assume χ is the mod 56 character induced by $\left(\frac{8}{\cdot}\right)$. Thus in this section

$$\begin{aligned} G(1,56,\chi) = G(1) &= \frac{1}{\eta_{56;1,9,15,17,23,25}(\tau)} \\ &= \frac{q^{11/8}}{(q,q^9,q^{15},q^{17},q^{23},q^{25},q^{31},q^{33},q^{39},q^{41},q^{47},q^{55};q^{56})_\infty}, \quad \text{and} \end{aligned}$$

$$\begin{aligned} H(1,56,\chi) = H(1) &= \frac{1}{\eta_{56;3,5,11,13,19,27}(\tau)} \\ &= \frac{q^{-13/8}}{(q^3,q^5,q^{11},q^{13},q^{19},q^{27},q^{29},q^{37},q^{43},q^{45},q^{51},q^{53};q^{56})_\infty} \end{aligned}$$

4.15.1 Type 1

$$G(2)\,H(1) + G(1)\,H(2) = \frac{\eta(2\tau)\eta(4\tau)\eta(14\tau)}{\eta(\tau)\eta(8\tau)\eta(56\tau)}, \qquad \Gamma_1(112), \qquad -B = 144. \tag{4.111}$$

4.15.2 Type 6

$$G(1)\,H^*(1) - G^*(1)\,H(1) = 2\,\frac{\eta(4\tau)\eta(14\tau)\eta(16\tau)\eta(112\tau)}{\eta(8\tau)^2\eta(56\tau)^2},$$
$$\Gamma_1(112), \quad -B = 144. \tag{4.112}$$

4.15.3 Type 7

$$G^*(1)\,G(1) - H^*(1)\,H(1) = -\frac{\eta(8\tau)\eta(14\tau)\eta(56\tau)}{\eta(16\tau)\eta(28\tau)\eta(112\tau)}, \quad \Gamma_1(112), \quad -B = 144. \tag{4.113}$$

4.15.4 Type 8

$$G(1)^2\,H(2) - H(1)^2\,G(2) = 2\,\frac{\eta(2\tau)\eta(4\tau)\eta(7\tau)\eta(16\tau)\eta(112\tau)}{\eta(\tau)\eta(8\tau)^2\eta(56\tau)^2},$$
$$\Gamma_1(112), \quad -B = 144. \tag{4.114}$$

4.16 Mod 60

There are three real non-principal characters mod 60 that satisfy $\chi(-1) = 1$.

(i) The character induced by $\left(\frac{\cdot}{5}\right)$.
(ii) The character $\chi_{60,2}(\cdot) = \left(\frac{60}{\cdot}\right)$.
(iii) The character $\chi_{60,3}(\cdot)$ induced by the mod 12 character $\left(\frac{12}{\cdot}\right)$.

Only (ii), (iii) seem to lead to new identities.

4.16.1 $\chi_{60,2}$

In this section

$$G(1, 60, \chi_{60,2}) = G(1) = \frac{1}{\eta_{60;1,7,11,17}(\tau)}$$
$$= \frac{q^{-35/6}}{(q, q^7, q^{11}, q^{17}, q^{43}, q^{49}, q^{53}, q^{59}; q^{60})_\infty}, \quad \text{and}$$

$$H(1, 60, \chi_{60,2}) = H(1) = \frac{1}{\eta_{60;13,19,23,29}(\tau)}$$
$$= \frac{q^{37/6}}{(q^{13}, q^{19}, q^{23}, q^{29}, q^{31}, q^{37}, q^{41}, q^{47}; q^{60})_\infty}.$$

Type 1

$$G(2)\,H(1) - G(1)\,H(2) = \frac{\eta(4\tau)\eta(6\tau)\eta(10\tau)\eta(30\tau)}{\eta(2\tau)\eta(60\tau)^3}, \qquad \Gamma_1(120), \qquad -B = 192. \tag{4.115}$$

Type 6

$$G(1)\,H^*(1) - G^*(1)\,H(1) = 2\,\frac{\eta(4\tau)\eta(12\tau)^2\eta(20\tau)^2\eta(30\tau)^3\eta(120\tau)^4}{\eta(2\tau)\eta(24\tau)\eta(40\tau)\eta(60\tau)^9},$$
$$\Gamma_1(120), \quad -B = 192. \tag{4.116}$$

Type 7

$$G^*(1)\,G(1) - H^*(1)\,H(1) = \frac{\eta(4\tau)\eta(6\tau)\eta(10\tau)\eta(24\tau)\eta(40\tau)\eta(60\tau)^3}{\eta(2\tau)\eta(12\tau)\eta(20\tau)\eta(30\tau)\eta(120\tau)^4},$$
$$\Gamma_1(120), \quad -B = 192. \tag{4.117}$$

Type 8

$$G(1)^2\,H(2) - H(1)^2\,G(2)$$
$$= 2\,\frac{\eta(3\tau)\eta(4\tau)\eta(5\tau)\eta(12\tau)^2\eta(20\tau)^2\eta(30\tau)^4\eta(120\tau)^4}{\eta(\tau)\eta(6\tau)\eta(10\tau)\eta(15\tau)\eta(24\tau)\eta(40\tau)\eta(60\tau)^9},$$
$$\Gamma_1(120), \quad -B = 192. \tag{4.118}$$

4.16.2 $\chi_{60,3}$

In this section

$$G(1, 60, \chi_{60,3}) = G(1) = \frac{1}{\eta_{60;1,11,13,23}(\tau)}$$
$$= \frac{q^{-17/6}}{(q, q^{11}, q^{13}, q^{23}, q^{37}, q^{47}, q^{49}, q^{59}; q^{60})_\infty}, \quad \text{and}$$

$$H(1, 60, \chi_{60,3}) = H(1) = \frac{1}{\eta_{60;7,17,19,29}(\tau)}$$
$$= \frac{q^{19/6}}{(q^7, q^{17}, q^{19}, q^{29}, q^{31}, q^{41}, q^{43}, q^{53}; q^{60})_\infty}.$$

Type 1

$$G(2)\,H(1) - G(1)\,H(2) = \frac{\eta(4\tau)\eta(6\tau)^2\eta(10\tau)}{\eta(2\tau)\eta(12\tau)^2\eta(60\tau)}, \qquad \Gamma_1(120), \qquad -B = 160. \tag{4.119}$$

Type 6

$$G(1)\,H^*(1) - G^*(1)\,H(1) = 2\,\frac{\eta(4\tau)\eta(6\tau)^2\eta(20\tau)^2\eta(24\tau)\eta(30\tau)\eta(120\tau)^2}{\eta(2\tau)\eta(12\tau)^3\eta(40\tau)\eta(60\tau)^4},$$
$$\Gamma_1(120), \quad -B = 160. \tag{4.120}$$

Type 7

$$G^*(1)\,G(1) - H^*(1)\,H(1) = \frac{\eta(4\tau)\eta(6\tau)\eta(10\tau)\eta(40\tau)\eta(60\tau)^2}{\eta(2\tau)\eta(20\tau)\eta(24\tau)\eta(30\tau)\eta(120\tau)^2},$$
$$\Gamma_1(120), \quad -B = 160. \tag{4.121}$$

Type 8

$$G(1)^2\,H(2) - H(1)^2\,G(2)$$
$$= 2\,\frac{\eta(3\tau)\eta(4\tau)\eta(5\tau)\eta(6\tau)\eta(20\tau)^2\eta(24\tau)\eta(30\tau)^2\eta(120\tau)^2}{\eta(\tau)\eta(10\tau)\eta(12\tau)^3\eta(15\tau)\eta(40\tau)\eta(60\tau)^4},$$
$$\Gamma_1(120), \quad -B = 160. \tag{4.122}$$

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The Generators of all Polynomial Relations Among Jacobi Theta Functions

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Abstract In this article, we consider the classical Jacobi theta functions $\theta_i(z)$, $i = 1, 2, 3, 4$ and show that the ideal of all polynomial relations among them with coefficients in $K := \mathbb{Q}(\theta_2(0|\tau), \theta_3(0|\tau), \theta_4(0|\tau))$ is generated by just two polynomials, that correspond to well known identities among Jacobi theta functions.

1 Introduction

Let $\theta_j(z|\tau)$ ($j = 1, \ldots, 4$, $z \in \mathbb{C}$, $\tau \in \mathbb{H}$) denote the four classical Jacobi theta functions where $\mathbb{H}$ denotes the upper complex half plane. In this article we show that if $p \in K[T_1, T_2, T_3, T_4]$ is a polynomial with coefficients in $K := \mathbb{Q}(\theta_2(0|\tau), \theta_3(0|\tau), \theta_4(0|\tau))$ such that for every $z \in \mathbb{C}$ and every $\tau \in \mathbb{H}$

$$p(\theta_1(z|\tau), \theta_2(z|\tau), \theta_3(z|\tau), \theta_4(z|\tau)) = 0, \tag{1}$$

then $p = p_1 b_1 + p_2 b_2$ for some $p_1, p_2 \in K[T_1, T_2, T_3, T_4]$ where

$$b_1 := \theta_2(0|\tau)^2\, T_2^2 - \theta_3(0|\tau)^2\, T_3^2 + \theta_4(0|\tau)^2\, T_4^2, \tag{2}$$

$$b_2 := \theta_2(0|\tau)^2\, T_1^2 + \theta_4(0|\tau)^2\, T_3^2 - \theta_3(0|\tau)^2\, T_4^2. \tag{3}$$

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Note that b_1 and b_2 correspond to [1, Eq. 20.7.1] and [1, Eq. 20.7.2], respectively.

The polynomials b_1 and b_2 form a Gröbner basis of the ideal of all such relations. Thus, one can check whether a relation of the form (1) holds by simply reducing p by b_1 and b_2. The result of the reduction is zero if and only if the identity holds.

After introducing some notation, we give the precise formulation of our problem in Sect. 2. In Sect. 3, we reduce the problem of finding relations among theta functions to finding relations among quotients of theta functions that, additionally are elliptic. In Sect. 4, we then show that the ideal of relations among elliptic theta quotients is generated by two elements. These two elements are then used to setup the generators for the ideal of polynomial relations among Jacobi theta functions in Sect. 5. To actually, compute the Gröbner basis of this ideal, we show computability of K in Sect. 6. Eventually, we show the steps to compute the polynomials b_1 and b_2 in the computer algebra system FriCAS.

2 Notation and Problem Formulation

The classical Jacobi theta functions $\theta_j(z|\tau)$ $(j = 1, \dots, 4)$ are defined as follows.

Definition 1 (*cf.* [1, Eq. 20.2(i)]) Let $\tau \in \mathbb{H} := \{z \in \mathbb{C} \mid \Im(z) > 0\}$ and $q := e^{\pi i \tau}$, then

$$\theta_1(z, q) := \theta_1(z|\tau) := 2\sum_{n=0}^{\infty}(-1)^n q^{(n+\frac{1}{2})^2}\sin((2n+1)z),$$

$$\theta_2(z, q) := \theta_2(z|\tau) := 2\sum_{n=0}^{\infty} q^{(n+\frac{1}{2})^2}\cos((2n+1)z),$$

$$\theta_3(z, q) := \theta_3(z|\tau) := 1 + 2\sum_{n=1}^{\infty} q^{n^2}\cos(2nz),$$

$$\theta_4(z, q) := \theta_4(z|\tau) := 1 + 2\sum_{n=1}^{\infty}(-1)^n q^{n^2}\cos(2nz).$$

For simplicity, we write $\theta_j(z) := \theta_j(z|\tau)$.

Throughout the paper, we use multi-index notation, i.e., for $n \in \mathbb{N}$, $\alpha \in \mathbb{Z}^n$ and objects $x_1, \dots, x_n$ we simply write x^α instead of $x_1^{\alpha_1} \dots x_n^{\alpha_n}$. We mostly use $n = 3$ or $n = 4$. In particular, if $\alpha \in \mathbb{Z}^4$,

$$\theta(z)^\alpha := \theta_1(z)^{\alpha_1}\theta_2(z)^{\alpha_2}\theta_3(z)^{\alpha_3}\theta_4(z)^{\alpha_4}. \tag{4}$$

If L is a ring and S is a subset of an L-module, we denote by $\langle S\rangle_L$ the set of L-linear combinations of elements of S. If L is a field, then $\langle S\rangle_L$ is a vector space. If $S \subset L$, then $\langle S\rangle_L$ is an ideal of L.

We define the field $K := \mathbb{Q}(\theta_2(0), \theta_3(0), \theta_4(0))$ and set

$$\begin{aligned}
&\theta := \{\theta_i(z) \mid i = 1, 2, 3, 4\}, \\
&T := \{T_1, T_2, T_3, T_4\}, \\
&\phi : K[T] \to K[\theta], \quad T_i \mapsto \theta_i(z), \quad i = 1, 2, 3, 4.
\end{aligned}$$

The problem we are dealing with in this article is to determine (algorithmically) the set $\ker\phi \subset K[T]$. Note that $\ker\phi$ is an ideal of $K[T]$ and, thus, by Hilbert's basis theorem, finitely generated.

In order to describe $\ker\phi$, we first consider the map

$$\Phi : K[T, T^{-1}] \to K[\theta, \theta^{-1}], \quad T_i \mapsto \theta_i(z), \quad i = 1, 2, 3, 4.$$

Note that $\phi = \Phi|_{K[T]}$ and $\ker\phi = \ker\Phi \cap K[T]$. Define $L := K[T, T^{-1}]$. For $p \in L$, we sometimes write $p(\theta)$ instead of $\Phi(p)$.

3 Reduction to Elliptic Theta Quotients

Definition 2 A meromorphic function f on $\mathbb{C}$ is called *elliptic*, if there are two non-complex numbers ω_1 and ω_2 with $\frac{\omega_1}{\omega_2} \notin \mathbb{R}$ such that $f(z + \omega_1) = f(z)$ and $f(z + \omega_2) = f(z)$ for all $z \in \mathbb{C}$.

In [2], an algorithm was given to decide whether $f = 0$ for $f \in K[\theta]$ by reducing the problem to such f that are additionally, "quasi-elliptic" functions. More precisely, for our problem it is enough to find all relations among quotients of theta functions that are elliptic.

In view of the following lemma, we can connect theta functions with elliptic functions. Note that whenever we say elliptic function, we mean elliptic function with respect to the argument z.

Lemma 1 (cf. [3, p. 465]) *Let $N := e^{-\pi i\tau - 2iz}$. For $j \in \{1, 2, 3, 4\}$ we have $\theta_j(z + \pi\tau|\tau) = \varepsilon_1(j)\theta_j(z|\tau)$ and $\theta_j(z + \pi|\tau) = \varepsilon_2(j)\theta_j(z|\tau)$ where $\varepsilon_1(j)$ and $\varepsilon_2(j)$ are defined in the following table.*

j	1	2	3	4
$\varepsilon_1(j)$	$-N$	N	N	$-N$
$\varepsilon_2(j)$	-1	-1	1	1

Definition 3 (*cf.* [2, Def. 2.2]) Given $\alpha, \beta \in \mathbb{Z}^4$, we say that α and β are similar, denoted by $\alpha \sim \beta$, if $\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 = \beta_1 + \beta_2 + \beta_3 + \beta_4$, $\alpha_1 + \alpha_2 \equiv \beta_1 + \beta_2 \pmod 2$, and $\alpha_1 + \alpha_4 \equiv \beta_1 + \beta_4 \pmod 2$.

It is easy to prove that $\sim$ is a congruence relation on the $\mathbb{Z}$-module $\mathbb{Z}^4$.

The conditions in Definition 3 have been chosen according to the table in Lemma 1, so that $\theta(z)^\alpha$ is elliptic if $\alpha \sim 0$, cf. Lemma 3.1 in [2]. Similar to Definition 4.1 in [2] we define $R^* := \left\{\alpha \in \mathbb{Z}^4 \,\middle|\, \alpha \sim 0\right\}$.

Theorem 2.7 from [2] can be formulated as follows.

Theorem 1 *Let M be a finite subset of $\mathbb{Z}^4$, $M/\!\sim = \{M_1, \ldots, M_n\}$. For $i \in \{1, \ldots, n\}$ let $p_i = \sum_{\alpha \in M_i} c_\alpha T^\alpha$ with $c_\alpha \in K$ and let $p = \sum_{i=1}^n p_i$. Then $p(\theta) = 0$ if and only if $p_i(\theta) = 0$ for all $i \in \{1, \ldots, n\}$.*

With the same notation as in Theorem 1 we can write

$$p = \sum_{i=1}^{n} p_i = \sum_{i=1}^{n} T^{\beta_i} \frac{p_i}{T^{\beta_i}} = \sum_{i=1}^{n} T^{\beta_i} \sum_{\alpha \in M_i} c_\alpha T^{\alpha - \beta_i}$$

for some $\beta_i \in M_i$. Note that if $\alpha \in M_i$, then $\alpha - \beta_i \in R^*$.

Let L^* be the set of K-linear combinations of monomials $T^\alpha \in L$ with $\alpha \in R^*$. Theorem 1 says that $\ker \Phi = \langle L^* \cap \ker \Phi \rangle_L$.

Lemma 2 (cf. [2, Lemma 4.2]) *The set R^* forms an (additive) $\mathbb{Z}$-module that is generated by the vectors $\iota_1 = (-2, 2, 0, 0)$, $\iota_2 = (-2, 0, 2, 0)$, $\iota_3 = (-3, 1, 1, 1)$, i.e., $R^* = \langle \iota_1, \iota_2, \iota_3 \rangle_{\mathbb{Z}}$.*

Proof Clearly, $\langle \iota_1, \iota_2, \iota_3 \rangle_{\mathbb{Z}} \subseteq R^*$. For $R^* \subseteq \langle \iota_1, \iota_2, \iota_3 \rangle_{\mathbb{Z}}$ note that if $\alpha \in R^*$, then

$$\alpha = \iota_1 \frac{\alpha_2 - \alpha_4}{2} + \iota_2 \frac{\alpha_3 - \alpha_4}{2} + \iota_3 \alpha_4.$$

4 The Ideal of Relations Among Elliptic Theta Quotients

From Lemma 2 follows $L^* = K[T^{\iota_1}, T^{\iota_2}, T^{\iota_3}]$, i.e.,

$$\ker \Phi = \langle K[T^{\iota_1}, T^{\iota_2}, T^{\iota_3}] \cap \ker \Phi \rangle_L \,.$$

In other words, any relation among theta functions can be expressed as a L-linear combination of polynomials in $T^{\iota_1}, T^{\iota_2}, T^{\iota_3}$ whose coefficients are in K. We would like to find polynomials p in $T^{\iota_1}, T^{\iota_2}, T^{\iota_3}$ such that $\Phi(p) = 0$.

Let us define the elliptic functions corresponding to the above generators.

$$\begin{aligned} j_1(z) &:= \Phi(T^{\iota_1}) = \theta(z)^{\iota_1} = \frac{\theta_2(z)^2}{\theta_1(z)^2}, \\ j_2(z) &:= \Phi(T^{\iota_1}) = \theta(z)^{\iota_2} = \frac{\theta_3(z)^2}{\theta_1(z)^2}, \end{aligned}$$

$$j_3(z) := \Phi(T^{\iota_1}) = \theta(z)^{\iota_2} = \frac{\theta_2(z)\theta_3(z)\theta_4(z)}{\theta_1(z)^3}.$$

Let $J = \{J_1, J_2, J_3\}$ be a new set of indeterminates. As an intermediate step to solve our original problem, we consider the map $\Psi : K[J, J^{-1}] \to K[\theta, \theta^{-1}]$, which is defined by $\Psi = \Phi \circ \sigma$ for the ring homomorphism $\sigma : K[J, J^{-1}] \to L^*$, $J_i \mapsto T^{\iota_i}$, $i = 1, 2, 3$. Note that because $L^* = K[T^{\iota_1}, T^{\iota_2}, T^{\iota_3}]$, σ is surjective, i.e., $p \in K[T^{\iota_1}, T^{\iota_2}, T^{\iota_3}] \cap \ker \Phi$, there exists $f \in K[J, J^{-1}]$ such that $\sigma(f) = p$. Therefore, $\sigma(\ker \Psi) = K[T^{\iota_1}, T^{\iota_2}, T^{\iota_3}] \cap \ker \Phi$.

Clearly, Ψ maps J_i to $j_i(z)$, $i = 1, 2, 3$. In the following we are going to show that $\ker \Psi$ is an ideal in $K[J, J^{-1}]$ that is generated by the two polynomial

$$h_1 := J_2 - c_3 J_1 - c_4, \tag{5}$$

$$h_2 := J_3^2 - J_1 J_2(c_4 J_1 + c_3) \tag{6}$$

where $c_3 = \frac{\theta_3(0)^2}{\theta_2(0)^2}$, $c_4 = \frac{\theta_4(0)^2}{\theta_2(0)^2}$.

Let $I_\Psi := \langle h_1, h_2 \rangle_{K[J,J^{-1}]}$. One can verify by Algorithm 6.6 from [2] that $\Psi(h_1) = 0$, and $\Psi(h_2) = 0$. Hence $I_\Psi \subseteq \ker \Psi$. In order to prove $\ker \Psi \subseteq I_\Psi$, assume that $f \in \ker \Psi$. Because $h_1 \in I_\Psi$, we have

$$f(J_1, J_2, J_3) + I_\Psi = f(J_1, c_3 J_1 + c_4, J_3) + I_\Psi = J_1^{\alpha_1} J_3^{\alpha_3}\, \tilde{f}(J_1, J_3) + I_\Psi$$

for some $\alpha_1, \alpha_3 \in \mathbb{Z}$ and $\tilde{f} \in K[J_1, J_3]$.

Clearly, we can split $\tilde{f}$ with respect to even and odd powers of J_3 in such a way that for some polynomials $\tilde{f}_1$ and $\tilde{f}_2$ we have the representation

$$\tilde{f}(J_1, J_3) = \tilde{f}_1(J_1, J_3^2) + J_3 \tilde{f}_2(J_1, J_3^2).$$

Since $h_1, h_2 \in I_\Psi$, we can replace J_3^2 by $J_1(c_3 J_1 + c_4)(c_4 J_1 + c_3) \in K[J_1]$ and obtain

$$\tilde{f}(J_1, J_3) + I_\Psi = f_1(J_1) + J_3 f_2(J_1) + I_\Psi$$

for some $f_1, f_2 \in K[J_1]$. Hence,

$$f(J_1, J_2, J_3) + I_\Psi = J_1^{\alpha_1} J_3^{\alpha_3}\, (f_1(J_1) + J_3 f_2(J_1)) + I_\Psi$$

From $f \in \ker \Psi$ and $I_\Psi \subseteq \ker \Psi$, we conclude

$$j_1^{\alpha_1} j_3^{\alpha_3}\, (f_1(j_1) + j_3 f_2(j_1)) = 0.$$

Since $j_1^{\alpha_1} j_3^{\alpha_3}$ is a nonzero meromorphic function, it follows that

$$f_1(j_1) + j_3 f_2(j_1) = 0. \tag{7}$$

Note that expanding $j_1(z)$ and $j_3(z)$ as Laurent series in z with coefficients in K, we observe that

$$j_1(z) = z^{-2} + \text{ higher order terms}$$

and

$$j_3(z) = z^{-3} + \text{ higher order terms.}$$

If we assume that $f_1, f_2 \neq 0$ and $\deg(f_1) = d_1$ and $\deg(f_2) = d_2$ for $d_1, d_2 \in \mathbb{N}$ then

$$f_1(j_1(z)) = c_1 z^{-2d_1} + \text{ higher order terms}$$

and

$$j_3(z) f_2(j_1(z)) = c_2 z^{-2d_2-3} + \text{ higher order terms}$$

for some $c_1, c_2 \in K \setminus \{0\}$.

Since $-2d_1$ is even and $-2d_2 - 3$ is odd, the leading terms cannot cancel and, therefore, $f_1(j_1(z)) + j_3(z) f_2(j_1(z)) \neq 0$. Thus, either $f_1 = 0$ or $f_2 = 0$. However, if one of these polynomials is zero, the other must also be zero, since otherwise the respective leading term of the Laurent series expansion cannot be made to vanish as required by (7).

In summary, for $f \in \ker \Psi$ we have shown

$$\begin{aligned} f(J_1, J_2, J_3) + I_\Psi &= J_1^{\alpha_1} J_3^{\alpha_3} \tilde{f}(J_1, J_3) + I_\Psi \\ &= J_1^{\alpha_1} J_3^{\alpha_3} (f_1(J_1) + J_3 f_2(J_1)) + I_\Psi \\ &= J_1^{\alpha_1} J_3^{\alpha_3} (0 + J_3 \cdot 0) + I_\Psi \\ &= 0 + I_\Psi. \end{aligned}$$

Therefore $f \in I_\Psi$ and $\ker \Psi = I_\Psi = \langle h_1, h_2 \rangle_{K[J,J^{-1}]}$.

5 The Ideal of Relations Among Theta Functions

From the previous section we have $\sigma(\ker \Psi) = K[T^{\iota_1}, T^{\iota_2}, T^{\iota_3}] \cap \ker \Phi$ and, therefore, $\ker \Phi = \langle \sigma(I_\Psi) \rangle_L$. Let $H^L := \left\{h_1^L, h_2^L\right\}$ for $h_1^L := \sigma(h_1)$, $h_2^L := \sigma(h_2)$.

We are left with the problem of computing $\left\langle H^L \right\rangle_L \cap K[T] = \ker \phi$.

A solution of this problem is well-known in the computer algebra community. Let us denote by $P = K[S, T]$ the polynomial ring in the indeterminates $S = \{S_1, S_2, S_3, S_4\}$ and $T = \{T_1, T_2, T_3, T_4\}$. Let $U = \{1 - S_i T_i \mid i \in \{1, 2, 3, 4\}\}$ and $I = \langle U \rangle_P$ be the ideal generated by the elements of U. By [4, Proposition 7.1], $\ker \chi = I$ for the surjective homomorphism $\chi : P \to L$ with $\chi(S_i) = T_i^{-1}$ and $\chi(T_i) = T_i$ for $i \in \{1, 2, 3, 4\}$, i.e., $P/I \cong L$.

Let $\chi' : L \to P$ be such that $\chi'(T_i) = T_i$, $\chi'(T_i^{-1}) = S_i$, i.e., $\chi(\chi'(p)) = p$ for every $p \in L$. Then $\ker \phi = \ker \Phi \cap K[T] = \left\langle \chi'(H^L) \cup U \right\rangle_P \cap K[T]$. Note that

$$\chi'(h_1^L) := S_1^2 T_3^2 - c_3 S_1^2 T_2^2 - c_4,$$
$$\chi'(h_2^L) := (S_1^3 T_1 T_2 T_3)^2 - (S_1^2 T_2^2)(S_1^2 T_3^2)(c_4 S_1^2 T_2^2 + c_3).$$

A generating set for the latter intersection can be computed by Buchberger's algorithm (cf. [5] or [6]) applied to $\chi'(H^L) \cup U$ with respect to a term ordering such that monomials with indeterminates exclusively from the set T are smaller than any monomial involving indeterminates from S. Then by [6, Cor. 5.51] the polynomials $g_1, \ldots, g_t$ in this Gröbner basis that only involve indeterminates from the set T form a Gröbner basis G of all the relations among the theta functions $\theta_1, \theta_2, \theta_3, \theta_3$ with coefficients in K.

6 Computability of *K*

Up to now the field of coefficients has not played an essential role in the derivation. However, in order to actually compute the Gröbner basis from the previous section, we must find a good representation of the elements of K. Note that $\theta_2(0)$, $\theta_3(0)$, and $\theta_4(0)$, and therefore, also c_3 and c_4 are actually Puiseux series in q.

In the following, we employ results from [7] in order to show that the well known Jacobi identity

$$\theta_2(0|\tau)^4 - \theta_3(0|\tau)^4 + \theta_4(0|\tau)^4 = 0$$

is a "factor" of any other identity among $\theta_2(0)$, $\theta_3(0)$, and $\theta_4(0)$ and then use it to model K in a finitary way.

Let

$$\eta : \mathbb{H} \to \mathbb{C}, \quad \tau \mapsto \exp\left(\frac{\pi i \tau}{12}\right) \prod_{n=1}^{\infty} (1 - e^{2\pi i n})$$

be the Dedekind eta function and denote for $\delta = 1, 2, 4$ by $\eta_\delta : \mathbb{H} \to \mathbb{C}$ the function $\eta_\delta(\tau) := \eta(\delta\tau)$.

By simple rewriting of formulas for theta functions in Section 21.42 of [3] or rewriting of q-series expansions from Entry 22 together with formulas (0.12) and (0.13) of Chapter 20 of [8], we can express the Jacobi theta functions in terms of in Dedekind η functions:

$$\theta_2(0|\tau) = \frac{2\eta(2\tau)^2}{\eta(\tau)}, \qquad \theta_3(0|\tau) = \frac{\eta(\tau)^5}{\eta(\frac{1}{2}\tau)^2 \eta(2\tau)^2}, \qquad \theta_4(0|\tau) = \frac{\eta(\frac{1}{2}\tau)^2}{\eta(\tau)}. \quad (8)$$

The relations among the theta functions are given by the kernel of the following map.

$$\xi : \mathbb{Q}[t_2, t_3, t_4] \to \mathbb{Q}[\theta_2(0), \theta_3(0), \theta_4(0)],$$
$$t_j \mapsto \theta_j(0), \quad j = 2, 3, 4,$$

where t_2, t_3, t_4 are indeterminates. In order to find $\ker \xi$, we extend this map to

$$\Xi : \mathbb{Q}[Y, E, t] \to \mathbb{Q}[\eta^{-1}, \eta, \theta],$$
$$Y_\delta \mapsto \eta_\delta(\tau/2)^{-1}, \quad E_\delta \mapsto \eta_\delta(\tau/2), \quad \delta = 1, 2, 4, \quad t_j \mapsto \theta_j(0|\tau), \quad j = 2, 3, 4.$$

Define $r := E_2^{24} - E_1^{16}E_4^8 - 16E_1^8 E4^{16}$ and the ideal $I = \langle W_1 \cup W_2 \cup W_3\rangle_{\mathbb{Q}[Y,E,t]}$ in $\mathbb{Q}[Y, E, t]$ where

$$\begin{aligned} W_1 &:= \left\{t_2 - 2Y_2E_4^2, t_3 - Y_1^2Y_4^2E_2^5, t_4 - Y_2E_1^2\right\}, \\ W_2 &:= \{Y_\delta E_\delta - 1 \mid \delta = 1, 2, 4\}, \\ W_2 &:= \{r\}. \end{aligned}$$

W_1 encodes the relations (8) and W_2 just says that Y_δ models the inverse of E_δ.

Computing the relations among eta functions of level 4 as described in [7] leads to an ideal that is generated by only one polynomial, namely r, i.e.,

$$\ker(\Xi|_{\mathbb{Q}[E]}) = \langle r\rangle_{\mathbb{Q}[E]} \tag{9}$$

where $\Xi|_{\mathbb{Q}[E]}$ denotes the restriction of the map Ξ to $\mathbb{Q}[E]$.

Clearly, $I \subseteq \ker \Xi$. To prove $\ker \Xi \subseteq I$, consider $f \in \ker \Xi$. By W_1 we can find a polynomial $f_1 \in \mathbb{Q}[Y, E]$ with $f + I = f_1 + I$. Note that by W_2 we have $Y_\delta E_\delta + I = 1 + I$. Thus, similar to "clearing a common denominator", by multiplication of each term of f_1 with an appropriate power of $Y_\delta E_\delta$, we can find a polynomial $f_2 \in \mathbb{Q}[E]$ and a vector $\alpha \in \mathbb{N}^3$ such that $f + I = Y^\alpha f_2 + I$. Since $\Xi(Y^\alpha) \neq 0$, it follows $\Xi(f_2) = 0$ and, thus, $f_2 \in \ker(\Xi|_{\mathbb{Q}[E]})$. From (9) we conclude that there is $\tilde{p} \in \mathbb{Q}[E]$ such that $f_2 = \tilde{p} \cdot r$. Therefore, $f \in I = \ker \Xi$.

Since we are actually interested in $\ker \xi = \ker \Xi \cap \mathbb{Q}[t]$, we can simply compute a Gröbner basis of I and intersect with $\mathbb{Q}[t]$. We find $I \cap \mathbb{Q}[t] = \left\langle t_2^4 - t_3^4 + t_4^4\right\rangle_{\mathbb{Q}[t]}$. This polynomial corresponds to [1, Eq. 20.7.5]. In particular, that result says that there is no polynomial $p \in \mathbb{Q}[t_2, t_4]$ such that $p(\theta_2(0), \theta_4(0)) = 0$. Hence, $F := \mathbb{Q}(t_2, t_4)$ is isomorphic to $\mathbb{Q}(\theta_2(0), \theta_4(0))$. Since $t_2^4 - t_3^4 + t_4^4$ is irreducible over $F[t_3]$, it follows from the First Isomorphism Theorem that

$$K \cong F(\theta_3(0|\tau)) \cong F[t_3]/\left\langle t_2^4 - t_3^4 + t_4^4\right\rangle. \tag{10}$$

7 Computation of the Ideal of Relations in FriCAS

Having a finite (and computable) representation for the coefficient field K, we now demonstrate the steps to compute $\ker \phi$ in the computer algebra system FriCAS.[1] Due to its type system, FriCAS allows to almost naturally enter the respective data structures in order to compute the Gröbner basis of $\ker \phi$.

[1]FriCAS 1.3.4 [9].

We try to use almost the same identifiers in the following FriCAS session as we use in the mathematical notation above.

Let us start with setting up the field K and the two coefficients c_3 and c_4 that are used in the definition of h_1 and h_2 in (5) and (6).

```
1 N ==> NonNegativeInteger; Q ==> Fraction Integer
2 D ==> HomogeneousDistributedMultivariatePolynomial([t2,t4], Q)
3 F ==> Fraction D; R ==> UnivariatePolynomial('t3, F)
4 r: R := t2^4 -t3^4 + t4^4;
5 K := SimpleAlgebraicExtension(F, R, r)
6 t2: K := 't2; t3: K := 't3; t4: K := 't4::K
7 c3 := (t3/t2)^2; c4 := (t4/t2)^2;
```

Next, we create the data structure for $P = K[S, T]$.

```
8 vars := [S1, S2, S3, S4, T1, T2, T3, T4];
9 E ==> SplitHomogeneousDirectProduct(8, 4, N)
10 P ==> GeneralDistributedMultivariatePolynomial(vars, K, E)
```

Now, we setup the generators of $\ker \Phi$ and compute a Gröbner basis.

```
11 U: List(P) := [S1*T1-1, S2*T2-1, S3*T3-1, S4*T4-1]
12 h1: P := (S1*T3)^2 - c3*(S1*T2)^2 - c4
13 h2: P := (S1^3*T2*T3*T4)^2 - (c4*S1^2*T2^2+c3)*S1^4*T2^2*T3^2
14 B := groebner(concat [U, [h1, h2]])
```

Eventually, we compute a Gröbner basis of the intersection $\ker \phi = \ker \Phi \cap K[T]$ and take advantage of the fact that, if B is a Gröbner basis with respect to a termorder where any term that involves only variables from the set T is smaller than any term that involves at least one variable from the set S, then $B \cap K[T]$ is a Gröbner basis. We have defined the terms E in line 9 in exactly such a way, i.e., we can simply extract all the polynomials from B that have a vanishing total degree in the indeterminates S.

```
15 G := [x for x in B | zero? reduce(_+, degree(x, vars(1..4)))]
16 G := [(t2::K)^2*x for x in G]  -- make it denominator-free
```

The computation returns the polynomials

$$g_1 := t_2^2 T_1^2 + t_4^2 T_3^2 - t_3^2 T_4^2,$$
$$g_2 := t_2^2 T_2^2 - t_3^2 T_3^2 + t_4^2 T_4^2.$$

as generators of $\ker \phi$, i.e., $G := \langle g_1, g_2 \rangle_{K[T]}$. In view of the isomorphism given in (10), these are exactly the polynomials b_1 and b_2 as given by (2) and (3).

Having a Gröbner basis of the ideal of all polynomial relations among the classical Jacobi theta functions with coefficients involving $\theta_2(0)$, $\theta_3(0)$, and $\theta_4(0)$, allows for a simple decision procedure to check whether a given polynomial expression p in $\theta_2(0)$, $\theta_3(0)$, $\theta_4(0)$, $\theta_1(z)$, $\theta_2(z)$, $\theta_3(z)$, $\theta_4(z)$ is zero or not. One would simply have to translate this expression into a polynomial p in $t_2, t_3, t_4, T_1, T_2, T_3, T_4$ and then apply the function `normalForm` in FriCAS.

As an example, take the identity [1, Eq. 20.7.3]. We can enter it into FriCAS like

```
17 p: P := t3^2*T1^2 + t4^2*T2^2 - t2^2*T4^2
18 normalForm(p, G)
```

FriCAS returns 0 if an only if identity $p(\theta) = 0$ holds. In this case 0 is indeed computed.

One can easily program an extended normalform computation that collects the cofactors during the normalform computation and that leads to a representation of the form $p = p_2 g_1 + p_2 g_2$. In the above, we get $p_1 = c_3$ and $p_2 = c_4$.

8 Conclusion

We have shown that any polynomial identity in Jacobi theta functions can be expressed as a $K[T]$-linear combination of just two polynomials. Moreover such a linear combination can be computed algorithmically by a simple reduction process.

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Numerical Evaluation of Elliptic Functions, Elliptic Integrals and Modular Forms

Fredrik Johansson

Abstract We describe algorithms to compute elliptic functions and their relatives (Jacobi theta functions, modular forms, elliptic integrals, and the arithmetic-geometric mean) numerically to arbitrary precision with rigorous error bounds for arbitrary complex variables. Implementations in ball arithmetic are available in the open source Arb library. We discuss the algorithms from a concrete implementation point of view, with focus on performance at tens to thousands of digits of precision.

1 Introduction

The elliptic functions and their relatives have many applications in mathematical physics and number theory. Among the elliptic family of special functions, we count the elliptic functions proper (i.e. doubly periodic meromorphic functions) as well as the quasiperiodic Jacobi theta functions, the closely related classical modular forms and modular functions on the upper half plane, and elliptic integrals which are the inverse functions of elliptic functions.

Our goal is to give a modern treatment of numerical evaluation of these functions, using algorithms that meet several criteria:

- *Full domain*. We should be able to compute the functions for arbitrary complex values of all parameters where this is reasonable, with sensible handling of branch cuts for multivalued functions.
- *Arbitrary precision*. Precision much higher than 16-digit (or 53-bit) machine arithmetic is sometimes needed for solving numerically ill-conditioned problems. For example, extremely high precision evaluations are employed in mathematical physics to find closed-form solutions for sums and integrals using integer relation methods [2]. Computations with elliptic functions and modular forms requiring hundreds or thousands of digits are commonplace in algebraic and analytic number

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theory, for instance in the construction of discrete data such as class polynomials from numerical approximations [10].

- *Rigorous error bounds*. When we compute an approximation $y \approx f(x)$, we should also be able to offer a bound $|y - f(x)| \le \varepsilon$, accounting for all intermediate rounding and approximation errors in the algorithm.
- *Efficiency*. The algorithms should be robust and efficient for arguments that are very small, large, or close to singularities. For arbitrary-precision implementations, a central concern is to ensure that the computational complexity as a function of the precision does not grow too quickly. At the same time, we must have in mind that the algorithms with the best theoretical asymptotic complexity are not necessarily the best in practice, and we should not sacrifice efficiency at moderate precision (tens to hundreds of digits).

It turns out that these goals can be achieved simultaneously and with reasonable implementation effort thanks to the remarkable amount of structure in the elliptic function family — in contrast to many other problems in numerical analysis!

The present author has implemented routines for elliptic functions, Jacobi theta functions, elliptic integrals and commonly-used modular forms and functions as part of the open source Arb library for arbitrary-precision ball arithmetic [16].[1] The idea behind ball arithmetic is to represent numerical approximations with error bounds attached, as in $\pi \in [3.14159265358979 \pm 3.57 \cdot 10^{-15}]$. The algorithms use ball arithmetic internally for automatic propagation of error bounds, in combination with some pen-and-paper bounds mainly for truncations of infinite series.[2]

The functions in Arb can be used directly in C or via the high-level wrappers in Sage [29] or the Julia package Nemo [12]. As an example, we use the Arb interface in Sage to evaluate the Weierstrass elliptic function $\wp$ on the lattice $(1, \tau)$ with $\tau = \frac{1}{2}(1 + \sqrt{3}i)$. We check $\wp(z) = \wp(z + 5 + 6\tau)$ at the arbitrarily chosen point $z = 2 + 2i$, here using 100-bit precision:

```
sage: C = ComplexBallField(100)
sage: tau = (1 + C(-3).sqrt())/2
sage: z = C(2 + 2*I)
sage: z.elliptic_p(tau)
[-13.7772161934928750714214345 +/- 6.41e-26] + [+/- 3.51e-26]*I
sage: (z + 5 + 6*tau).elliptic_p(tau)
[-13.777216193492875071421435 +/- 9.69e-25] + [+/- 4.94e-25]*I
```

This text covers the algorithms used in Arb and discusses some of the implementation aspects. The algorithms are general and work well in most situations. However,

[1] Available at http://arblib.org. The functionality for modular forms and elliptic functions can be found in the `acb_modular` (http://arblib.org/acb_modular.html) and `acb_elliptic` (http://arblib.org/acb_elliptic.html) modules.

[2] Of course, for applications that do not require rigorous error bounds, all the algorithms can just as well be implemented in ordinary floating-point arithmetic.

we note that the code in Arb does not use the best available algorithms in all cases, and we will point out some of the possible improvements.

There is a vast body of literature on elliptic functions and integrals, and we will not be able to explore the full breadth of computational approaches. We will, in particular, focus on arbitrary-precision arithmetic and omit techniques that only matter in machine precision. A good overview and a comprehensive bibliography can be found in chapters 19, 20, 22 and 23 of the NIST Handbook of Mathematical Functions [23] or its online counterpart, the Digital Library of Mathematical Functions.[3] Cohen's book on computational number theory [5] is also a useful resource.

Many other packages and computer algebra systems also provide good support for evaluating elliptic and related functions, though not with rigorous error bounds; we mention Pari/GP [28] and of course Maple and Mathematica. For a nice application of Weierstrass elliptic functions in astrodynamics and a fast machine-precision implementation of these functions, we mention the work by Izzo and Biscani [13].

The algorithms that we review are well known, but they are sometimes described without discussing arbitrary complex variables, variable precision, or error bounds. We attempt to provide an account that is complementary to the existing literature, and we also discuss some minor improvements to the algorithms as they are usually presented. For example, we have optimized Carlson's algorithm for symmetric elliptic integrals to reduce the asymptotic complexity at high precision (Sect. 6.3), and we make several observations about the deployment of ball arithmetic.

2 General Strategy

Algorithms for evaluating mathematical functions often have two stages: argument reduction, followed by evaluation of a series expansion [3, 21].

Minimax polynomial or rational function approximations are usually preferred for univariate functions in machine precision, but truncated Taylor series expansions are the tools of choice in arbitrary-precision arithmetic, for two reasons. First, precomputing minimax approximations is not practical, and second, we can exploit the fact that the polynomials arising from series expansions of special functions are typically not of generic type but highly structured.

Argument reduction consists of applying functional equations to move the argument to a part of the domain where the series expansion converges faster. In many cases, argument reduction is needed to ensure convergence in the first place. Argument reduction also tends to improve numerical stability, in particular by avoiding alternating series with large terms that would lead to catastrophic cancellation.

The classical elliptic and modular functions are no exception to this general pattern, as shown in Table 1. For elliptic integrals, the argument reduction consists of using contracting transformations to reduce the distance between the function arguments, and the series expansions are hypergeometric series (in one or several

[3] https://dlmf.nist.gov/.

Table 1 Methods for computation of elliptic functions and integrals. This table illustrates the analogies between the elliptic function and elliptic integral cases, and the simplifications between the general (arbitrary parameters) and special (some parameters fixed at special values) cases

	Elliptic functions	Elliptic integrals
General case	Elliptic functions, Jacobi theta functions	Incomplete elliptic integrals
Argument reduction	Reduction to standard domain (modular transformations, periodicity)	Contraction of parameters (linear symmetric transformations)
Series expansions	Theta function q-series	Multivariate hypergeometric series
Special case	Modular forms and functions, theta constants	Complete elliptic integrals, arithmetic-geometric mean
Argument reduction	Reduction to standard domain (modular transformations)	Contraction of parameters (quadratic transformations)
Series expansions	Theta constant and eta function q-series	Classical ${}_2F_1$ hypergeometric series

variables). For the elliptic and modular functions, the argument reduction consists of using modular transformations and periodicity to move the lattice parameter to the fundamental domain and the argument to a lattice cell near the origin, and the series expansions are the sparse q-series of Jacobi theta functions.

In the following text, we will first discuss the computation of elliptic functions starting with the special case of modular forms and functions before turning to general elliptic and Jacobi theta functions. Then, we discuss elliptic integrals, first covering the easier case of complete integrals before concluding with the treatment of incomplete integrals.

We comment briefly on error bounds. Since ball arithmetic automatically tracks the error propagation during series evaluation and through argument reduction steps, the only error analysis that needs to be done by hand is to bound the series truncation errors. If $f(x) = \sum_{k=0}^{\infty} t_k(x)$, we compute $\sum_{k=0}^{N} t_k(x)$ and then add the ball $[\pm\varepsilon]$ or $[\pm\varepsilon] + [\pm\varepsilon]i$ where ε is an upper bound for $|R_N(x)| = |\sum_{k=N+1}^{\infty} t_k(x)|$. Such a bound is often readily obtained by comparison with a geometric series, i.e. if $|t_k(x)| \le AC^k$ with $0 \le C < 1$, then $|R_N(x)| \le \sum_{k=N+1} AC^k = AC^N/(1-C)$. In some cases, further error analysis can be useful to improve the quality (tightness) of the ball enclosures.

For arbitrary-precision evaluation, we wish to minimize the computational complexity as a function of the precision p. The complexity is often measured by counting arithmetic operations. The actual time complexity must account for the fact that arithmetic operations have a bit complexity of $\widetilde{O}(p)$ (where the $\widetilde{O}$ notation ignores logarithmic factors). In some situations, it is better to use a model of complexity that distinguishes between "scalar" arithmetic operations (such as addition of two p-bit numbers or multiplication of a p-bit number by a small integer) and "nonscalar" arithmetic operations (such as multiplication of two general p-bit numbers).

2.1 The Exponential Function

We illustrate these principles with a commonly used algorithm to compute the exponential function e^x of a real argument x to p-bit precision.

- *Argument reduction.* We first use $e^x = 2^n e^t$ with $t = x - n\log(2)$ and $n = \lfloor x/\log(2)\rfloor$ which ensures that $t \in [0, \log(2))$. At this point, the usual Taylor series $e^t = 1 + t + \frac{1}{2}t^2 + \cdots$ does not suffer from cancellation, and we only need $O(p/\log p)$ terms for a relative error of 2^{-p} independent of the initial size of $|x|$. As a second argument reduction step, we write $e^t = (e^u)^{2^r}$ with $u = t/2^r$, which reduces the number N of needed Taylor series terms to $O(p/r)$.
  Balancing $N = O(p/r)$ against the number r of squarings needed to reconstruct e^t from e^u, it is optimal to choose $r \approx p^{0.5}$. This gives an algorithm for e^x requiring $O(p^{0.5})$ arithmetic operations on p-bit numbers, which translates to a time complexity of $\widetilde{O}(p^{1.5})$.
- *Series evaluation.* As an additional improvement, we can exploit the structure of the Taylor series of the exponential function. For example, $\sum_{k=0}^{8}\frac{1}{k!}x^k$ can be evaluated as

$$1 + x + \tfrac{1}{2}\left(x^2 + \tfrac{1}{3}x^3\left(1 + \tfrac{1}{4}\left(x + \tfrac{1}{5}\left(x^2 + \tfrac{1}{6}x^3\left(1 + \tfrac{1}{7}\left(x + \tfrac{1}{8}x^2\right)\right)\right)\right)\right)\right) \qquad (1)$$

where we have extracted the power x^3 repeatedly and used the fact that the ratios between successive coefficients are small integers. As a result, we only need four nonscalar multiplications involving x (to compute x^2, x^3, and for the two multiplications by x^3), while the remaining operations are scalar divisions. With further rewriting, the scalar divisions can be replaced by even cheaper scalar multiplications.

In general, to evaluate a polynomial of degree N with scalar coefficients at a nonscalar argument x, we can compute $x^2, \ldots, x^m$ once and then use Horner's rule with respect to x^m, for $m \approx N^{0.5}$, which reduces the total number of nonscalar multiplications to about $2N^{0.5}$ [24]. This trick is sometimes called *rectangular splitting*. To motivate this terminology, picture the terms of the polynomial laid out as a matrix with m columns and N/m rows.

In view of this improvement to the series evaluation, it turns out to be more efficient in practice to choose the tuning parameter r used for argument reduction $e^t = (e^{t/2^r})^{2^r}$ slightly smaller, say about $r \approx p^{0.4}$ for realistic p. The algorithm combining optimal argument reduction with rectangular splitting for evaluation of elementary functions such as e^x is due to Smith [26].

There are asymptotically faster algorithms that permit evaluating elementary functions using only $O(\log p)$ arithmetic operations (that is, in $\widetilde{O}(p)$ time), for instance based on the AGM (discussed in Sect. 5 for computing elliptic integrals), but Smith's algorithm is more efficient in practice for moderate p, and in some situations still wins for p as large as 10^5.

3 Modular Forms and Functions

A modular transformation g is a linear fractional transformation on the upper half plane $\mathbb{H} = \{\tau : \mathbb{C} : \mathrm{Im}(\tau) > 0\}$ of the form $g(\tau) = (a\tau + b)/(c\tau + d)$ where a, b, c, d are integers with $ad - bc = 1$. We can assume that $c \geq 0$. The group of modular transformations (known as the modular group) can be identified with the projective special linear group $\mathrm{PSL}(2, \mathbb{Z})$, where g is represented by the matrix $\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ and composition corresponds to matrix multiplication.

A modular form (of weight k) is a holomorphic function on $\mathbb{H}$ satisfying the functional equation $f(g(\tau)) = (c\tau + d)^k f(\tau)$ for every modular transformation g, with the additional technical requirement of being holomorphic as $\tau \to i\infty$. A modular form of weight $k = 0$ must be a constant function, but nontrival solutions of the above functional equation are possible if we allow poles. A meromorphic function on $\mathbb{H}$ satisfying $f(g(\tau)) = f(\tau)$ is called a modular function.

Every modular form or function is periodic with $f(\tau + 1) = f(\tau)$ and has a Fourier series (or q-series)

$$f(\tau) = \sum_{n=-m}^{\infty} a_n q^n, \quad q^{2\pi i \tau} \tag{2}$$

where $m = 0$ in the case of a modular form. The fundamental tool in numerical evaluation of modular forms and functions is to evaluate a truncation of such a q-series. Since τ has positive imaginary part, the quantity q always satisfies $|q| < 1$, and provided that an explicit bound for the coefficient sequence a_n is known, tails of (2) are easily bounded by a geometric series.

3.1 Argument Reduction

The q-series (2) always converges, but the convergence is slow for τ close to the real line where $|q| \approx 1$. However, we can always find a modular transformation g that moves τ to the fundamental domain $\{\tau \in \mathbb{H} : |\tau| \geq 1, |\mathrm{Re}(\tau)| \leq \frac{1}{2}\}$ (see Fig. 1). This ensures $|q| \leq e^{-\pi\sqrt{3}} \approx 0.00433$ which makes the convergence extremely rapid.

Technically, the fundamental domain does not include half of the boundary (meaning that $\mathbb{H}$ is tiled by copies of the fundamental domain under the action of the modular group), but this does not matter for the algorithm. In fact, it is sufficient to put τ within some small distance ε of the fundamental domain, and this relaxation is especially useful in ball arithmetic since a ball may overlap with the boundary.

The well-known algorithm to construct g (see Cohen [5, Algorithm 7.4.2]) repeatedly applies the generators $\tau \to \tau + 1$ and $\tau \to -1/\tau$ of the modular group:

1. Set $g \leftarrow \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$.
2. Set $\tau \leftarrow \tau + n$, $g \leftarrow \left(\begin{smallmatrix} 1 & n \\ 0 & 1 \end{smallmatrix}\right) g$ where $n = -\left\lfloor \mathrm{Re}(\tau) + \frac{1}{2} \right\rfloor$.

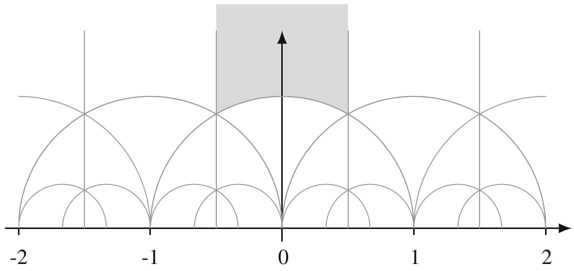


Fig. 1 The shaded region shows the canonical fundamental domain for the action of the modular group on the upper half plane

3. If $|\tau| < 1 - \varepsilon$, set $\tau \leftarrow -1/\tau$ and $g \leftarrow \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right) g$ and go to step 2; otherwise, stop.

Exact integer operations should be used for the matrices, but we can perform all operations involving τ in this algorithm using heuristic floating-point approximations, starting with the midpoint of the initial ball. Once g has been constructed, we evaluate $g(\tau)$ and $f(g(\tau))$ as usual in ball arithmetic.

Indeed, it is important to construct the transformation matrix g separately and then apply the functional equation for the modular form in a single step rather than applying the generating transformations iteratively in ball arithmetic. This both serves to minimize numerical instability and to optimize performance. The precision needed to construct g only depends on the size of the entries of g and not on the precision for evaluating $f(\tau)$. If $\tau \approx 2^{-p}i$, we only need about $2p$ bits to construct g even if the overall precision is thousands of digits. The implementation in Arb uses virtually costless machine floating-point arithmetic to construct g when 53-bit arithmetic is sufficient, switching to arbitrary-precision arithmetic only when necessary.

3.2 *Standard Functions*

Several commonly-used modular forms and functions are implemented in Arb. The basic building blocks are the Dedekind eta function

$$\eta(\tau) = e^{\pi i \tau/12} \sum_{n=-\infty}^{\infty} (-1)^n q^{(3n^2-n)/2}, \quad q = e^{2\pi i \tau}, \tag{3}$$

and the theta constants $\theta_j \equiv \theta_j(\tau)$,

$$\theta_2(\tau) = e^{\pi i \tau/4} \sum_{n=-\infty}^{\infty} q^{n(n+1)}, \quad \theta_3(\tau) = \sum_{n=-\infty}^{\infty} q^{n^2}, \quad \theta_4(\tau) = \sum_{n=-\infty}^{\infty} (-1)^n q^{n^2} \tag{4}$$

in which (as a potential source of confusion) $q = e^{\pi i \tau}$.

It is useful to represent other modular forms in terms of these particular functions since their q-series are extremely sparse (requiring only $O(p^{0.5})$ terms for p-bit accuracy, which leads to $\widetilde{O}(p^{1.5})$ bit complexity) and only have coefficients ± 1. We give a few examples of derived functions:

- Modular functions are precisely the rational functions of the j-invariant

$$j(\tau) = 32\frac{(\theta_2^8 + \theta_3^8 + \theta_4^8)^3}{(\theta_2\theta_3\theta_4)^8}, \quad j\left(\frac{a\tau + b}{c\tau + d}\right) = j(\tau). \tag{5}$$

- The modular discriminant is a modular form of weight 12, given by

$$\Delta(\tau) = \eta(\tau)^{24}, \quad \Delta\left(\frac{a\tau + b}{c\tau + d}\right) = (c\tau + d)^{12}\Delta(\tau). \tag{6}$$

- Eisenstein series are modular forms of weight $2k$ for $k \geq 2$, given by

$$G_{2k}(\tau) = \sum_{m^2+n^2 \neq 0} \frac{1}{(m + n\tau)^{2k}}, \quad G_{2k}\left(\frac{a\tau + b}{c\tau + d}\right) = (c\tau + d)^{2k} G_{2k}(\tau) \tag{7}$$

where we compute $G_4(\tau)$, $G_6(\tau)$ via theta constants using

$$G_4(\tau) = \frac{\pi^4}{90}\left(\theta_2^8 + \theta_3^8 + \theta_4^8\right), \quad G_6(\tau) = \frac{\pi^6}{945}\left(-3\theta_2^8(\theta_3^4 + \theta_4^4) + \theta_3^{12} + \theta_4^{12}\right)$$

and obtain the higher-index values using recurrence relations.

The Dedekind eta function itself transforms as

$$\eta\left(\frac{a\tau + b}{c\tau + d}\right) = \varepsilon(a, b, c, d)\sqrt{c\tau + d}\,\eta(\tau) \tag{8}$$

where $\varepsilon(a, b, c, d) = \exp(\pi i R/12)$ is a 24th root of unity. The integer R (mod 24) can be computed using Kronecker symbols [25, section 74]. The modular transformations for theta constants are a special case of the formulas for theta functions given below in Sect. 4.1. However, we avoid using these transformations directly when computing the functions (5)–(7): it is better to apply the simpler argument reductions for the top-level functions and then evaluate the series expansions (3) or (4) when τ is already reduced.

3.3 Fast Evaluation of q-Series

The powers of q appearing in (3) and (4) are easily generated using two multiplications per term since the exponents are successive values of quadratic polynomials.

The cost can nearly be halved using short addition sequences [11, Algorithm 2]. The cost can be reduced even further by combining addition sequences with rectangular splitting[11, section 5]. Here, the idea is to factor out some power q^m as in (1), but m must be chosen in a particular way — for example, in the case of the theta series $\sum_{n=1}^{\infty} q^{n^2}$, m is chosen so that there are few distinct quadratic residues modulo m. In Arb, these optimizations save roughly a factor four over the naive algorithm.

4 Elliptic and Theta Functions

An elliptic function with respect to a lattice in $\mathbb{C}$ with periods ω_1, ω_2 is a meromorphic function satisfying $f(z + m\omega_1 + n\omega_2) = f(z)$ for all $z \in \mathbb{C}$ and all $m, n \in \mathbb{Z}$. By making a linear change of variables, we can assume that $\omega_1 = 1$ and $\omega_2 = \tau \in \mathbb{H}$. The elliptic functions with a fixed lattice parameter τ form a field, which is generated by the Weierstrass elliptic function

$$\wp(z, \tau) = \frac{1}{z^2} + \sum_{n^2+m^2 \neq 0} \left[\frac{1}{(z + m + n\tau)^2} - \frac{1}{(m + n\tau)^2} \right] \tag{9}$$

together with its z-derivative $\wp'(z, \tau)$.

The building blocks for elliptic functions are the Jacobi theta functions

$$\begin{aligned}
\theta_1(z, \tau) &= \sum_{n=-\infty}^{\infty} e^{\pi i[(n+\frac{1}{2})^2\tau + (2n+1)z + n - \frac{1}{2}]} = 2q_4 \sum_{n=0}^{\infty} (-1)^n q^{n(n+1)} \sin((2n+1)\pi z) \\
&= -iq_4 \sum_{n=0}^{\infty} (-1)^n q^{n(n+1)} (w^{2n+1} - v^{2n+1}), \\
\theta_2(z, \tau) &= \sum_{n=-\infty}^{\infty} e^{\pi i[(n+\frac{1}{2})^2\tau + (2n+1)z]} = 2q_4 \sum_{n=0}^{\infty} q^{n(n+1)} \cos((2n+1)\pi z) \\
&= q_4 \sum_{n=0}^{\infty} q^{n(n+1)} (w^{2n+1} + v^{2n+1}), \qquad (10) \\
\theta_3(z, \tau) &= \sum_{n=-\infty}^{\infty} e^{\pi i[n^2\tau + 2nz]} = 1 + 2\sum_{n=1}^{\infty} q^{n^2} \cos(2n\pi z) = 1 + \sum_{n=1}^{\infty} q^{n^2} (w^{2n} + v^{2n}), \\
\theta_4(z, \tau) &= \sum_{n=-\infty}^{\infty} e^{\pi i[n^2\tau + 2nz + n]} = 1 + 2\sum_{n=1}^{\infty} (-1)^n q^{n^2} \cos(2n\pi z) \\
&= 1 + \sum_{n=1}^{\infty} (-1)^n q^{n^2} (w^{2n} + v^{2n}),
\end{aligned}$$

where $q = e^{\pi i \tau}$, $q_4 = e^{\pi i \tau/4}$, $w = e^{\pi i z}$, $v = w^{-1}$. The theta functions are quasielliptic functions of z, having period or half-period 1 and quasiperiod τ (a shift by τ introduces an exponential prefactor). With $z = 0$, the theta functions $\theta_2, \theta_3, \theta_4$ reduce to the corresponding theta constants, while $\theta_1(0, \tau) = 0$ identically.

Arb provides a complete implementation of the Jacobi theta functions themselves as well as the Weierstrass elliptic function which is computed as

$$\wp(z, \tau) = \pi^2 \theta_2^2(0, \tau)\theta_3^2(0, \tau)\frac{\theta_4^2(z, \tau)}{\theta_1^2(z, \tau)} - \frac{\pi^2}{3}\left[\theta_2^4(0, \tau) + \theta_3^4(0, \tau)\right]. \tag{11}$$

For all these functions, Arb also allows computing an arbitrary number of z-derivatives. Derivatives are handled by working with $\theta_j(z + x, \tau)$ and $\wp(z + x, \tau)$ as elements of $\mathbb{C}[[x]]$ (truncated to some length $O(x^D)$), using power series arithmetic.

Arb also implements the quasielliptic Weierstrass zeta and sigma functions $\zeta(z, \tau)$ and $\sigma(z, \tau)$ as well as the lattice invariants g_2, g_3 (which are essentially Eisenstein series) and lattice roots $4z^3 - g_2 z - g_3 = 4(z - e_1)(z - e_2)(z - e_3)$ arising in the differential equation $[\wp'(z, \tau)]^2 = 4[\wp(z, \tau)]^3 - g_2\wp(z, \tau) - g_3$. The inverse Weierstrass elliptic function is also available; see Sect. 6.

The Jacobi elliptic functions sn, cn, ... are not currently part of the library, but users can compute them via theta functions using formulas similar to (11).

4.1 Argument Reduction

As the first step when computing theta functions or elliptic functions, we reduce τ to the fundamental domain using modular transformations. This gives us a new lattice parameter τ' and a new argument z'. As a second step, we reduce z' modulo τ', giving an argument z'' with smaller imaginary part (it is not necessary to reduce z' modulo 1 since this is captured by the oscillatory part of exponentials). We can then compute $\theta_j(z'', \tau')$ using the theta series (10).

These steps together ensure that both $|q|$ and $\max(|w|, |w|^{-1})$ will be small. It is important to perform both transformations. Consider $\tau = 0.07 + 0.003i$ and $z = 3.14 + 2.78i$: without the modular transformation, the direct series evaluation would use 3710 terms for machine precision.[4] With the modular transformation alone, it would use 249 terms. With both reductions, only 6 terms are used! Depending on the arguments, the numerical stability may also be improved substantially.

Modular transformations have the effect of permuting the theta functions and introducing certain exponential prefactors. It is easy to write down the transformations for the generators $\tau + 1$, $-1/\tau$, but the action of a composite transformation involves

[4]The number is somewhat smaller if the series is truncated optimally using a relative rather than an absolute tolerance.

a certain amount of bookkeeping. The steps have been worked out by Rademacher [25, chapter 10]. We reproduce the formulas below.[5]

We wish to write a theta function with lattice parameter τ in terms of a theta function with lattice parameter $\tau' = g(\tau)$, given some $g = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in \mathrm{PSL}(2, \mathbb{Z})$. For $j = 0, 1, 2, 3$, there are $R_j, S_j \in \mathbb{Z}$ depending on g such that

$$\theta_{1+j}(z, \tau) = \exp(\pi i R_j/4) \cdot A \cdot B \cdot \theta_{1+S_j}(z', \tau') \tag{12}$$

where if $c = 0$,

$$z' = z, \quad A = 1, \quad B = 1, \tag{13}$$

and otherwise (if $c > 0$),

$$z' = \frac{-z}{c\tau + d}, \quad A = \sqrt{\frac{i}{c\tau + d}}, \quad B = \exp\left(-\pi i c \frac{z^2}{c\tau + d}\right). \tag{14}$$

We always have $B = 1$ when computing theta constants which have $z = 0$.

The parameters R_j, S_j are computed from g as follows. If $c = 0$, we have $\theta_j(z, \tau) = \exp(-\pi i b/4)\theta_j(z, \tau + b)$ for $j = 1, 2$, whereas θ_3 and θ_4 remain unchanged when b is even and swap places with each other when b is odd. For the $c > 0$ case, it is helpful to define the function $\theta_{m,n}(z, \tau)$ for $m, n \in \mathbb{Z}$ by

$$\begin{aligned} \theta_{0,0}(z, \tau) &= \theta_3(z, \tau), & \theta_{0,1}(z, \tau) &= \theta_4(z, \tau), \\ \theta_{1,0}(z, \tau) &= \theta_2(z, \tau), & \theta_{1,1}(z, \tau) &= i\theta_1(z, \tau), \\ \theta_{m+2,n}(z, \tau) &= (-1)^n \theta_{m,n}(z, \tau) & \theta_{m,n+2}(z, \tau) &= \theta_{m,n}(z, \tau). \end{aligned} \tag{15}$$

With this notation, we have

$$\begin{aligned} \theta_1(z, \tau) &= \varepsilon_1 AB\theta_1(z', \tau'), & \theta_2(z, \tau) &= \varepsilon_2 AB\theta_{1-c,1+a}(z', \tau'), \\ \theta_3(z, \tau) &= \varepsilon_3 AB\theta_{1+d-c,1-b+a}(z', \tau'), & \theta_4(z, \tau) &= \varepsilon_4 AB\theta_{1+d,1-b}(z', \tau') \end{aligned} \tag{16}$$

where ε_k is an 8th root of unity. If we denote by $\varepsilon(a, b, c, d) = \exp(\pi i R(a, b, c, d)/12)$ the 24th root of unity in the transformation (8) of the Dedekind eta function, then

$$\begin{aligned} \varepsilon_1(a, b, c, d) &= \exp(\pi i [R(-d, b, c, -a) + 1]/4), \\ \varepsilon_2(a, b, c, d) &= \exp(\pi i [-R(a, b, c, d) + (5 + (2 - c)a)]/4), \\ \varepsilon_3(a, b, c, d) &= \exp(\pi i [-R(a, b, c, d) + (4 + (c - d - 2)(b - a))]/4), \\ \varepsilon_4(a, b, c, d) &= \exp(\pi i [-R(a, b, c, d) + (3 - (2 + d)b)]/4). \end{aligned} \tag{17}$$

[5] We give the inverse form of the transformation.

Finally, to reduce z', we compute $n = \lfloor \mathrm{Im}(z')/\mathrm{Im}(\tau') + 1/2 \rfloor$ and set $z'' = z' - n\tau'$. In this step, all theta functions pick up a prefactor $\exp(\pi i[-\tau n^2 - 2nz])$ (this data may be combined with B) while θ_1 and θ_2 pick up the additional prefactors $(-1)^n$ (this data may be combined with R_j).

When computing z-derivatives of theta functions, the same formulas are applied in power series arithmetic. That is, if the initial argument consists of the formal power series $z + x$, then the scaling factor $-1/(c\tau + d)$ is applied coefficient by coefficient, while $B = B_0 + B_1 x + \cdots$ is obtained by squaring the power series $z + x$, scaling, and then evaluating a power series exponential.

As with modular forms, the transformations should be applied at the highest possible level. For example, when computing a quotient of two theta functions of the same z, τ, the prefactors A and B in (12) cancel out (and the leading roots of unity possibly also simplify). We should then simplify the expression symbolically and avoid computing A and B altogether, since this both saves time and improves numerical stability in ball arithmetic (in particular, $e^{f(z)}/e^{f(z)}$ evaluated in ball arithmetic will not give 1 but rather a ball which can be extremely wide).

Since the description of the algorithm given above is quite terse, the reader may find it helpful to look at the code in Arb to see the concrete steps.

4.2 Theta Function Series Evaluation

Algorithm 1 implements the expansions (10), with the optimization that we combine operations to save work when computing all four functions and their derivatives simultaneously (a single theta function could be computed slightly faster, but computing all four functions is barely more work than it would be to compute a pair containing either θ_1 or θ_2 and either θ_3 or θ_4). This is essentially the algorithm used in Arb for $z \neq 0$, while more optimized code is used for theta constants.

The main index k runs over the terms in the following order:

$$\begin{array}{llll}
 & \theta_1, \theta_2 & q^0 & (w^1 \pm w^{-1}) \\
k = 0 & \theta_3, \theta_4 & q^1 & (w^2 \pm w^{-2}) \\
k = 1 & \theta_1, \theta_2 & q^2 & (w^3 \pm w^{-3}) \\
k = 2 & \theta_3, \theta_4 & q^4 & (w^4 \pm w^{-4}) \\
k = 3 & \theta_1, \theta_2 & q^6 & (w^5 \pm w^{-5}) \\
k = 4 & \theta_3, \theta_4 & q^9 & (w^6 \pm w^{-6}) \\
k = 5 & \theta_1, \theta_2 & q^{12} & (w^7 \pm w^{-7})
\end{array}$$

The algorithm outputs the range of scaled derivatives $\theta_j^{(r)}(z, \tau)/r!$ for $0 \le r < D$. The term of index k in the main summation picks up a factor $\pm(k + 2)^r$ from r-fold differentiation of w^{k+2}. Another factor $(\pi i)^r/r!$ is needed to convert to a z-derivative and a power series coefficient, but we postpone this to a single rescaling pass at the end of the computation. In the main summation, we write the even cosine terms as $w^{2n} + w^{-2n}$, the odd cosine terms as $w(w^{2n} + w^{-2n-2})$, and the sine terms as $w(w^{2n} - w^{-2n-2})$, postponing a multiplication by w for θ_1 and θ_2 until the end, so that only even powers of w and w^{-1} are needed.

For some integer $N \geq 1$, the summation is stopped just before term $k = N$. Let $Q = |q|, W = \max(|w|, |w^{-1}|), E = \lfloor (N+2)^2/4 \rfloor$ and $F = \lfloor (N+1)/2 \rfloor + 1$. The error of the zeroth derivative can be bounded as

$$2Q^E W^{N+2} \left[1 + Q^F W + Q^{2F} W^2 + \cdots \right] = \frac{2Q^E W^{N+2}}{1 - Q^F W} \tag{18}$$

provided that the denominator $1 - Q^F W$ is positive. For the rth derivative, including the factor $(k+2)^r$ gives the error bound

$$2Q^E W^{N+2} (N+2)^r \left[1 + Q^F W \frac{(N+3)^r}{(N+2)^r} + Q^{2F} W^2 \frac{(N+4)^r}{(N+2)^r} + \cdots \right] \tag{19}$$

which by the inequality $(1 + m/(N+2))^r \leq \exp(mr/(N+2))$ can be bounded as

$$\frac{2Q^E W^{N+2} (N+2)^r}{1 - Q^F W \exp(r/(N+2))}, \tag{20}$$

again valid when the denominator is positive.

Algorithm 1 Computation of Jacobi theta functions (using series evaluation)

Require: $z, \tau \in \mathbb{C}$ with $\mathrm{Im}(\tau) > 0$ (can be arbitrary, but should be reduced for best performance), integer $D \geq 1$ to output the D first terms in the Taylor expansions with respect to z, precision p

Ensure: $\theta_j = [\alpha_0, \ldots, \alpha_{D-1}]$ represents $\theta_j(z + x, \tau) = \alpha_0 + \alpha_1 x + \cdots + \alpha_{D-1} x^{D-1}$, for $1 \leq j \leq 4$

$q_4 \leftarrow e^{\pi i \tau/4};\ q \leftarrow q_4^4;\ w \leftarrow e^{\pi i z};\ v \leftarrow w^{-1};\ Q \leftarrow |q|;\ W \leftarrow \max(|w|, |v|)$

Choose N with $E = \lfloor (N+2)^2/4 \rfloor$ and $F = \lfloor (N+1)/2 \rfloor + 1$ such that $Q^E W^{N+2} < 2^{-p}$ and $\alpha = Q^F W \exp(r/(N+2)) < 1$

for $0 \leq r < D$ **do** $\varepsilon[r] \leftarrow 2Q^E W^{N+2} (N+2)^r / (1 - \alpha)$ **end for** ▷ Error bounds

$\mathbf{w} \leftarrow [1, w^2, w^4, \ldots, w^{2K-2}];\ \mathbf{v} \leftarrow [1, v^2, v^4, \ldots, v^{2K}]$ for $K = \lfloor (N+3)/2 \rfloor$ ▷ Precompute powers

$\theta_1 \leftarrow [0, \ldots, 0];\ \theta_2 \leftarrow [0, \ldots, 0];\ \theta_3 \leftarrow [0, \ldots, 0];\ \theta_4 \leftarrow [0, \ldots, 0];$ ▷ Arrays of length D

for $0 \leq k < N$ **do**

  $m \leftarrow \lfloor (k+2)^2/4 \rfloor;\ n \leftarrow \lfloor k/2 \rfloor + 1$

  Compute q^m ▷ Use addition sequence [11, Alg. 2] to build q^m from previous powers.

  $t \leftarrow (\mathbf{w}[n] + \mathbf{v}[n + (k \bmod 2)]) q^m$

  $u \leftarrow (\mathbf{w}[n] - \mathbf{v}[n + (k \bmod 2)]) q^m$ ▷ Skip when $k \bmod 2 = 0$ if $D = 1$.

  if $k \bmod 2 = 0$ **then**

    for $0 \leq r < D$ **do**

      if $r \bmod 2 = 0$ **then**

        if $r \neq 0$ **then** $t \leftarrow 4n^2 t$ **end if**

        $\theta_3[r] \leftarrow \theta_3[r] + t;\ \theta_4[r] \leftarrow \theta_4[r] + (-1)^{\lfloor (k+2)/2 \rfloor} t$

      else

        if $r = 1$ **then** $u \leftarrow 2nu$ **else** $u \leftarrow 4n^2 u$ **end if**

$\theta_3[r] \leftarrow \theta_3[r] + u;\ \theta_4[r] \leftarrow \theta_4[r] + (-1)^{\lfloor (k+2)/2 \rfloor} u$
end if
end for
else
for $0 \le r < D$ **do**
if $r \bmod 2 = 0$ **then**
$\theta_1[r] \leftarrow \theta_1[r] + (-1)^{\lfloor (k+1)/2 \rfloor} u;\ \theta_2[r] \leftarrow \theta_2[r] + t$
else
$\theta_1[r] \leftarrow \theta_1[r] + (-1)^{\lfloor (k+1)/2 \rfloor} t;\ \theta_2[r] \leftarrow \theta_2[r] + u$
end if
$t \leftarrow (2n+1)t;\ u \leftarrow (2n+1)u$
end for
end if
end for
for $0 \le r < D$ **do**
$\theta_1[r] \leftarrow \theta_1[r]w + (w - (-1)^r v)$ ▷ Adjust power of w and add leading terms
$\theta_2[r] \leftarrow \theta_2[r]w + (w + (-1)^r v)$
for $1 \le j \le 4$ **do** $\theta_j[r] \leftarrow \theta_j[r] + [\pm\varepsilon[r]] + [\pm\varepsilon[r]]i$ **end for** ▷ Add error bounds
$C \leftarrow (\pi i)^r / r!$ ▷ Final scaling factors
$\theta_1[r] \leftarrow -iq_4 C\theta_1[r];\ \theta_2[r] \leftarrow q_4 C\theta_2[r];\ \theta_3[r] \leftarrow C\theta_3[r];\ \theta_4[r] \leftarrow C\theta_4[r]$
end for
$\theta_3[0] \leftarrow \theta_3[0] + 1;\ \theta_4[0] \leftarrow \theta_4[0] + 1$ ▷ Add leading terms

end

The time complexity of the algorithm is $\widetilde{O}(p^{1.5})$ (with all inputs besides p fixed). By employing fast Fourier transforms cleverly, the complexity of evaluating theta functions from their series expansions can be reduced to $\widetilde{O}(p^{1.25})$, but that method is only faster in practice for p exceeding 200 000 bits [22]. See also Sect. 8.1 below concerning methods that are even faster asymptotically.

5 Complete Elliptic Integrals and the AGM

Complete elliptic integrals arise in period relations for elliptic functions. The complete elliptic integral of the first kind is $K(m) = \frac{1}{2}\pi\,{}_2F_1(\frac{1}{2}, \frac{1}{2}, 1, m)$ and the complete elliptic integral of the second kind is $E(m) = \frac{1}{2}\pi\,{}_2F_1(-\frac{1}{2}, \frac{1}{2}, 1, m)$ where ${}_2F_1$ denotes the Gauss hypergeometric function, defined for $|z| < 1$ by

$$ {}_2F_1(a, b, c, z) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} \frac{z^k}{k!}, \quad (x)_k = x(x+1)\cdots(x+k-1) \tag{21} $$

and elsewhere by analytic continuation with the standard branch cut on $[1, \infty)$.

The ${}_2F_1$ function can be computed efficiently for any $z \in \mathbb{C}$ using a combination of argument transformations, analytic continuation techniques, and series expansions (where the rectangular splitting trick (1) and other accelerations methods are applicable). A general implementation of ${}_2F_1$ exists in Arb [15]. However, it is more efficient to compute the complete elliptic integrals by exploiting their connection with the arithmetic-geometric mean (AGM) described below.

A third complete elliptic integral $\Pi(n, m)$ is also encountered, but this is a more complicated function that is not a special case of ${}_2F_1$, and we handle it later in terms of an incomplete integral without using a dedicated algorithm for the complete case.

The arithmetic-geometric mean $M(x, y)$ of two nonnegative real numbers x, y is defined as the common limit of the sequences

$$a_{n+1} = \frac{a_n + b_n}{2}, \quad b_{n+1} = \sqrt{a_n b_n} \tag{22}$$

with initial values $a_0 = x$, $b_0 = y$. In different words, the AGM can be computed by repeatedly applying the functional equation $M(x, y) = M\left((x + y)/2, \sqrt{xy}\right)$. It is a well known fact that each step of the AGM iteration roughly doubles the number of accurate digits in the approximation $a_n \approx b_n \approx M(x, y)$, so it only costs $O(\log(p))$ arithmetic operations to compute the AGM with an accuracy of p bits, resulting in a bit complexity of $\widetilde{O}(p)$.

For complex x, y, defining the AGM becomes more difficult since there are two possible choices for the square root in each step of the iteration, and these choices lead to different limits. However, it turns out that there is an "optimal" choice which leads to a well-defined and useful extension of the AGM to complex variables. We rely on several properties of this function proved in earlier work [6–8].

With complex variables, it is convenient to work with the univariate function $M(z) = M(1, z)$, with a branch cut on $(-\infty, 0]$. The general case can be recovered as $M(x, y) = xM(1, y/x)$. The complete elliptic integrals (with the conventional branch cuts on $[1, \infty)$) are now given by

$$K(m) = \frac{\pi}{2M(\sqrt{1-m})}, \quad E(m) = (1 - m)(2mK'(m) + K(m)). \tag{23}$$

For implementing the function $M(z)$, we can further assume that $\operatorname{Re}(z) \geq 0$ holds. If this is not the case, we first apply the functional equation $M(z) = (z + 1)M(u)/2$ where $u = \sqrt{z}/(z + 1)$. The correct square root in the AGM iteration is now always equal to $\sqrt{a_n}\sqrt{b_n}$, written in terms of the usual principal square root function. This can be computed as $\sqrt{a_n b_n}$, $i\sqrt{-a_n b_n}$, $-i\sqrt{-a_n b_n}$, $\sqrt{a_n}\sqrt{b_n}$ respectively if both a_n and b_n have positive real part, nonnegative imaginary part, nonpositive imaginary part, or otherwise. When the iteration is executed in ball arithmetic, the computed balls may end up containing points with negative real part, but this just inflates the final result and does not affect correctness.

The iteration should be terminated when a_n and b_n are close enough. For positive real variables, we can simply take lower and upper bounds to get a correct enclosure. For complex variables, it can be shown [8, p. 87] that $|M(z) - a_n| \leq |a_n - b_n|$ if $\operatorname{Re}(z) \geq 0$, giving a convenient error bound. However, instead of running the AGM iteration until a_n and b_n agree to p bits, it is slightly better to stop when they agree to about $p/10$ bits and end with a Taylor series. With $t = (a - b)/(a + b)$, we have

$$M(a,b) = \frac{(a+b)\pi}{4K(t^2)}, \quad \frac{\pi}{4K(t^2)} = \tfrac{1}{2} - \tfrac{1}{8}t^2 - \tfrac{5}{128}t^4 - \tfrac{11}{512}t^6 - \tfrac{469}{32768}t^8 + \cdots \quad (24)$$

which is valid at least when $|t| < 1$ and a, b have nonnegative real part, and where the tail $(\ldots)$ is bounded by $\sum_{k=10}^{\infty} |t|^k/64$.

This algorithm follows the pattern of argument reduction and series evaluation. However, unlike the elementary functions and the incomplete elliptic integrals described below, there is no asymptotic benefit to using more terms of the series. The quadratic convergence of the AGM iteration is so rapid that we only get a speedup from trading $O(1)$ of the $O(\log p)$ square roots for lower-overhead multiplications. Although there is no asymptotic improvement, the order-10 series expansion nevertheless gives a significant speedup up to a few thousand bits.

For computing the second elliptic integral $E(m)$ or the first derivative $M'(z)$ of the AGM, a simple method is to use a central finite difference to compute $(M(z), M'(z)) \approx (M(z+h) + M(z-h))/2, (M(z+h) - M(z-h))/(2h)$. This requires two evaluations at 1.5 times increased precision, which is about three times as expensive as evaluating M once. Error bounds can be obtained using the Cauchy integral formula and the inequality $|M(z)| \le \max(1, |z|)$ which is an immediate consequence of the AGM iteration. This method has been implemented in Arb. A more efficient method is to compute $E(m)$ using an auxiliary sequence related to the AGM iteration, which also generalizes to computing $\Pi(n, m)$ [23, 19.8.6 and 19.8.7]. This method has not yet been implemented in Arb since it requires some additional error analysis and study for complex variables.

Higher derivatives of the arithmetic-geometric mean or the complete elliptic integrals can be computed using recurrence relations. Writing $W(z) = 1/M(z)$ and $W(z+x) = \sum_{k=0}^{\infty} c_k x^k$, we have $-2z(z^2-1)c_2 = (3z^2-1)c_1 + zc_0$, $-(k+2)(k+3)z(z^2-1)c_{k+3} = (k+2)^2(3z^2-1)c_{k+2} + (3k(k+3)+7)zc_{k+1} + (k+1)^2 c_k$ when $z \ne 1$ and $-(k+2)^2 c_{k+2} = (3k(k+3)+7)c_{k+1} + (k+1)^2 c_k$ when $z = 1$.

6 Incomplete Elliptic Integrals

A general elliptic integral is an integral of the form $\int_a^b R(t, \sqrt{P(t)})dt$ where R is a bivariate rational function and P is a cubic or quartic polynomial without repeated roots. It is well known that any elliptic integral can be expressed in terms of integrals of rational functions and a finite set of standard elliptic integrals.

Such a set of standard integrals is given by the Legendre incomplete elliptic integrals of the first, second and third kind

$$F(\phi, m) = \int_0^{\phi} \frac{dt}{\sqrt{1 - m\sin^2 t}}, \quad E(\phi, m) = \int_0^{\phi} \sqrt{1 - m\sin^2 t}\, dt, \quad (25)$$

$$\Pi(n, \phi, m) = \int_0^{\phi} \frac{dt}{(1 - n\sin^2 t)\sqrt{1 - m\sin^2 t}}. \tag{26}$$

The complete elliptic integrals are the special cases $E(m) = E(\pi/2, m)$, $K(m) = F(\pi/2, m)$, and $\Pi(n, m) = \Pi(n, \pi/2, m)$.

The definitions for complex variables do not appear to be standardized in the literature, but following the conventions used in Mathematica [31], we may fix an interpretation of (25)–(26) on $-\pi/2 \le \mathrm{Re}(\phi) \le \pi/2$ and use the quasiperiodic extensions $F(\phi + k\pi, m) = 2kK(m) + F(\phi, m)$, $E(\phi + k\pi, m) = 2kE(m) + E(\phi, m)$, $\Pi(n, \phi + k\pi, m) = 2k\Pi(n, m) + \Pi(n, \phi, m)$ for $k \in \mathbb{Z}$.[6]

The Legendre forms of incomplete elliptic integrals are widely used by tradition, but they have some practical drawbacks. Since they have a complicated (and not standardized) complex branch structure, transforming their arguments using functional equations or using them to represent other functions often requires making complicated case distinctions. As a result, it is cumbersome both to compute the functions themselves and to apply them, outside of a restricted parameter range.

We remark that F and E can be expressed in terms of the Appell F_1 hypergeometric function of two variables, while Π can be expressed in terms of the three-variable Lauricella hypergeometric function $F_D^{(3)}$, generalizing the ${}_2F_1$ representations for the complete integrals. Such formulas are by themselves mainly useful when the hypergeometric series converge, and provide no insight into the analytic continuations.

In the 1960s, Carlson introduced an alternative set of standard elliptic integrals in which all or some of the variables are symmetric [4]. The Carlson incomplete elliptic integrals are

$$R_F(x, y, z) = \frac{1}{2}\int_0^{\infty} \frac{dt}{\sqrt{(t + x)(t + y)(t + z)}} \tag{27}$$

and

$$R_J(x, y, z, p) = \frac{3}{2}\int_0^{\infty} \frac{dt}{(t + p)\sqrt{(t + x)(t + y)(t + z)}} \tag{28}$$

together with three special cases $R_D(x, y, z) = R_J(x, y, z, z)$, $R_C(x, y) = R_F(x, y, y)$, and

$$R_G(x, y, z) = zR_F(x, y, z) - \frac{1}{3}(x - z)(y - z)R_D(x, y, z) + \frac{\sqrt{x}\sqrt{y}}{\sqrt{z}}. \tag{29}$$

The Carlson forms have several advantages over the Legendre forms. Symmetry unifies and simplifies the argument transformation formulas, and the Carlson forms also have a simpler complex branch structure, induced by choosing the branch of the square root in (27) and (28) to extend continuously from $+\infty$. We can define and compute the Legendre forms from the Carlson forms using

[6] For Π, Mathematica restricts this quasiperiodicity relation to hold only for $-1 \le n \le 1$.

$$\begin{aligned} F(\phi, m) &= s R_F(x, y, 1), \\ E(\phi, m) &= s R_F(x, y, 1) - \tfrac{1}{3} m s^3 R_D(x, y, 1), \\ \Pi(n, \phi, m) &= s R_F(x, y, 1) + \tfrac{1}{3} n s^3 R_J(x, y, 1, p) \end{aligned} \tag{30}$$

on $-\pi/2 \le \operatorname{Re}(\phi) \le \pi/2$ (with the quasiperiodic extensions elsewhere) where $x = c^2, y = 1 - ms^2, p = 1 - ns^2$ and $s = \sin(\phi), c = \cos(\phi)$. This is the approach used to implement the Legendre forms in Arb. The Carlson forms themselves are also exposed to users. Formulas for other elliptic integrals can be found in [4].

Elliptic integrals can also be characterized as the inverse functions of elliptic functions. For example, the inverse of the Weierstrass elliptic function, which by definition satisfies $\wp(\wp^{-1}(z, \tau), \tau) = z$, is given by the elliptic integral

$$\wp^{-1}(z, \tau) = \frac{1}{2} \int_z^\infty \frac{dt}{\sqrt{(t - e_1)(t - e_2)(t - e_3)}} = R_F(z - e_1, z - e_2, z - e_3). \tag{31}$$

The implementation in Arb simply computes the lattice roots e_1, e_2, e_3 using theta constants and then calls R_F. The inverses of Jacobi's elliptic functions can be computed similarly, but at this time they are not implemented in Arb.

Carlson gives algorithms for computing R_F and R_J using argument reduction and series evaluation [4]. The algorithm for R_F is correct for all complex x, y, z (Carlson restricts to the cut plane with $(-\infty, 0)$ removed, but it is clear that the algorithm also works on the branch cut by continuity). The algorithm for R_J is not correct for all values of the variables, but it is always correct when computing R_D (otherwise, a sufficient condition is that x, y, z have nonnegative real part while p has positive real part). Carlson also provides modifications of the algorithms for computing the Cauchy principal values of the integrals.

We will now describe Carlson's algorithm for R_F and adapt it to the setting of arbitrary precision and ball arithmetic. The algorithm given in [4] for R_J and R_D works analogously, but we do not reproduce all the steps here since the formulas would be too lengthy (the code in Arb can be consulted for concrete details).

6.1 Argument Reduction

Argument reduction for R_F uses the symmetric "duplication formula"

$$R_F(x, y, z) = R_F\left(\frac{x + \lambda}{4}, \frac{y + \lambda}{4}, \frac{z + \lambda}{4}\right) \tag{32}$$

where $\lambda = \sqrt{x}\sqrt{y} + \sqrt{y}\sqrt{z} + \sqrt{z}\sqrt{x}$. Each application of (32) reduces the distance between the arguments by roughly a factor 4. The analogous formula for R_J reads

$$R_J(x, y, z, p) = \frac{1}{4} R_J\left(\frac{x + \lambda}{4}, \frac{y + \lambda}{4}, \frac{z + \lambda}{4}, \frac{p + \lambda}{4}\right) + \frac{6}{d} R_C(1, 1 + e) \tag{33}$$

where λ is defined as above and d, e are certain auxiliary terms (see [4, (24)–(28)]). The formulas (32) and (33) are iterated until all the parameters are close so that a series expansion can be used, as detailed in the next subsection. It is interesting to note the similarity between (32) and the AGM iteration, although the convergence rate of (32) only is linear.

When computing R_C or R_D, some redundant operations in the reductions for R_F and R_J can be avoided. $R_C(x, y)$ can also be expressed piecewise using inverse trigonometric and hyperbolic functions. The special case $R_C(1, 1+t) = \operatorname{atan}(\sqrt{t})/\sqrt{t} = {}_2F_1(1, \frac{1}{2}, \frac{3}{2}, -t)$ is particularly important, as it is needed in the evaluation of R_J. This function is better computed via the inverse tangent function (or a direct Taylor series for small $|t|$) than by invoking Carlson's general method for R_F.

6.2 Series Expansions

Carlson's incomplete elliptic integrals are special cases of a multivariate hypergeometric function that may be written as

$$R_{-a}(z_1, \ldots, z_n) = A^{-a} \sum_{N=0}^{\infty} \frac{(a)_n}{(\frac{1}{2}n)_N} T_N(Z_1, \ldots, Z_n) \tag{34}$$

where $A = \frac{1}{n} \sum_{j=1}^{n} z_j$, $Z_j = 1 - z_j/A$, and

$$T_N(Z_1, \ldots, Z_n) = \sum_{\substack{m_1+\cdots+m_n=N \\ m_1,\ldots,m_n \geq 0}} \prod_{j=1}^{n} \frac{(\frac{1}{2})_{m_j}}{m_j!} Z_j^{m_j}. \tag{35}$$

We have $R_F(x, y, z) = R_{-1/2}(x, y, z)$ and $R_J(x, y, z, p) = R_{-3/2}(x, y, z, p, p)$. The crucial property of this hypergeometric representation is that the expansion point is the arithmetic mean of the arguments. After sufficiently many argument reduction steps have been performed, we will have $z_1 \approx z_2 \approx \ldots \approx z_n$ which ensures $|Z_1|, \ldots, |Z_n| \ll 1$ and rapid convergence of the series. A trivial bound for the terms is $|T_N(Z_1, \ldots, Z_n)| \leq p(N) \max(|Z_1|, \ldots, |Z_n|)^N$, where $p(N)$ denotes the number of partitions of N which is bounded by $O(c^N)$ for any $c > 1$. An explicit calculation shows, for example, that the error when computing either R_F or R_J is bounded by

$$2A^{-a} \sum_{N=B}^{\infty} \left(\tfrac{9}{8} \max(|Z_1|, \ldots, |Z_n|)\right)^N \tag{36}$$

if the summation in (34) includes the terms of order $N < B$.

For the evaluation of (35), Carlson noted that it is more efficient to work with elementary symmetric polynomials $E_j = E_j(Z_1, \ldots, Z_n)$ instead of the direct variables $Z_1, \ldots, Z_n$, giving

$$T_N(Z_1, \ldots, Z_n) = \sum_{\substack{m_1+2m_2+\cdots+nm_n=N \\ m_1,\ldots,m_n \geq 0}} (-1)^{M+N} (\tfrac{1}{2})_M \prod_{j=1}^{n} \frac{E_j^{m_j}}{m_j!}. \tag{37}$$

The key observation is that the symmetric choice of expansion variables Z_j with respect to $z_1, \ldots, z_n$ implies that $E_1 = 0$, which eliminates most of the terms in (37).[7] This dramatically reduces the amount of work to compute T_N compared to (35). For the $R_{-1/2}$ series, there are $(N+1)(N+2)/2$ terms in (35) and roughly $N/6$ terms in (37); for example, if $N = 8$, there are 45 terms in the former and only two nonzero terms (with monomials $E_1 E_2^2$ and E_1^4) in the latter.

6.3 *Series Evaluation and Balanced Argument Reduction*

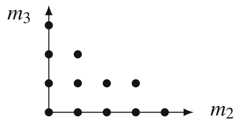
The argument reduction effectively adds $2B$ bits per step if a series expansion of order B is used. In other words, roughly $p/(2B)$ argument reduction steps are needed for p-bit precision. Carlson suggests using a precomputed truncated series of order $B = 6$ or $B = 8$, which is a good default at machine precision and up to a few hundred bits. At higher precision, we make the observation that it pays off to vary B dynamically as a function of p and evaluate the series with an algorithm.

Algorithm 2 Computation of $R_F(x, y, z)$

Choose series truncation order B optimally depending on the precision p
Apply argument reduction (32) until x, y, z are close (until $\varepsilon \approx 2^{-p}$ below)
$A \leftarrow (x + y + z)/3$; $(X, Y, Z) \leftarrow (1 - x/A, 1 - y/A, 1 - z/A)$; $(E_2, E_3) \leftarrow (XY - Z^2, XYZ)$
$\varepsilon \leftarrow 2 \sum_{k=B}^{\infty} \left(\frac{9}{8} \max(|X|, |Y|, |Z|)\right)^k$ ▷ Series error bound
procedure RSUM(E_2, E_3, B) ▷ Compute $R = \sum_{N=0}^{B-1} \left[(\frac{1}{2})_N/(\frac{3}{2})_N\right] T_N$
  Precompute E_2^k for $2 \leq k \leq \lfloor (B-1)/2 \rfloor$
  $R \leftarrow 0$; $c_3 \leftarrow (\frac{1}{2})_{\lfloor (B-1)/3 \rfloor} / (\lfloor (B-1)/3 \rfloor)!$
  for $(m_3 \leftarrow \lfloor (B-1)/3 \rfloor;\ m_3 \geq 0;\ m_3 \leftarrow m_3 - 1)$ **do**
    if $m_3 \neq \lfloor (B-1)/3 \rfloor$ **then**
      $c_3 \leftarrow c_3 \cdot (2m_3 + 2)/(2m_3 + 1)$
    end if
    $s \leftarrow 0$; $c_2 \leftarrow c_3$
    for $(m_2 \leftarrow 0;\ 2m_2 + 3m_3 < B;\ m_2 \leftarrow m_2 + 1)$ **do**
      $s \leftarrow s + E_2^{m_2} \cdot (-1)^{m_2} c_2/(4m_2 + 6m_3 + 1)$
      $c_2 \leftarrow c_2 \cdot (2m_2 + 2m_3 + 1)/(2m_2 + 2)$
    end for
    $R \leftarrow (R \cdot E_3) + s$
  end for
  return R
end procedure
return $A^{-1/2}$ (RSUM$(E_2, E_3, B) + [\pm\varepsilon] + [\pm\varepsilon]i$) ▷ Include prefactor and error bound
end

[7] This is an algebraic simplification, so we can take $E_1 = 0$ even if the input argument are represented by inexact balls.

Fig. 2 Exponents $2m_2 + 3m_3 < B$ appearing for $B = 10$



Algorithm 2 gives pseudocode for the method implemented in Arb to compute R_F using combined argument reduction and series evaluation. The subroutine RSum evaluates the series for $R_{-1/2}$ truncated to an arbitrary order B using rectangular splitting combined with recurrence relations for the coefficients (one more optimization used in the implementation but omitted from the pseudocode is to clear denominators so that all coefficients are small integers). The exponents of $E_2^{m_2} E_3^{m_3}$ appearing in the series (Fig. 2) are the lattice points $m_2, m_3 \in \mathbb{Z}_{\geq 0}$ with $2m_2 + 3m_3 < B$: we compute powers of E_2 and then use Horner's rule with respect to E_3.

We now consider the choice of B. Since the series evaluation costs $O(B^2)$ operations and the argument reduction costs $O(p/B)$ operations, the overall cost is $O(N^2 + p/N)$ operations, which is minimized by setting $B \approx p^{1/3}$; this gives us an $O(p^{1.667})$ bit complexity algorithm for evaluating R_F. With rectangular splitting for the series evaluation, the optimal B should be closer to $B \approx p^{0.5}$ for moderate p. Timings in Arb show that expanding to order $B = 2p^{0.4}$ for real variables and $B = 2.5p^{0.4}$ for complex variables is nearly optimal in the range $10 \leq p \leq 10^6$ bits. Compared to the fixed order $B = 8$, this results in a measured speedup of 1.5, 4.0, 11 and 31 times at a precision of 100, 1000, 10 000 and 100 000 decimal digits respectively.

The algorithm for the R_J series is essentially the same, except that the summation uses four nested loops instead of two to iterate over the exponents with $2m_2 + 3m_3 + 4m_4 + 5m_5 < B$, with corresponding nested recurrence relations to update coefficients c_2, c_3, c_4, c_5 (see the Arb source code for details). In this case, rectangular splitting is used to split the number of variables in half by precomputing a twodimensional array of powers $E_2^{m_2} E_3^{m_3}$ and using the Horner scheme with respect to E_4 and E_5. The speedup of combining rectangular splitting with optimal argument reduction is smaller for R_J than for R_F but still appreciable at very high precision.

7 Arb Implementation Benchmarks

Table 2 compares the performance of different functions implemented in Arb.

The complete elliptic integrals of the first and second kind are about as fast as the elementary functions at high precision due to the $\widetilde{O}(p)$ AGM algorithm.[8] The modular forms and functions which use $\widetilde{O}(p^{1.5})$ algorithms with very low overhead are nearly as fast as complete elliptic integrals in practice.

[8]At precision up to about 1000 digits, the elementary functions in Arb are significantly faster than the AGM due to using precomputed lookup tables and many low-level optimizations [14].

Table 2 Time in seconds to evaluate the function (or tuple of function values simultaneously) at d decimal digits of precision ($p = \lceil d \log_2 10 \rceil$ bits) for d between 10 and 100 000. The arguments are set to generic complex numbers $x = \sqrt{2} + \sqrt{3}i$, $y = \sqrt{3} + \sqrt{5}i$, $z = \sqrt{5} + \sqrt{7}i$, $t = \sqrt{7} + i/\sqrt{11}$

	Function	$d = 10$	$d = 10^2$	$d = 10^3$	$d = 10^4$	$d = 10^5$
Elementary functions	$\exp(x)$	$7.7 \cdot 10^{-7}$	$2.9 \cdot 10^{-6}$	0.00011	0.0062	0.24
	$\log(x)$	$8.1 \cdot 10^{-7}$	$2.8 \cdot 10^{-6}$	0.00011	0.0077	0.27
Modular forms and functions	$\eta(t)$	$6.2 \cdot 10^{-6}$	$1.99 \cdot 10^{-5}$	0.00037	0.015	0.69
	$j(t)$	$6.3 \cdot 10^{-6}$	$2.3 \cdot 10^{-5}$	0.00046	0.022	1.1
	$(\theta_i(0,t))_{i=1}^4$	$7.6 \cdot 10^{-6}$	$2.7 \cdot 10^{-5}$	0.00044	0.022	1.1
Elliptic and theta functions	$(\theta_i(x,t))_{i=1}^4$	$2.8 \cdot 10^{-5}$	$8.1 \cdot 10^{-5}$	0.0016	0.089	5.4
	$\wp(x,t)$	$3.9 \cdot 10^{-5}$	0.00012	0.0021	0.11	6.6
	$(\wp(x,t), \wp'(x,t))$	$5.6 \cdot 10^{-5}$	0.00017	0.0026	0.13	7.3
	$\zeta(x,t)$	$7.5 \cdot 10^{-5}$	0.00022	0.0028	0.14	7.8
	$\sigma(x,t)$	$7.6 \cdot 10^{-5}$	0.00022	0.0030	0.14	8.1
Complete elliptic integrals	$K(x)$	$5.4 \cdot 10^{-6}$	$2.0 \cdot 10^{-5}$	0.00018	0.0068	0.23
	$E(y)$	$1.7 \cdot 10^{-5}$	$6.1 \cdot 10^{-5}$	0.00072	0.025	0.71
	$\Pi(x,y)$	$7.0 \cdot 10^{-5}$	0.00046	0.014	3.6	563
Incomplete elliptic integrals	$\wp^{-1}(x,t)$	$3.1 \cdot 10^{-5}$	0.00014	0.0025	0.20	20
	$F(x,y)$	$2.4 \cdot 10^{-5}$	0.00011	0.0022	0.19	19
	$E(x,y)$	$5.6 \cdot 10^{-5}$	0.00030	0.0070	0.76	97
	$\Pi(x,y,z)$	0.00017	0.00098	0.030	5.6	895
	$R_F(x,y,z)$	$1.6 \cdot 10^{-5}$	$9.5 \cdot 10^{-5}$	0.0020	0.18	18
	$R_G(x,y,z)$	$4.7 \cdot 10^{-5}$	0.00027	0.0067	0.75	95
	$R_D(x,y,z)$	$2.1 \cdot 10^{-5}$	0.00016	0.0046	0.57	78
	$R_J(x,y,z,t)$	$3.4 \cdot 10^{-5}$	0.00031	0.012	2.6	428

Elliptic functions and Jacobi theta functions, also implemented with $\widetilde{O}(p^{1.5})$ algorithms, are some 5–10 times slower than the special case of theta constants or modular forms. The incomplete elliptic integrals based on the R_F function implemented with $O(p^{1.667})$ complexity have similar performance to the elliptic functions at moderate precision with a slight divergence becoming visible only at several thousand digits. Indeed, $\wp(x,t)$ and $\wp^{-1}(x,t)$ have virtually identical performance although the algorithms are completely independent.

The incomplete elliptic integrals based on the R_J function stand out as being noticeably slower than the other functions, as a result of the more complicated argument reduction and high-dimensional series expansion.

8 Other Methods

Many numerical techniques apart from those covered in this text are useful in connection with elliptic functions and modular forms. Without going into detail, we sketch a few important ideas.

8.1 Quadratically Convergent Methods and Newton Iteration

The algorithms described above for complete elliptic integrals have quasioptimal $\widetilde{O}(p)$ bit complexity owing to the quadratically convergent AGM iteration, while the algorithms for all other functions have $\widetilde{O}(p^{1.5})$ or worse bit complexity. In fact, it is possible to compute general elliptic functions, modular forms and incomplete elliptic integrals with $\widetilde{O}(p)$ bit complexity using generalizations of the AGM iteration together with Newton's method for inverse functions. We have omitted these methods in the present work since they are more complicated, especially for complex variables, and not necessarily faster for p encountered in practice.

The asymptotically fast computation of modular forms and modular functions is discussed by Dupont [9], and Labrande [18] has given algorithms for general theta functions and elliptic functions. An important special case is the inverse Weierstrass elliptic function in the form of the elliptic logarithm, which can be computed using a simple AGM-type algorithm [7]. For the Legendre incomplete elliptic integrals, algorithms based on the quadratic Landen transformations are classical and have been described in several other works; they have the disadvantage of involving trigonometric functions, not having a straightforward extension to complex variables, and in some regions suffering from precision loss.

8.2 Numerical Integration

Direct numerical integration is a viable way to compute elliptic integrals. Numerical integration is generally slower than the more specialized algorithms already presented, but with a robust general-purpose integration algorithm, we can just plug in the formula for any particular elliptic integral. Specifying an explicit contour of integration also provides full control over branch cuts.

The double exponential or tanh-sinh quadrature method [1, 27] is ideal for elliptic integrals since it is extremely simple and converges rapidly even if the integrand has algebraic singularities of unknown type at one or both endpoints. The quadrature error in the double exponential method can be estimated quite reliably using heuristics, and effective rigorous error bounds are also known [19]. Alternatively, Gauss-Jacobi quadrature can be used for integrals with known algebraic singularities. Recently, Molin and Neurohr have studied use of both double exponential and Gauss-Jacobi quadrature with rigorous error bounds for integration of algebraic functions in the context of computing period matrices for hyperelliptic curves [20]. Rigorous numerical integration code also exists in Arb [17], but endpoint singularities require manual processing.

For integrals of smooth periodic functions, including integrals of analytic functions on closed circular contours, direct application of the trapezoidal rule is often the best choice. We conclude with the anecdote that Poisson already in the 1820s demonstrated the use of the trapezoidal rule to approximate the elliptic integral

$$\frac{1}{2\pi}\int_0^{2\pi}\sqrt{1-0.36\sin^2(\theta)}d\theta$$

which is equal to $\frac{2}{\pi}E(0.36)$ in the Legendre notation. Poisson derived an error bound for the N-point trapezoidal approximation and showed that $N = 16$ gives an error less than $4.84 \cdot 10^{-6}$ for this integral (in fact, nine digits are correct). Due to symmetry, just three nontrivial evaluations of the integrand are required for this level of accuracy! Trefethen and Weideman [30] discuss this example and provide a general error analysis for the trapezoidal rule applied to periodic functions.

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Multi-valued Feynman Graphs and Scattering Theory

Dirk Kreimer

Abstract We outline ideas to connect the analytic structure of Feynman amplitudes to the structure of Karen Vogtmann's and Marc Culler's *Outer Space*. We focus on the role of cubical chain complexes in this context, and also investigate the bordification problem in the example of the 3-edge banana graph.

1 Motivation and Introduction

This is a write-up of two talks given recently in Zeuthen and in Les Houches. It contains results and ideas which are partially published and which will be elaborated on in future work.

We want to establish a conceptual relation between scattering theory for Feynman amplitudes (see for example [1] and references there for an introduction) and the structure of suitable Outer Spaces, motivated by [2–5].

In particular we want to incorporate in the analysis the structure of amplitudes as multi-valued functions. We use this term for the study of functions defined by the evaluation of a Feynman graph $\Gamma \in H$ by renormalized Feynman rules,

$$\Phi_R : H \to \mathbb{C}.$$

Here, H is a suitable Hopf algebra of Feynman graphs.

$\Phi_R(\Gamma)$, $\forall \Gamma \in H$ depends on kinematics: $p \in Q_\Gamma$, $\Phi_R(\Gamma) = \Phi_R(\Gamma)(p)$, where Q_Γ is a real vectorspace [6],

$$Q_\Gamma \sim \mathbb{R}^{v_\Gamma(v_\Gamma-1)/2+e_\Gamma},$$

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generated by all scalar products of external momenta, and internal masses of Γ. Here, v_Γ, e_Γ are the number of vertices and edges of Γ. We assign an external momentum to each vertex of the graph. They can be set to zero when needed.

The analysis will proceed by regarding such an amplitude $\Phi_R(\Gamma)$ as an iterated integral. What is to be iterated are not differential one-forms though, as in the example of the study of generalized polylogarithms, but elementary amplitudes $\Phi_R(\gamma)$ built from particularly simple Feynman graphs γ: one-loop graphs which form the basis primitive elements of the core Hopf algebra H_{core} defined below.

$\Phi_R(\Gamma)$ is not uniquely defined as an iterated integral as there are many distinct flags [7, 8] which describe possible sequences of iteration to obtain $\Phi_R(\Gamma)$.

We will remedy this below by defining a suitable equivalence relation using equality along principal sheets. The latter equality reflects Fubini's theorem in the context of renormalized amplitudes.

Our claim is that this iteration gives $\Phi_R(\Gamma)$ -the evaluation of Γ by renormalized Feynman rules- a structure which reflects the structure of a suitable Outer Space built on graphs. Here, the graphs are metric marked graphs with colored edges, and without mono- or bi-valent vertices.

The full amplitude contributing at a given loop order is obtained by summing graphs which all have the same loop order and the same number of external edges. Suitably interpreted, the full amplitude is obtained as an integral over all cells of Outer Space, in a piecewise linear manner as exhibited in [9].

Such Outer Spaces are used in mathematics to study, amongst many things, the representation theory of the free group F_{n_Γ}. In the course of such studies graph complexes arise which have bearing in their own right in the investigation of $\Phi_R(\Gamma)$. This includes

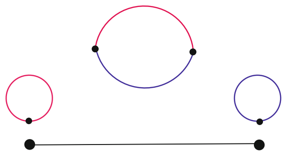
- Outer Space itself as a cell-complex with a corresponding spine and partial order defined from shrinking edges [2];
- a cubical chain complex resulting from a boundary d which acts on pairs (Γ, F), F a spanning forest of Γ [3];
- a bordification which blows up missing cells at infinity [4].

The use of metric graphs suggests itself in the study of amplitudes upon using the parametric representation: the parametric integral is then the integral over the volume of the open simplex σ_Γ, the cell assigned to each graph Γ in Outer Space, which itself is a union of such cells.

Colored edges reflect the possibility of different masses in the propagators assigned to edges. External edges are not drawn in the coming pictures. Momentum conservation allows us to incorporate them by connecting external vertices to a distinguished vertex v_∞. We come back to this elsewhere.

2 b_2: The Bubble

We first discuss the elementary monodromy of the simplest one-loop graph.[1] So we start with the 2-edge banana b_2, a bubble on two edges with two different internal masses m_b, m_r, indicated by two different colors:



The incoming external momenta at the two vertices of b_2 are $q, -q$.

We assign to b_2 a one-dimensional cell, an open line segment, and glue in its two boundary endpoints, to which the two tadpoles on the two different masses are assigned, obtained by either shrinking the blue or red edge. The vertex at each tadpole is then 4-valent, with no external momentum flow through the graph.

The fundamental group

$$\Pi_1(b_2) \sim \mathbb{Z}$$

of b_2 has a single generator. This matches with the monodromy of the function $\Phi_R(b_2)$ as we see in a moment.

Indeed, the Feynman integral we consider is coming from renormalized Feynman rules $\Phi_R(b_2)$, where we implement a kinematic renormalization scheme by subtraction at $\mu^2 < (m_b - m_r)^2$ (so that the subtracted terms does not have an imginary part, as μ^2 is even below the pseudo threshold):

$$\Phi_R(b_2) = \int d^4k \left(\underbrace{\frac{1}{k^2 - m_r^2}}_{Q_1} \underbrace{\frac{1}{(k+q)^2 - m_b^2}}_{Q_2} - \{q^2 \to \mu^2\} \right).$$

We set $s := q^2$ and demand $s > 0$, and also set $s_0 := \mu^2$.

We write $k = (k_0, \mathbf{k})^T$, $t := \mathbf{k} \cdot \mathbf{k}$. As the 4-vector q is assumed time-like (as $s > 0$) we can work in a coordinate system where $q = (q_0, 0, 0, 0)^T$ and get

$$\Phi_R(b_2) = 4\pi \int_{-\infty}^{\infty} dk_0 \int_0^{\infty} \sqrt{t} dt \left(\frac{1}{k_0^2 - t - m_r^2} \frac{1}{(k_0 + q_0)^2 - t - m_b^2} - \{s \to s_0\} \right).$$

We define the Kȧllen function

$$\lambda(a, b, c) := a^2 + b^2 + c^2 - 2(ab + bc + ca),$$

[1] This material is standard for physicists. It is included here for the benefit of mathematicians who are usually not exposed to the monodromy of Feynman amplitudes.

and find by explicit integration

$$\Phi_R(b_2)(s,s_0;m_r^2,m_b^2) = \\ = \left(\underbrace{\frac{\sqrt{\lambda(s,m_r^2,m_b^2)}}{2s} \ln \frac{m_r^2+m_b^2-s-\sqrt{\lambda(s,m_r^2,m_b^2)}}{m_r^2+m_b^2-s+\sqrt{\lambda(s,m_r^2,m_b^2)}} - \frac{m_r^2-m_b^2}{2s} \ln \frac{m_r^2}{m_b^2}}_{B_2(s)} \right. \\ \left. - \underbrace{\{s \to s_0\}}_{B_2(s_0)} \right).$$

The principal sheet of the above logarithm is real for $s \leq (m_r+m_b)^2$ and free of singularities at $s=0$ and $s=(m_r-m_b)^2$. It has a branch cut for $s \geq (m_r+m_b)^2$.

The threshold divisor defined by the intersection $Q_1 \cap Q_2$ where the zero locii of the quadrics meet is at $s=(m_b+m_r)^2$. This is an elementary example of the application of Picard–Lefschetz theory [6, 10].

Off the principal sheet, we have a pole at $s=0$ and a further branch cut for $s \leq (m_r-m_b)^2$.

It is particularly interesting to compute the variation using Cutkosky's theorem [6]

$$\mathrm{Var}(\Phi_R(b_2)) = 4\pi \int_0^\infty \sqrt{z}dz \int_{-\infty}^\infty dk_0 \delta_+(k_0^2-t-m_r^2)\delta_+((k_0-q_0)^2-t-m_b^2).$$

Integrating k_0 using $k_0+q_0>0$ and $k_0=-q_0+\sqrt{t+m_b^2}$, delivers

$$\mathrm{Var}(\Phi_R(b_2)) = \int_0^\infty \sqrt{t}dt\delta((q_0-\sqrt{t+m_b^2})^2-t-m_r^2)\frac{1}{\sqrt{t+m_b^2}}.$$

With

$$\left(q_0-\sqrt{t+m_b^2}\right)^2 - t - m_r^2 = s - 2\sqrt{s}\sqrt{t+m_b^2} + m_b^2 - m_r^2,$$

we have from the remaining δ-function,

$$0 \leq t = \frac{\lambda(s,m_r^2,m_b^2)}{4s},$$

whenever the Kȧllen $\lambda(s,m_r^2,m_b^2)$ function is positive.

The integral gives

$$\mathrm{Var}(\Phi_R(b_2))(s, m_r^2, m_b^2) = \overbrace{\left(\frac{\sqrt{\lambda(s, m_r^2, m_b^2)}}{2s}\right)}^{=:V_{rb}(s;m_r^2,m_b^2)} \times \Theta(s - (m_r + m_b)^2).$$

We emphasize that V_{rb} has a pole at $s = 0$ with residue $|m_r^2 - m_b^2|/2$ and note $\lambda(s, m_r^2, m_b^2) = (s - (m_r + m_b)^2)(s - (m_r - m_b)^2)$.

We regain $\Phi_R(b_2)$ from $\mathrm{Var}(\Phi_R(b_2))$ by a subtracted dispersion integral:

$$\Phi_R(b_2) = \frac{s - s_0}{\pi} \int_0^\infty \frac{\mathrm{Var}(\Phi_R(b_2)(x))}{(x - s)(x - s_0)} dx.$$

Below we will also study the contributions of non-principal sheets and relate them to the bordification of Outer Space.

In preparation we note that non-principal sheets give a contribution

$$2j\pi\imath V_{rb}(s),\ j \in \mathbb{Z}^\times,$$

where $\imath$ is the imaginary unit, $\imath^2 = -1$.

We hence define a multi-valued function

$$\Phi_R(b_2)^{\mathrm{mv}}(s, m_r^2, m_b^2) := \Phi_R(b_2)(s, m_r^2, m_b^2) + 2\pi\imath\mathbb{Z}V_{rb}(s).$$

Sometimes it is convenient to write this as

$$\Phi_R(b_2)^{\mathrm{mv}}(s, m_r^2, m_b^2) := \Phi_R(b_2)(s, m_r^2, m_b^2) + 2\pi\imath\mathbb{Z}\left(J_1^{rb}(s) + J_2^{rb}(s) + J_3^{rb}(s)\right),$$

with

$$J_1^{rb}(s) := V_{rb}(s)\Theta((m_r - m_b)^2 - s), \tag{1}$$
$$J_2^{rb}(s) := V_{rb}(s)\Theta(s - (m_r - m_b)^2)\Theta((m_r + m_b)^2 - s), \tag{2}$$
$$J_3^{rb}(s) := V_{rb}(s)\Theta(s - (m_r + m_b)^2). \tag{3}$$

From the definition of the Kållen function, we conclude:

$J_1^{rb} \in \mathbb{R}_+$ is positive real,
$J_3^{rb}(s) \in \mathbb{R}_+$ likewise and
$J_2^{rb}(s) \in \imath\mathbb{R}_+$ is positive imaginary.

3 The Pole at $s = 0$

In the above, we saw already a pole in s appear for the evaluation along non-principal sheets for the amplitudes coming from the graph b_2. Actually, such poles are a general phenomenon as we want to exhibit now before we discuss the relation between the sheet structure of amplitudes and the structure of graph complexes apparent in colored variants of Outer Spaces.

We proceed using the parametric representation of amplitudes through graph polynomials as for example given in [11].

Let

$$\Phi_\Gamma = \phi_\Gamma + A \cdot M\psi_\Gamma,$$

be the second Symanzik polynomial with masses and consider the amplitude

$$A_\Gamma := \int_{\mathbb{P}_\Gamma} \frac{\ln \frac{\Phi_\Gamma}{\Phi_\Gamma^0}}{\psi_\Gamma^2} \Omega_\Gamma.$$

As ψ_Γ and Φ_Γ^0 are both strictly positive in the domain of integration (the latter by choice of a renormalization scheme which subtracts at a kinematic point $p_0 \in Q_\Gamma$ below all thresholds), we conclude

$$\Im A_\Gamma := \int_{\mathbb{P}_\Gamma} \frac{\Theta(\Phi_\Gamma)}{\psi_\Gamma^2} \Omega_\Gamma.$$

Let dA_Γ^1 be the affine measure setting $A_1 = 1$, and let $e \neq e_1$ be an edge $e \in E_\Gamma$, and $\mathbb{A}^1$ be the corresponding positive hypercube.

We have $\psi_\Gamma = A_e \psi_{\gamma - e} + \psi_{\Gamma/e}$. Then,

$$\Im A_\Gamma = \int_{\mathbb{A}^1} \frac{\partial_{A_e} \Theta(\Phi_\Gamma)}{\psi_\Gamma \psi_{\Gamma - e}} dA_\Gamma^1 + \text{boundary},$$

where we note $\partial_{A_e} \Theta(\Phi_\Gamma) = -\delta(\Phi_\Gamma)\partial_{A_e}(\Phi_\Gamma)$. With Φ_Γ being a quadratic polynomial in A_e,

$$\Phi_\Gamma = Z A_e^2 - Y A_e - X = Z\left(A_e + \frac{\tilde{Y}}{2} + \frac{1}{2}\sqrt{\tilde{Y}^2 - 4\tilde{X}}\right)\left(A_e + \frac{\tilde{Y}}{2} - \frac{1}{2}\sqrt{\tilde{Y}^2 - 4\tilde{X}}\right),$$

we set

$$A_e^{\pm} := -\frac{\tilde{Y}}{2} \pm \frac{1}{2}\sqrt{\tilde{Y}^2 - 4\tilde{X}}.$$

As $\delta(f(x)) = \sum_{\{x_0|f(x_0)=0\}} \frac{1}{|f'(x_0)|}\delta(x-x_0)$, we get

$$\Im A_\Gamma = \int_{\mathbb{A}_e^1} \sum_{\pm} \frac{-\partial_{A_e}(\Phi_\Gamma)(A_e^\pm)}{|-\partial_{A_e}(\Phi_\Gamma)(A_e^\pm)|} \frac{1}{(\psi_\Gamma \psi_{\Gamma-e})(A_e^\pm)}.$$

At $A_e = A_e^\pm$, we have $\Phi_\Gamma = 0$, and therefore $\phi_\Gamma = A \cdot M \psi_\Gamma$, or

$$\psi_\Gamma = \frac{\phi_\Gamma}{A \cdot M},$$

hence

$$\frac{1}{\psi_\Gamma \psi_{\Gamma-e}} = \frac{1}{\psi_{\Gamma-e}} \frac{A \cdot M}{\phi_\Gamma}.$$

For a two-point function associated to a two-point graph Γ we have $\phi_\Gamma = s\psi_{\Gamma_\bullet}$. Here $\Gamma_\bullet$ is the graph where the two external edges of Γ are identified. We conclude

$$\Im A_\Gamma \sim \frac{1}{s}.$$

For a n-point function, regarded as a function of a kinematical scale s and angles $\vartheta_{ij} = q_i \cdot q_j / s$ [11], we find similarly[2]

$$\frac{1}{\psi_\Gamma \psi_{\Gamma-e}} = \frac{1}{s} \frac{1}{\psi_{\Gamma-e}} \frac{A \cdot M}{\phi_\Gamma(\{\vartheta_{ij}\})}.$$

An immediate calculation gives that the boundary term remaining from the above,

$$\int_{\mathbb{P}_{\Gamma/e}} \frac{\Theta(\Phi_{\Gamma/e})}{\psi_{\Gamma/e} \psi_{\Gamma-e}} \Omega_{\Gamma/e},$$

leads to an iteration akin to linear reduction as studied by Brown and Panzer [12–14].

We have just proven that the two point function has a pole at $s = 0$ in its imaginary part. This will have consequences below when we investigate in particular the analytic structure of the multi-edge banana graphs b_3, the story is similar for generic b_n.

4 The Basic Set-Up: Outer Space

We now first describe Outer Space. What we use is actually a variant in which there are external edges at vertices, and internal edges are colored to allow for different

[2] This explains the Omnès factor $1/\sqrt{\lambda(q_1^2, q_2^2, q_3^2)}$ in the computation of the anomalous threshold of the triangle graph.

types of internal propagators. Here, different colors indicate generic different internal masses, but could also be used as placeholders for different spin and more.[3]

4.1 The Set-Up of Colored Outer Space

Outer Space can be regarded as a collection of open simplices. For a graph with k edges, we assign an open simplex of dimension $k-1$. We can either demand that the sum of edge lengths (given by parametric variables A_e) adds to unity, or work in projective space $\mathbb{P}^{k-1}(\mathbb{R}_+)$ in such a cell. Each graph comes with a metric, and one moves around the cell by varying the edge lengths.

Edge lengths are allowed to become zero but we are not allowed to shrink loops.

When an edge say between two three-valent vertices shrinks to zero length, there are several ways to resolve the resulting 4-valent vertex to obtain a new nearby graph: assume we have a 4-valent vertex in a graph G sitting in a $(k-1)$-dimensional cell. Then, this cell can be glued in as a common boundary of three other k-dimensional cells with corresponding graphs G_i, $i \in \{s, t, u\}$, which have an edge e connecting two 3-valent vertices, such that $G_i/e = G$, where G_i/e is the graph where edge e shrinks to zero length.

For a formal definition of Outer Space we refer to [2]. We emphasize that a crucial role is played by the fundamental group of the graph, generated by its loops. A choice of a spanning tree T of a graph with m independent loops l_i determines m edges e_i not in the spanning tree. The loops $l_i = l_i(e_i)$ are uniquely given by the edge e_i and the path in T connecting the two endpoints of e_i. An orientation of e_i orients the loop, and shrinking all edges of T to zero length gives a rose R_m, a graph with one vertex and m oriented petals e_i. The inverse of this map gives a marking to the graph, which for us determines a choice for a basis of loops we integrate in a Feynman integral. The homotopy equivalence of such markings is reflected by the invariance of the Feynman integral under the choice how we route our momenta through the graph.

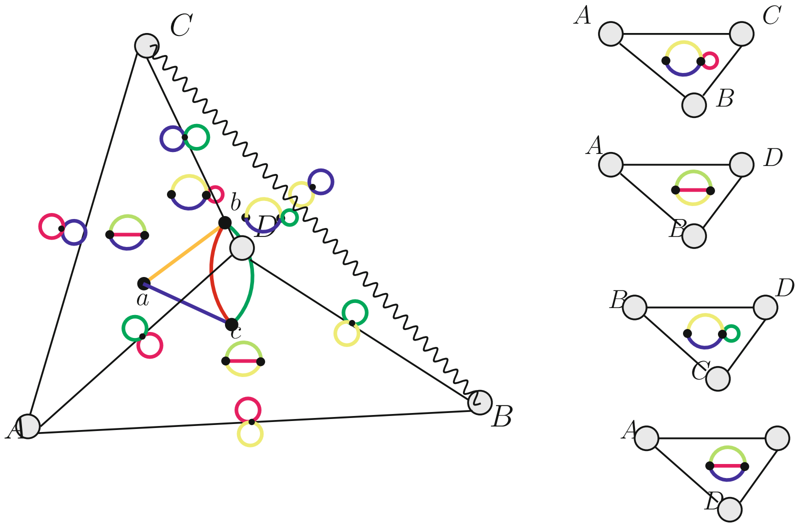
In Outer Space graphs are metric graphs, where the metric comes from assigning an edge length to each edge, and using the parametric integrand for Feynman graph, the Feynman integral becomes an integral over the volume of the open simplex assigned to the graph, with a measure defined by the parametric representation. All vertices we assume to be of valence three or higher.

Each edge-path $l_i(e_i)$ defines a one-loop sub-integral which is multi-valued and an ordered sequence of petals of R_m defines an iterated integral of multi-valued one-loop integrals. Using Fubini this is a well-defined integral for any ordering of the loops along the principal sheets of these loop evaluations.

Let us discuss these notions on the example of the Dunce's cap graph, to which just one of the many simplices of Outer Space is assigned. It is a graph dc on four edges, accordingly, the open simplex assigned to it is a tetrahedron. The codimension-one

[3]See [15] for first introductory explorations of Outer Space with colored edges in this context.

boundaries are four triangles, to which we assign reduced graphs dc/e in which one of the four edges e has zero length.



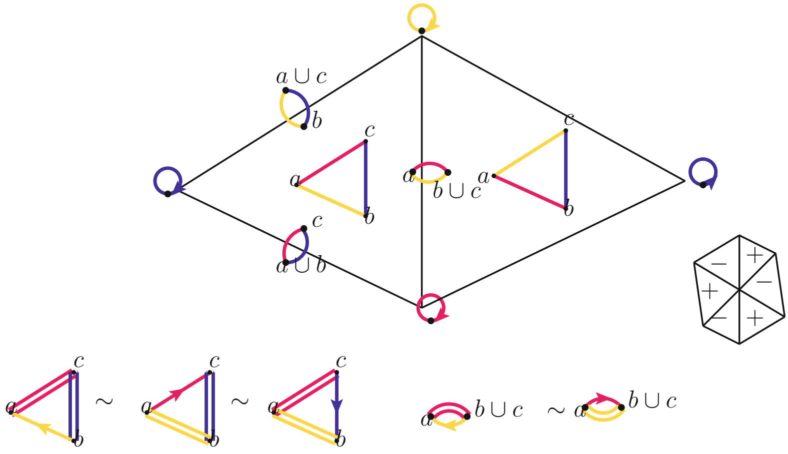
The codimension-two boundaries are six edges, to which in five cases a two-petal rose R_2 is assigned, of the form $\mathrm{dc}/e/f$, by shrinking two of the four edges. We can not shrink the green and red edges, as this would shrink a loop. So the edge BC (indicated by a wavy line) with the rose on blue and yellow petals is actually not part of Outer Space.

The codimension-three boundaries are the four corners A, B, C, D and are not part of Outer Space either. The graph dc allows for five spanning trees, each of which determines a loop basis for $H^1(\mathrm{dc})$. For any of the five choices of a spanning tree, there are two edges e, f say not in the spanning tree. They define two loops l_e, l_f, by the edge path through the spanning tree which connects the endpoints of e and f.

To translate this to Feynman graphs, we route all external momenta through edges of the spanning tree, and assign a loop momentum to each loop l_e, l_f. Any choice of order in which to carry out the loop integrations defines an iterated integral over two four-forms given by the corresponding loop integrals.

4.2 Example: The Triangle Graph

The above example discusses the structure of one cell together with its boundary components. We now look at the example of a triangle graph, and discuss its appearance in different cells.



Here, the boundaries of the triangular cell belong themselves to OS: the three edges of the triangular cell are a cell for the indicated 1-loop graphs on two graph-edges, the vertices correspond to colored 1-petal roses.

We have given two triangular cells in the picture. Both are associated to a triangle graph. The boundary in between is associated to the graph on a red and yellow edge as indicated. It is obtained by shrinking the blue edge. On the left- and righthand side of the boundary the triangle has permuted its internal red and yellow edge, with a corresponding orientation change $x \to x^{-1}$ of the single marking assigned to the graph. Gluing cells for the six possible permutations we obtain a hexagon, with alternating orientations as indicated.

We also give the OS equivalence relation where spanning trees are indicated by double-edges, for the triangle and for the example of the red-yellow graph on the boundary.

We omit the triangular cells corresponding to not bridge-free (not core) graphs.

Each choice of a spanning tree and choice of an ordering of its (two) edges gives rise to a Hodge matrix corresponding to the evaluation of this graph as a dilogarithm [7]. The entries are formed from the graphs apparent in the corresponding cubical cell complex which we describe in a moment.

The sheet structure of the normal threshold of a two-edge graph on a boundary edge of the triangular cell is a $2\pi\imath\mathbb{Z}$ logarithmic ambiguity, the triangle provides a further anomalous threshold which is of similar nature.

In this way the generators of the simple fundamental group of this one-loop graph map to generators of the monodromy generated by the normal or anomalous threshold divisors of the amplitude obtained from the graph.

4.3 Analytic Structure

We consider the Feynman integral in momentum space and define the following quadrics.

$$
\begin{aligned}
Q_1 &:= k_0^2 - t - m_1^2 + i\eta,\\
Q_2 &:= (k_0 + q_0)^2 - t - m_2^2 + i\eta,\\
Q_3 &:= (k_0 + p_0)^2 - t - \mathbf{p}^2 - 2\sqrt{t\mathbf{p}^2}z - m_1^2 + i\eta,
\end{aligned}
$$

where $s = q_0^2$. The independent external momenta are p and q. $q^2 = q_0^2$ is time-like as before, and we compute in the rest-frame of q. q is the momentum at vertex a, p the momentum at vertex c and $-(q + p)$ the momentum incoming at vertex b.

The measure d^4k is transferred to $dk_0d^3\mathbf{k}$, and in the three-dimensional space-like part we choose spherical coordinates with $\mathbf{k}^2 =: t$. $z = \cos(\Theta) = \mathbf{p}\cdot\mathbf{k}/\sqrt{\mathbf{p}^2\mathbf{k}^2}$ the cosine of the angle between $\mathbf{k}$, $\mathbf{p}$.

We are interested in the following integrals (subtractions at s_0 understood when necessary):

(i)

$$\int_{\infty}^{\infty} dk_0 \int_0^{\infty} \sqrt{t}dt \int_{-1}^{1} dz \int_0^{2\pi} d\phi \frac{1}{Q_1 Q_2} = \Phi_R(b_2),$$

(ii)

$$\int_{\infty}^{\infty} dk_0 \int_0^{\infty} \sqrt{t}dt \int_{-1}^{1} dz \int_0^{2\pi} d\phi \delta_+(Q_1)\delta_+(Q_2) = \mathrm{Var}(\Phi_R(b_2)),$$

(iii)

$$\int_{\infty}^{\infty} dk_0 \int_0^{\infty} \sqrt{t}dt \int_{-1}^{1} dz \int_0^{2\pi} d\phi \frac{1}{Q_1 Q_2 Q_3} =: I_3(s, p^2, (p+q)^2; m_b^2, m_r^2, m_y^2),$$

(iv)

$$\mathrm{Var}^{12}(I_3) := \int_{\infty}^{\infty} dk_0 \int_0^{\infty} \sqrt{t}dt \int_{-1}^{1} dz \int_0^{2\pi} d\phi \delta_+(Q_1)\delta_+(Q_2)\frac{1}{Q_3}.$$

(v)

$$\mathrm{Var}^{123}(I_3) := \int_{\infty}^{\infty} dk_0 \int_0^{\infty} \sqrt{t}dt \int_{-1}^{1} dz \int_0^{2\pi} d\phi \delta_+(Q_1)\delta_+(Q_2)\delta_+(Q_3).$$

Note that for (i), (ii) the integrand neither depends on z, nor on ϕ, so these integrals have a factor $4\pi = \mathrm{Vol}(S^2)$ in their evaluation.

Most interesting are the integrals in (iii)–(v). I_3 is a dilogarithm, see [7] for its properties.

Let us start with $\mathrm{Var}^{12}(I_3)$. The two δ_+-functions constrain the k_0- and t-variables, so that the remaining integrals are over the compact domain S^2.

As the integrand does not depend on ϕ, this gives a result of the form

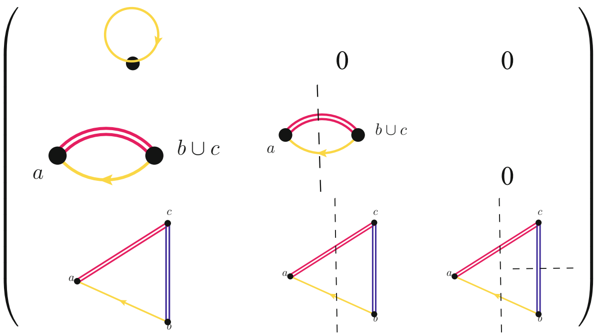
$$2\pi C \underbrace{\int_{-1}^{1} \frac{1}{\alpha+\beta z} dz}_{:=J(z)} = 2\pi C \frac{\ln \frac{\alpha+\beta}{\alpha-\beta}}{\beta},$$

where C is intimately related to $\mathrm{Var}(\Phi_R(b_2)) = 2C$, and the factor 2 here is $\mathrm{Vol}(S^2)/\mathrm{Vol}(S^1)$.

Then, we get a Hodge matrix for a triangle graph Δ

$$\begin{pmatrix} 1 & 0 & 0 \\ \Phi_R(b_2)(s, m_r^2, m_y^2) & V_{ry}(s, m_r^2, m_y^2) & 0 \\ I_3 & V_{ry}(s, m_r^2, m_y^2) \frac{\ln \frac{\alpha+\beta}{\alpha-\beta}}{\beta} & \underbrace{\frac{1}{\sqrt{s, p^2, (p+q)^2}}}_{=V_{ry}(s, m_r^2, m_y^2) \times \mathrm{Var} J(z)} \end{pmatrix}$$

$\sim$



Here, α and β are given through $l_1 := \lambda(s, p_b^2, p_c^2)$ and $l_2 := \lambda(s, m_y^2, m_r^2)$ as

$$\alpha := (m_y^2 - m_r^2 - s - p_a.p_c)^2 - l_1 - l_2, \ \beta := 2\sqrt{l_1 l_2}.$$

The amplitude of the triangle graph in a chosen triangular cell is the lower left entry in this Hodge matrix. The leftmost column of this matrix was obtained by first shrinking the blue edge, and then the red one. This fixes the other columns which are defined by the Cutkosky cuts -the variations- of the column to the left.

The triangle graph has a single loop and its fundamental group a single generator. Accordingly, we find a single generator for the monodromy in the complement of the threshold divisors: either for the normal threshold at $s_0 = (m_r + m_y)^2$ or for the anomalous threshold at s_1, with $l_r = p^2 - m_r^2 - m_b^2$, $l_y = (p+q)^2 - m_y^2 - m_b^2$, $\lambda_1 = \lambda(p^2, m_r^2, m_b v^2)$, $\lambda_1 = \lambda((p+q)^2, m_y^2, m_b v^2)$ it is [6] given as,

$$s_1 = (m_r + m_y)^2 + \frac{4m_b^2(\sqrt{\lambda_2}m_r - \sqrt{\lambda_1}m_y)^2 - (\sqrt{\lambda_1}l_y + \sqrt{\lambda_2}l_r)^2}{4m_b^2\sqrt{\lambda_1}\sqrt{\lambda_2}}. \tag{4}$$

The function $J(z)$ has no pinch singularity and does not generate a new vanishing cycle. In general, a one-loop graph generates one pinch singularity through its normal threshold given by a reduced graph b_2, and as many anomalous thresholds as there are further edges in the graph.

This structure iterates upon iterating one-loop graphs to multi-loop graphs. For multi-loop graphs, we discuss later only the example of the three-edge banana b_3, which only has a normal cut on the principal sheet, but a rather interesting structure on other sheets. The general picture will be discussed elsewhere. An algorithm to compute anomalous thresholds as s_1 is contained in [6].

Returning to the triangle graph, there are three different spanning trees on two edges for the triangle graph, and for each spanning tree two possibilities which edge to shrink first. This gives us six such matrices. To see the emergence of such matrices from the set-up of Outer Space turn to the cubical chain complex associated to the spine of Outer Space [3].

5 The Cubical Chain Complex

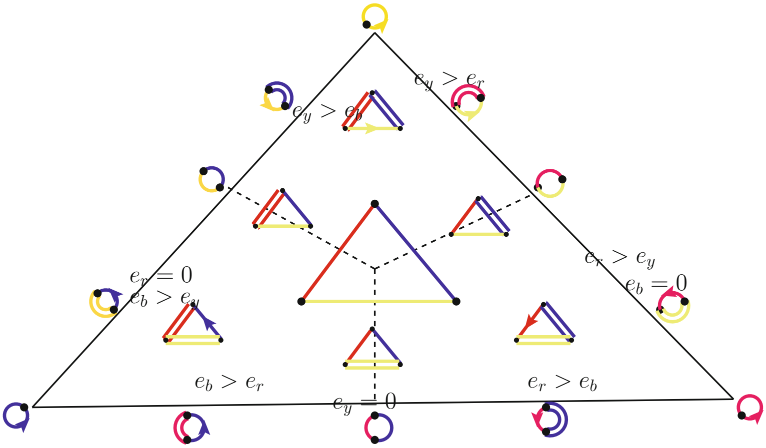
Consider the cell (itself an open triangle) assigned to one triangle graph. Let us assume we put the graph in the barycentric middle of the cell. At the codimension-one boundaries of the cell we glue edges, and put the corresponding graphs in their (barycentric) middle.

These boundaries correspond to edges $e_i = 0$, $i \in \{r, b, y\}$ as indicated in the figure.

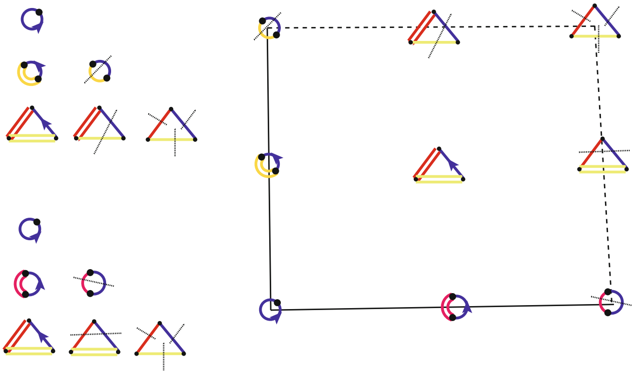
At the codimension-two corners we find tadpoles. When we move the triangle towards the blue corner say, its spanning tree must be on the yellow and red edges (edges in spanning trees are indicated by a double edge in the figure), which are the ones allowed to shrink.

When we move towards say the barycentric middle of the boundary defined by $e_y = 0$, only the yellow edge is part of a spanning forest, to the left of it the red edge is spanning as well, to the right the blue one.

The dashed lines connecting the barycentre of the triangular cell with the barycentres of its codimension-one boundaries partitions the triangular cell into three regions. Each such region has four corners and four line segments connections them, and an interior, to which pairs of the triangle graph Δ and a spanning tree are assigned as indicated.



Such a decomposition of sectors exists for any cell in Outer space. If a graph Γ has m spanning trees on n edges, we have $m \times n!$ paths from the barycentre of the Γ-cell to a rose. To this, we can assign m cubes, which decompose into $n!$ simplices, and we get $m \times n!$ Hodge matrices as well, $n!$ for each cosen spanning tree, for example two for a pair of a triangle and a chosen spanning tree (containing two edges) for it:



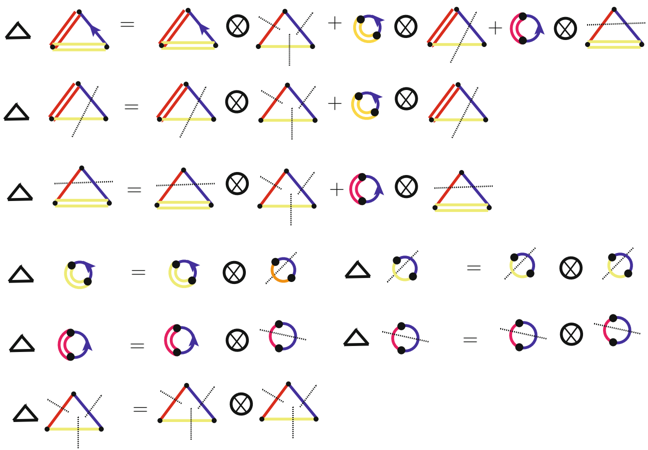
In the figure, we have marked the edges connecting different components of a spanning forest by cuts. The two triangular Hodge matrices on the left in the figure correspond to the two possible choices which edge to shrink first. Both Hodge matrices contain the three graphs as entries which populate the diagonal of the cube. The other entries are from above or below the diagonal.

The entries of the cube, and therefore the entries of the Hodge matrices describing variations of the accompanying Feynman integrals, are generated from a boundary operator d, $d \circ d = 0$, which acts on pairs (Γ, F) of a graph and a spanning forest [3].

$$d(\Gamma, F) = \sum_{j=1}^{|E_F|}(-1)^j\,((\Gamma/e, F/e) \otimes (\Gamma, F\backslash e))$$

In our Hodge matrices, the left-most columns are distinguished, as in them only pairs (Γ, F) appear in which F is a spanning tree of Γ, while all other entries have spanning forests consisting of more than a single tree, corresponding to graphs with Cutkosky cuts.

This suggests to bring this into a form of coaction (see also [16]), which looks as follows:



(5)

Before we comment on this in any further detail, we have to collect a few more algebraic properties of Feynman graphs.

6 Hopf Algebra Structure for 1PI Graphs

We start with the renormalization and core Hopf algebras.

6.1 Core and Renormalization Hopf Algebras

Consider the free commutative $\mathbb{Q}$-algebra

$$H = \oplus_{i\geq 0} H^{(i)},\ H^{(0)} \sim \mathbb{Q}\mathbb{I}, \tag{6}$$

generated by 2-connected graphs as free generators (disjoint union is product m, labelling of edges and of vertices by momenta as declared).

Consider the Hopf algebras $H(m, \mathbb{I}, \Delta, \hat{\mathbb{I}}, S)$ and $H(m, \mathbb{I}, \Delta_{\text{core}}, \hat{\mathbb{I}}, S_c)$, given by

$$\mathbb{I} : \mathbb{Q} \to H, q \to q\mathbb{I}, \tag{7}$$

$$\Delta : H \to H \otimes H, \Delta(\Gamma) = \Gamma \otimes \mathbb{I} + \mathbb{I} \otimes \Gamma + \sum_{\gamma \subsetneq \Gamma, \gamma = \cup_i \gamma_i, w(\gamma_i) \geq 0} \gamma \otimes \Gamma/\gamma, \tag{8}$$

$$\Delta_{\text{core}} : H \to H \otimes H, \Delta_{\text{core}}(\Gamma) = \Gamma \otimes \mathbb{I} + \mathbb{I} \otimes \Gamma + \sum_{\gamma \subsetneq \Gamma, \gamma = \cup_i \gamma_i} \gamma \otimes \Gamma/\gamma, \tag{9}$$

$$\hat{\mathbb{I}} : H \to \mathbb{Q}, q\mathbb{I} \to q, H_> \to 0, \tag{10}$$

$$S : H \to H, S(\Gamma) = -\Gamma - \sum_{\gamma \subsetneq \Gamma, \gamma = \cup_i \gamma_i, w(\gamma_i) \geq 0} S(\gamma)\Gamma/\gamma, \tag{11}$$

$$S_{\text{core}} : H \to H, S(\Gamma) = -\Gamma - \sum_{\gamma \subsetneq \Gamma, \gamma = \cup_i \gamma_i} S_{\text{core}}(\gamma)\Gamma/\gamma, \tag{12}$$

where $H_> = \oplus_{i \geq 1} H^{(i)}$ is the augmentation ideal.

Both Hopf algebras will be needed in the following for renormalization in the presence of variations.

They both have a co-radical filtration, which for the renormalization Hopf algebra delivers the renormalization group, and for the core Hopf algebra the flags of all decompositions of a graph into iterated integrals of one-loop graphs. We often use Sweedler's notation: $\Delta\Gamma = \Gamma' \otimes \Gamma''$.

6.2 *Hopf Algebras and the Cubical Chain Complex of Graphs*

Let us return to graphs with spanning forests. For a spanning tree of length j, there are $j!$ orderings of it edges. To such a spanning tree, we assign a j-dimensional cube and to each of the $j!$ ordering of its edges a matrix as follows. We follow [6].

Let (Γ, T) be a pair of a graph and a spanning tree for it with a choice of ordering for its edges. Let $\mathscr{F}_{(\Gamma,T)}$ be the set of corresponding forests obtained by removing edges from T in order.

Then, to any pair (Γ, F), with F a k-forest $(1 \leq k \leq v_\Gamma)$, $F \in \mathscr{F}_{(\Gamma,T)}$ we can assign a set of k disjoint graphs Γ^F. We let $\Gamma_F := \Gamma/\Gamma^F$ be the graph obtained by shrinking all internal edges of these graphs.

For each such F, we call E_{Γ_F} a cut. In particular, for F the unique 2-forest assigned to T (by removing the first edge from the ordered edges of T), we call $\varepsilon_2 = E_{\Gamma_F}$ the normal cut of (Γ, T).

Note that the ordering of edges defines an ordering of cuts $\emptyset = \varepsilon_1 \subsetneq \varepsilon_2 \subsetneq \cdots \subsetneq \varepsilon_k = E_\Gamma$.

For a normal cut, we have $\Gamma^F = (\Gamma_1, \Gamma_2)$ and we call

$$s = \left(\sum_{v \in V_{\Gamma_1}} q_v\right)^2 = \left(\sum_{v \in V_{\Gamma_2}} q_v\right)^2 \tag{13}$$

the channel associated to (Γ, T).

These notions are recursive in an obvious way: the difference between a k and a $k+1$ forest defines a normal cut for some subgraph.

We then get a lower triangular matrix with entries from pairs (Γ, F) by shrinking edges of the spanning tree from bottom to top in order, and removing edges from the spanning tree from left to right in reverse order.

To set up Feynman rules for pairs (Γ, F) we need an important lemma.

We define $|\Gamma^F| = \sum_{\gamma \in \Gamma^F} |\gamma|$. Also, we let $\mathscr{F}_k(\Gamma)$ be the set of all k-forests for a graph Γ.

For a disjoint union of r graphs $\gamma = \cup_{i=1}^r \gamma_i$, we say a disjoint union of trees $T = \cup_i t_i$ spans γ and write $T|\gamma$, if t_i is a spanning tree for γ_i.

We have then an obvious decomposition of all possible spanning forests using the coproduct Δ_{core}. A spanning forest decomposes into a spanning forest which leaves no loop intact in the cograph together with spanning trees for the subgraph [17, 18]:

Lemma 1

$$\sum_{T|\Gamma'} \left(\Gamma, T \cup \sum_{k=2}^{v_\Gamma} \sum_{F \in \mathscr{F}_k(\Gamma''), |\Gamma_F|=0} F\right) = \sum_{k=2}^{v_\Gamma} \sum_{F \in \mathscr{F}_k(\Gamma)} (\Gamma, F). \tag{14}$$

Remark 1 On the right, we have a sum over all $(k \geq 2)$-forests, and therefore a sum over all possible Cutkosky cuts. On the left, we have the same using that the set of all sub-graphs Γ' which have loops left intact appear on the lhs of the core Hopf algebra co-product, with intact spanning trees T, whilst Γ'' has no loops left intact, $|\Gamma_F| = 0$.

Remark 2 The lemma ensures that uncut subgraphs which have loops can have their loops integrated out. The resulting integrals are part of the integrand of the full graph and its variations determined by the cut edges. Understanding the variations for cuts which leave no loop intecat suffices to understand the variations in the general case.

We set

$$\sum_{k=1}^{v_\Gamma} \sum_{F \in \mathscr{F}_k(\Gamma)} (\Gamma, F) =: \text{Disc}(\Gamma),$$

for the sum of all cuts at a graph.

6.3 *Graph Polynomials and Feynman Rules*

We turn to Feynman rules, therefore from graphs and their combinatorial properties to the analytic structure of the amplitudes associated to graphs.

6.3.1 Renormalized Feynman Rules

For graphs of a renormalizable field theory, we get renormalized Feynman rules for an overall logarithmically divergent graph Γ ($w(\Gamma) = 0$) with logarithmically divergent subgraphs as

$$\Phi_R = \int_{\mathbb{P}_\Gamma} \sum_{F \in \mathscr{F}_\Gamma} (-1)^{|F|} \frac{\ln \frac{\Phi_{\Gamma/F}\psi_F + \Phi^0_F \psi_{\Gamma/F}}{\Phi^0_{\Gamma/F}\psi_F + \Phi^0_F \psi_{\Gamma/F}}}{\psi^2_{\Gamma/F}\psi^2_F} \Omega_\Gamma. \tag{15}$$

Formula for other degrees of divergence for sub- and cographs can be found in [11]. In particular, also overall convergent graphs are covered. It is important that we use a kinematic renormalization scheme such that tadpole integrals vanish [11, 19].

The Hopf algebra in use in the above is based on the renormalization coproduct Δ.

The antipode $S(\Gamma)$ in this Hopf algebra can be written as a forest sum:

$$S(\Gamma) = -\Gamma - \sum_{F \in \mathscr{F}_\Gamma} (-1)^{|F|} F \times (\Gamma/F). \tag{16}$$

6.3.2 Renormalized Feynman Rulesfor Pairs (Γ, F)

We now give the Feynman rules for a graph with some of its internal edges cut. This can be regarded as giving Feynman rules for a pair (Γ, F).

$$\Upsilon^F_\Gamma := \int \left(\Phi_R(\Gamma') \prod_{e \in (\Gamma'' - E_{\Gamma_F})} \frac{1}{P(e)} \prod_{e \in E_{\Gamma_F}} \delta^+(P(e)) \right) d^{4|\Gamma/\Gamma'|}k. \tag{17}$$

We use Sweedler's notation for the copoduct provided by Δ_{core}.

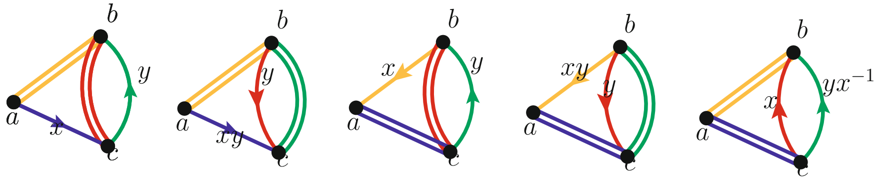
Note that in this formula $\Phi_R(\Gamma')$ has to stay in the integrand. The internal loops of Γ' have been integrated out by Φ_R, but $\Phi_R(\Gamma')$ is still an obvious function of loop momenta apparent in Γ/Γ'. The existence of this factorization into integrated subgraphs times cut cographs is a consequence of Lemma 1.

7 Graph Amplitudes and Fubini's Theorem

This section just mentions an important point often only implicitly assumed. For a k-loop graph Γ, acting with Δ^{k-1} gives a sum over k-fold tensorproducts of one-loop graphs, each of which corresponding to a possibility to write $\Phi_R(\Gamma)$ as an iterated integral of one-loop amplitudes.

Below, we study the 3-edge banana as an explicit example. Each of these possibilities evaluate to the same physical amplitude $\Phi_R(\Gamma)$ uniquely defined on the principal sheet. We need Fubini's theorem for that, and the existence of the operator product expansion (OPE).

Consider the Dunce's cap.



Its five spanning trees give five choices for a basis for its two loops. The loop to be integrated out first is a function of the next loop's loop momentum.

If we integrate out first the loop based on three edges, say $l_x : e_b, e_r, e_y$ (a triangle), this is a finite integral which does not need renormalization. The second loop is $l_y : e_r, e_g$ and carries the overall divergence after integrating l_x.

Still, the counterterm for the subloop based on the two edges e_r, e_g is needed. Indeed, it corresponds to a limit where vertices b, c collapse, a limit in which the Hopf algebra of renormalization needs to provide the expected counterterm, even if the iterated integral $l_y \circ l_x$ has no divergent subintegral.

We need the operator product expansion to work precisely in the way it does to have the freedom to use Fubini to come to uniquely defined renormalized amplitudes.

8 Cutkosky's Theorem

In [6], Cutkosky's theorem for a graph G is proven in a particular straightforward way for cuts which leave no loop intact, so $|G^F| = 0$. We quote

Theorem 1 (Cutkosky) *Assume G_F has a non-degenerate physical singularity at an external momentum point $p'' \in Q_{G_F}$. Let $p \in Q_G$ be an external momentum point for G lying over p''. Then the variation of the amplitude $I(G)$ around p is given by Cutkosky's formula*

$$var(I(G)) = (-2\pi i)^{\#E_{G_F}} \int \frac{\prod_{e\in E_G\setminus E_{G_F}} \delta^+(\ell_e)}{\prod_{e\in E_{G_F}} \ell_e}. \tag{18}$$

For the set-up of Cutkosky's theorem in general, we can proceed using Lemma 1:

- either a renormalized subgraph is smooth at the threshold divisors of the co-graph: then we can apply Cutkosky's theorem on the nose, and get a variation which is parametrized by the renormalization conditions for these subgraphs with loops;
- or it is not smooth. Then, necessarily, its disconitinuity is described by a cut on this subgraph, and hence it has no loops, adding its cut to the cut for the total.

9 Galois Co-actions and Symbols

In the above, we allow $|E_{\Gamma_F}|$ internal edges $e \in E_{\Gamma_F}$ to be on-shell. Other authors [16] also allow to put internal edges on shell such that they do not separate the graph. This gives no physical variation as one easily proves [6]. If one allows for variations of masses as well, in particular in the context of non-kinematical renormalization schemes, then such more general cuts can be meaningful though. Here, we restrict to variations coming from varying external momenta for amplitudes renormalized with kinematic renormalization schemes.

It is of interest to study a coaction. It is often simply written as a Hopf algebra [16, 20] and then for general cuts the coproduct Δ_{co} has the incidence form

$$\Delta_{\mathrm{co}}(\Gamma, E) = \sum_{F \subseteq (E_\Gamma \setminus E)} (\Gamma/(E_\Gamma \setminus (E \cup F)), E) \otimes (\Gamma, E \cup F),$$

where E is a set of edges, and F a subset of the complement $E_\Gamma \setminus E$. A pair (Γ, E) is to be regarded as a graph with the set of edges E put on-shell.

Restricting on-shell edges to originate from cuts E_{Γ_F} allows to read off Δ_{co} from our lower triangular Hodge matrices in an obvious way, as in the example for the triangle above (Eq. (5)).

This co-product fulfills

$$\Delta_{\mathrm{co}} \circ \mathrm{Disc} = (\mathrm{Disc} \otimes \mathrm{id}) \circ \Delta_{\mathrm{co}},$$

and

$$\Delta_{\mathrm{co}} \circ /e = (\mathrm{id} \otimes /e) \circ \Delta_{\mathrm{co}},$$

where Disc as before is the map which sends a Feynman graph to a sum over all cut graphs obtained from all spanning k-forests of the graph, $k \geq 2$. Furthermore, $/e$ is the map which sums over all ways of shrinking an (uncut) edge.

We can make this into a proper coaction (see [20, 21] for an overview of coactions in the context of Feynman amplitudes)

$$\rho : V \to V \otimes H, (\rho \otimes \mathrm{id}) \circ \rho = (\mathrm{id} \otimes \Delta) \circ \rho.$$

Here, it suggests itself to take for V the vector space of uncut Feynman graphs, and for H the Hopf algebra of cut graphs with a coproduct as above.

For one-loop graphs, these graphical coactions are in accordance with the structure of the dilogarithms into which these graphs evaluate as was observed by Abreu et.al., see [16].

The Hodge matrices resulting from the cubical chain complex can be constructed for every graph, and from it the corresponding coaction can be constructed. On the analytic side, the hope is that this confirms the set-up suggested by Brown [21].

For cuts, these coactions in accordance with the cubical chain complex.

Iterating this coaction in accordance with the co-radical filtration of the Hopf algebra suggests then to define symbols graphically, a theme to be pursued further.

10 3-Edge Banana

In the process of the blow-up of missing cells in Outer Space a graph polytope is generated [4]. Such polytopes combine to jewels. One can use the blow-up to store the complete sheet structure of the amplitude.

As an example we consider the construction of colored jewel J_2, generated by the 3-edge banana graph.

10.1 Existence of the Banana Monodromy

Let us first collect an elementary result.

Lemma 2 *The integral for the cut n-edge banana*

$$\int_{\mathbb{M}^{D(n-1)}} d^{D(n-1)}k \prod_{i=1}^{n} \delta_+(k_i) \equiv \mathrm{Var}(\Phi_R(b_n))$$

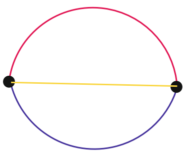
exists for any positive integer D.

Proof We have $n-1$ loop momenta $k_1, \ldots, k_{n-1}$, and the measure is $d^{D(n-1)}x = d^Dk_1 \cdots d^Dk_{n-1}$. The δ_+-distributions give n constraints. The $n-1$ integrations over the 0-components of the loop momenta can be constrained by $n-1$ of the δ_+ distributions. The remaining spacelike integrals are over an Euclidean space $\mathbb{R}^{(D-1)(n-1)}$ and can be done in spherical coordinates. The angle integrations are over a compact sphere, and the one remaining δ_+-distribution fixes the radial integration.

The argument obviously generalizes to graphs with $n-1$-loops in which n cuts cut all the loops.

10.2 b_3: Three Edges

We now consider the 3-edge banana b_3 on three different masses.



As we will see, the resulting function $\Phi_R(b_3)$ has a structure very similar to the dilogarithm function $\mathrm{Li}_2(z)$. As a multi-valued function, we can write the latter as

$$\mathrm{Li}_2^{\mathrm{mv}}(z) = \mathrm{Li}_2(z) + 2\pi\imath\mathbb{Z}\ln z + (2\pi\imath)^2\mathbb{Z}\times\mathbb{Z},$$

or more explicitly

$$\mathrm{Li}_2^{\mathrm{mv}}(z)(n_1, n_2) = \mathrm{Li}_2(z) + 2\pi\imath n_1 \ln z + (2\pi\imath)^2 n_1 n_2.$$

The variable n_1 stores the sheet for the evaluation of the sub-integral $\mathrm{Li}_1(x)$ apparent in the iterated integral representation

$$\mathrm{Li}_2(z) = \int_0^z \frac{\mathrm{Li}_1(x)}{x} dx.$$

The sheet for the evaluation of $\ln z$ is stored by n_2 and only contributes for $n_1 \neq 0$.

Very similarly we will establish the structure of the multi-valued functions assigned to b_3 as iterated integrals, with $\Phi_R(b_2)^{\mathrm{mv}}(k^2, m_i^2, m_j^2)$ apparent as a one-loop sub-integral in the two-loop integration assigned to b_3 and playing the role of $\mathrm{Li}_1(x)$.

We will find multi-valued functions

$$\mathrm{I}_k^{ij}(n_1, n_2)(s) = \Phi_R(b_3)(s) + 2\pi\imath n_1 \int \frac{\mathrm{Var}(\Phi_R(b_2))(k^2; m_i^2, m_j^2)}{(k+q)^2 - m_k^2} d^4k \quad (19)$$
$$+ (2\pi\imath)^2 \frac{|m_k^2 - s||m_i^2 - m_j^2|}{2s} n_1 n_2.$$

Here, i, j, k take values in the index set $\{b, y, r\}$ labelling the three different masses, and we regard the three functions

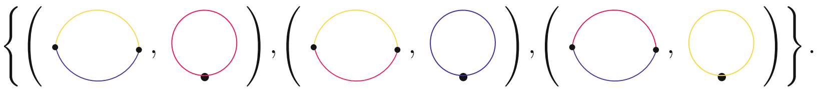
$$\mathrm{I}_r^{by}(n_1, n_2)(s) \sim \mathrm{I}_b^{yr}(n_1, n_2)(s) \sim \mathrm{I}_y^{rb}(n_1, n_2)(s)$$

as equivalent, with equivalence established by equality along the principal sheet.

Let us come back to b_3. Here, the fundamental group has two generators, the interesting question is how to compare this with the generators of monodromy for $\Phi_R(b_3)$ and how this defines corresponding multi-valued functions as above.

We start by using the fact that we can disassemble b_3 in three different ways into a b_2 sub-graph, with a remaining edge providing the co-graph.

Any two of the three edges of the graph b_3 can be regarded as a subgraph $b_2 \subsetneq b_3$. This is in accordance with the flag structure of b_3 generated from an application of Δ_{core}, which gives a set of three flags (see [7]):



Let us compute

$$\operatorname{Var}(\Phi_R(b_3)(s, m_r^2, m_b^2, m_y^2)) = \int d^4k d^4l \delta_+(k^2 - m_b^2)\delta_+(l^2 - m_r^2)\delta_+((k - l + q)^2 - m_y^2),$$

an integral which exists by the above Lemma.

Using Fubini, this can be written in three different ways in accordance with the flag structure:

$$\operatorname{Var}(\Phi_R(b_3)) = \int d^4k \operatorname{Var}(\Phi_R(b_2))(k^2, m_r^2, m_b^2)\delta_+((k + q)^2 - m_y^2),$$

or

$$\operatorname{Var}(\Phi_R(b_3)) = \int d^4k \operatorname{Var}(\Phi_R(b_2))(k^2, m_b^2, m_y^2)\delta_+((k + q)^2 - m_r^2),$$

or

$$\operatorname{Var}(\Phi_R(b_3)) = \int d^4k \operatorname{Var}(\Phi_R(b_2))(k^2, m_y^2, m_r^2)\delta_+((k + q)^2 - m_b^2).$$

The integrals are well-defined by the above Lemma and give the variation and hence imaginary part of $\Phi_R(b_3)$, which can be obtained from it by a twice subtracted dispersion integral (the renormalized function and its first derivative must vanish as $s = s_0$)

$$\Phi_R(b_3)(s, s_0) = \frac{(s - s_0)^2}{\pi} \int_0^\infty \frac{\operatorname{Var}(\Phi_R(b_3)(x))}{(x - s)(x - s_0)^2} dx.$$

Computing $\Phi_R(b_3)$ directly from $\Phi_R(b_2)$ as an iterated integral can be done accordingly in three different ways:

$$\Phi_R(b_3)(s, s_0; m_r^2, m_b^2, m_y^2) =$$
$$= \int d^4k \frac{B_2(k^2, m_r^2, m_b^2)}{(k + q)^2 - m_y^2} = \int d^4k \frac{B_2(k^2, m_b^2, m_y^2)}{(k + q)^2 - m_r^2} = \int d^4k \frac{B_2(k^2, m_y^2, m_r^2)}{(k + q)^2 - m_b^2},$$

with subtractions at $s = s_0$ understood.

There is a subtlety here: this is only correct in a kinematic renormalization scheme where subtractions are done by a Taylor expansion of the integrand around $s = s_0$ [11, 19].

This implies that the co-graphs in the flag structure of b_3 fulfil

$\Phi_R\Big($  $\Big) = \Phi_R\Big($ $\Big) = \Phi_R\Big($  $\Big) = 0,$

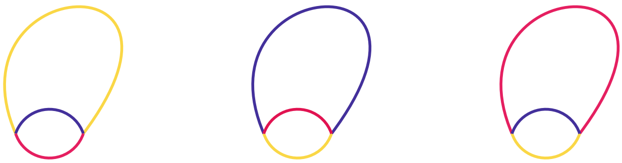
as tadpoles are independent of the kinematic variable s. Hence b_3 can be regarded as a primitive element under renormalization.

To study the sheet structure for b_3 we now define three different multi-valued functions as promised above

$$I_k^{ij} = I_k^{ji} = \int \frac{\Phi_R^{\mathrm{mv}}(b_2)(k^2, m_i^2, m_j^2)}{(k+q)^2 - m_k^2 + i\eta} d^4k,$$

with subtractions at $s = s_0$ understood as always such that the integrals exist.

For later use in the context of Outer Space we represent them as



I_y^{br} I_b^{yr} I_r^{by}

It is convenient to rewrite them as,

$$I_k^{ij} = \int \frac{\Phi_R(b_2)(k^2, m_i^2, m_j^2)}{(k+q)^2 - m_k^2 + i\eta} d^4k + 2\pi\imath\mathbb{Z}\sum_{u=1}^{3} J_k^{ij;u},$$

with

$$J_k^{ij;u} = \int d^4k \frac{J_u^{ij}(k^2)}{(k+q)^2 - m_k^2 + i\eta},$$

see Eqs. (1)–(3).

Note that by the above,

$$\Phi_R(b_3) = \int \frac{\Phi_R(b_2)(k^2, m_i^2, m_j^2)}{(k+q)^2 - m_k^2 + i\eta} d^4k,$$

is well-defined no matter which of the two edges we choose as the sub-graph, and Cutkosky's theorem defines a unique function $V_{rby}(s)$,

$$\Im(\Phi_R(b_3)(s)) = V_{rby}(s)\Theta(s - (m_r + m_b + m_y)^2).$$

Before we start computations, we note that we expect that the integrals for $J_k^{ij;2}$, $J_k^{ij;3}$ have no monodromy as there are no endpoint singularities as the integrand vanishes at the endpoints of the domain of integration, and there are no pinch singularities by inspection.

But for $J_k^{ij;1}$ we expect monodromy: The denominator of V_{ij} is k^2. So we get monodromy from the intersection of the zero locus $k^2 = 0$ (which now lies in the domain of integration as k^2 is only bounded from the above by $(m_i - m_j)^2$) and the zero locus $(k+q)^2 - m_k^2 = 0$.

10.3 Computation

We now give computational details for the 3-edge banana graph.[4] We start by computing $\Im(\Phi_R(b_3)(s)) = V_{rby}(s)\Theta(s - (m_r + m_b + m_y)^2)$, or equivalently $\Im(J_k^{ij;3})(s)$. Consider

$$\int d^4k \frac{\Theta(k^2 - (m_i + m_j)^2)}{2k^2} \delta_+((k+q)^2) - m_k^2).$$

The δ_+ distribution demands that $k_0 + q_0 > 0$, and therefore we get

$$\int_{-q_0}^{\infty} dk_0 \int_0^{\infty} dt \sqrt{t} \frac{\Theta(k_0^2 - t - (m_i + m_j)^2)\sqrt{\lambda(k_0^2 - t, m_i^2, m_j^2)}}{2(k_0^2 - t)} \delta((k_0 + q_o)^2 - t - m_k^2).$$

As a function of k_0, the argument of the δ-distribution has two zeroes: $k_0 = -q_0 \pm \sqrt{t + m_k^2}$.

As $k_0 + q_0 > 0$, it follows $k_0 = -q_0 + \sqrt{t + m_k^2}$. Therefore, $k_0^2 - t = q_0^2 + m_k^2 - 2q_0\sqrt{t + m_k^2}$.

For our desired integral, we get

$$\int_0^{\infty} dt \sqrt{t} \Theta(q_0^2 + m_k^2 - 2q_0\sqrt{t + m_k^2} - (m_i + m_j)^2) \times$$

$$\times \frac{\sqrt{\lambda(q_0^2 + m_k^2 - 2q_0\sqrt{t + m_k^2}, m_i^2, m_j^2)}}{2(q_0^2 + m_k^2 - 2q_0\sqrt{t + m_k^2})\sqrt{t + m_k^2}}.$$

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[4]Further computational results can be found in [22, 23].

The Θ-distribution requires

$$q_0^2 + m_k^2 - (m_i + m_j)^2 \geq 2q_0\sqrt{t + m_k^2}.$$

Solving for t, we get

$$t \leq \frac{\lambda(s, m_k^2, (m_i + m_j)^2)}{4s}$$

As $t \geq 0$, we must have for the physical threshold $s > (m_k + m_i + m_j)^2$ (which is indeed completely symmetric under permutations of i, j, k, in accordance for what we expect for $\Im(\Phi_R(b_3)(s))$). We then have

$$\Im(J_k^{ij;3})(s) = \int_0^{\frac{\lambda(s,m_k^2,(m_i+m_j)^2)}{4s}} \frac{\sqrt{\lambda(s + m_k^2 - 2\sqrt{s}\sqrt{t + m_k^2}, m_i^2, m_j^2)}}{2(s + m_k^2 - 2\sqrt{s}\sqrt{t + m_k^2})\sqrt{t + m_k^2}}\sqrt{t}dt.$$

There is also a pseudo-threshold at $s < (m_k - m_i - m_j)^2$.

Note that the integrand vanishes at the upper boundary $\frac{\lambda(s,m_k^2,(m_i+m_j)^2)}{4s}$, and the integral has a pole at $s = 0$ (see below) as for $s = 0$ the integral would not converge. The integrand is positive definite in the interior of the integration domain and free of singularities.

The computation of $\Im(J_k^{ij;2})(s)$ proceeds similarly and gives

$$\Im(J_k^{ij;2})(s) = \int_{\frac{\lambda(s,m_k^2,(m_i+m_j)^2)}{4s}}^{\frac{\lambda(s,m_k^2,(m_i-m_j)^2)}{4s}} \frac{\sqrt{\lambda(s + m_k^2 - 2\sqrt{s}\sqrt{t + m_k^2}, m_i^2, m_j^2)}}{2(s + m_k^2 - 2\sqrt{s}\sqrt{t + m_k^2})\sqrt{t + m_k^2}}\sqrt{t}dt.$$

The integrand vanishes at the upper and lower boundaries. The integrand is positive definite in the interior of the integration domain and free of singularities.

Most interesting is the computation of $\Im(J_k^{ij;1})(s)$. It gives

$$\Im(J_k^{ij;1})(s) = \int_{\frac{\lambda(s,m_k^2,(m_i-m_j)^2)}{4s}}^{\infty} \frac{\sqrt{\lambda(s + m_k^2 - 2\sqrt{s}\sqrt{t + m_k^2}, m_i^2, m_j^2)}}{2(s + m_k^2 - 2\sqrt{s}\sqrt{t + m_k^2})\sqrt{t + m_k^2}}\sqrt{t}dt.$$

The integrand vanishes at the lower boundary $\frac{\lambda(s,m_k^2,(m_i-m_j)^2)}{4s}$, and the integral again has a pole at $s = 0$. But now the integrand has a pole as $q_0^2 + m_k^2 - 2q_0\sqrt{t + m_k^2}$ is only constrained to $\leq (m_i - m_j)^2$, and hence can vanish in the domain of integration.

This gives us a new variation apparent in the integration of the loop in the co-graph

$$\mathrm{Var}(J_k^{ij;1})(s) = \int \sqrt{\lambda(k^2, m_i^2, m_j^2)}\delta(k^2)\delta_+((k+q)^2 - m_k^2)d^4k,$$

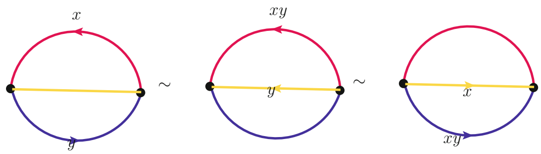
which evaluates to

$$\mathrm{Var}(J_k^{ij;1})(s) = \overbrace{|m_i^2 - m_j^2|}^{\sqrt{\lambda(0,m_i^2,m_j^2)}} \overbrace{\frac{|s-m_k^2|}{2s}}^{\sqrt{\lambda(s,m_k^2,0)}} \Theta(s - m_k^2)\,.$$

Adding the contributions, we confirm our expectations Eq. (19).

11 Markings and Monodromy

Consider the equivalence relation for b_3 in Outer Space.



The three possible choices for a spanning tree of b_3 result in three different but equivalent markings of b_3 regarded as a marked metric graph in (colored) Outer Space.[5] Each different choice corresponds to a different choice of basis for $H^1(b_3)$. The markings given in this picture determine all markings in subsequent picture, where they are omitted.

The choice of a spanning tree together with an ordering of the roses then determines uniquely a single element in the set of ordered flags of subgraphs, and hence determines one iterated Feynman integral describing the amplitude in question.

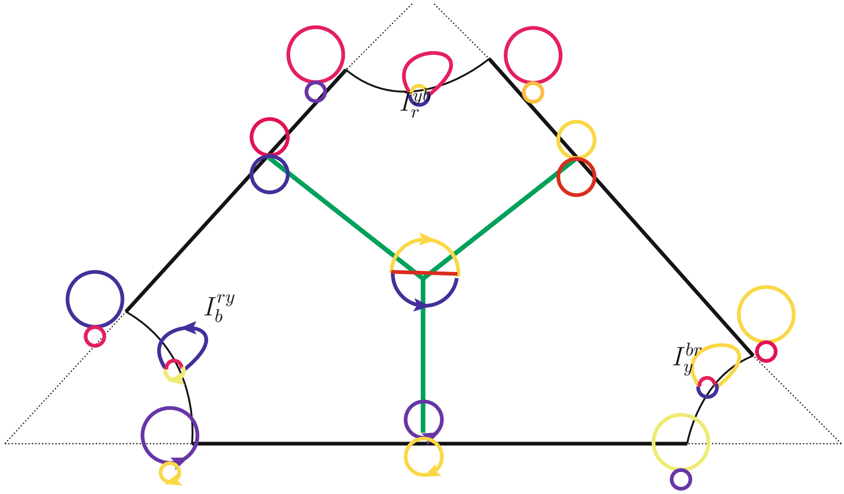
For their evaluation along principal sheets equality of these integrals follows by Fubini, which gives equality along the principal sheet and implies an equivalence relation for evaluation along the non-principal sheets.

On the level of amplitudes, a basis for the fundamental group of the graph, provided by a marking, translates to a basis for the fundamental group for the complement of the threshold divisors of the graph.

Concretely, for the amplitude generated by b_2, this is trivial: we have a single generator for the one loop, and this maps to a generator for the monodromy of the corresponding amplitude.

[5]For the notion of equivalence in Outer Space refer to [2].

For b_3, we get two generators. A choice as which two edges form the subgraph b_2 then determines the iterated integral. The equivalence of markings in Outer Space becomes the Fubini theorem of iterated integrals for the evaluation along principal sheets, and the corresponding equivalence off principal sheets else.



Let us have a closer look at this corresponding cell in Outer Space. In the barycenter of the triangle we indicate the graph b_3. The green lines form the spine, connecting the graph at the barycenter to the barycenters of the codimension-one edges of the triangle, which are cells marked by the indicated colored 2-petal roses.

The corners of the triangle are not part of Outer Space, as we are not allowed to shrink loops. In fact, they are blown up to arcs, which are cells populated by graphs for which the choice is obvious as to which two edges are the subgraphs - the corners are the intersections of two edge variables becoming small as compared to the third. The three different iterated integrals are hence assigned to those arcs in a natural manner.

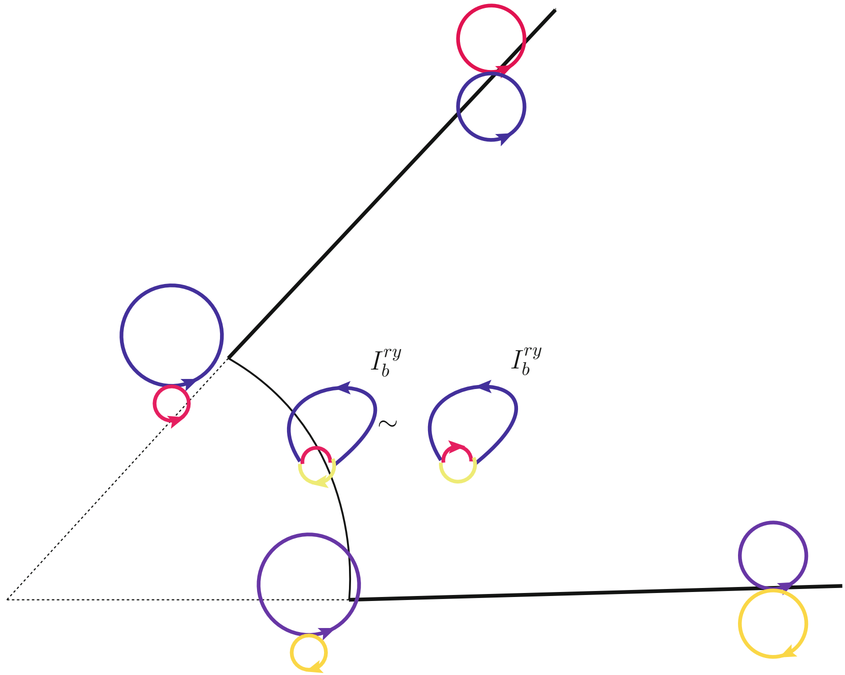
For example for the lower left corner, the edge variable A_b is much greater than the edge variables A_r, A_y. Along the arc, an equivalence relation operates as well, as the loop formed by edges e_r, e_y can have either of the two edges as its spanning tree. The endpoints of these arcs form the vertices of the cell, which is a hexagon. To those vertices we assign roses as indicated, with one small and one big petal, which indicates an order on the petals.

Note that moving along an arc can be regarded as movement in a fibre given by the chosen subgraph b_2, while moving the arc away or toward the barycenter of the triangle is movement in the base.

Moving from one corner to another utilizes a non-trivial equivalence of our iterated integrals.

We indicate the markings only for some of the graphs, and only for the choice of the red edge as the spanning tree.

Let us have a still closer look at the corners:



The equivalence relation is an equivalence relation for the two marked metric graphs, which is indeed coming from an equivalence relation for the two choices of a spanning tree for the 2-edge subgraph on the red and yellow edges, while the corresponding analytic expression is equal for both choices: I_b^{ry}.

Moving to a different corner by shrinking the size of the blue edge and increasing say the size of the red edge moves to a different corner while leaving the marking equal. This time we have an equivalence relation between the analytic expressions:

$$I_b^{ry} \sim I_r^{by}.$$

Moving along an arc uses equivalence based on homotopy of the graph, moving along an edge leaves the marking equal, but uses equivalence of analytic expressions $I^{\gamma}_{\Gamma/\gamma}$, here $I_b^{ry} \sim I_r^{by}$.[6]

The complete sheet structure including non-principal sheets is always rather subtle and is reflected by a jewelled space J_2 as we discuss now.

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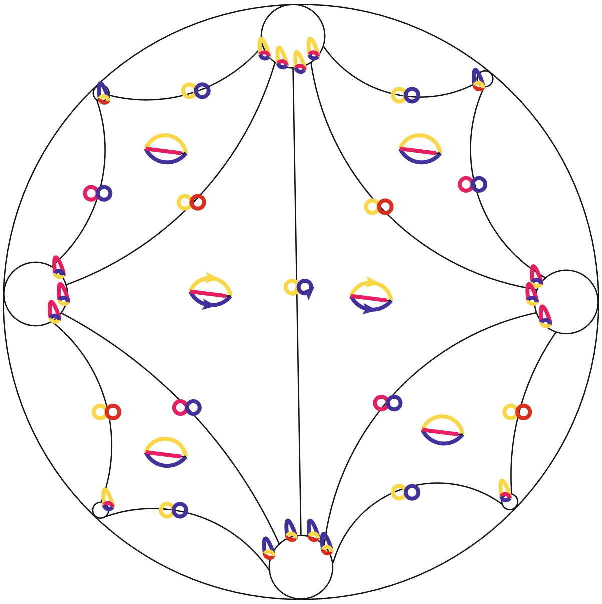
[6]In this example the cograph was always a single-edge tadpole whose spanning tree is a single vertex and therefore the equivalence relation from the 1-petal rose R_1 to the co-graph is in fact the identity. In general, the decomposition of a graph into a subgraph γ and cograph Γ/γ corresponds to a factorization into equivalence classes for the subgraph and equivalence classes for the cograph familiar from [5].

A crucial aspect of Outer Space is that cells combine to spaces, and that these spaces provide information, for example on the representation theory of the free group in the case of traditional Outer Space, and on the sheet structure of amplitudes in our case. In particular, the bordification of Outer Space as studied by [4], motivates to glue the cell studied above to a 'jewel':



The Euclidean simplices are put in a Poincaré disk as hyperbolic triangles. We only give markings for a few graphs in the center. To not clutter the figure, we have not given the graphs for the vertices in this figure which are all marked ordered roses as indicated above, by a result of [4].

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Interpolated Sequences and Critical L-Values of Modular Forms

Robert Osburn and Armin Straub

Abstract Recently, Zagier expressed an interpolated version of the Apéry numbers for $\zeta(3)$ in terms of a critical L-value of a modular form of weight 4. We extend this evaluation in two directions. We first prove that interpolations of Zagier's six sporadic sequences are essentially critical L-values of modular forms of weight 3. We then establish an infinite family of evaluations between interpolations of leading coefficients of Brown's cellular integrals and critical L-values of modular forms of odd weight.

1 Introduction

For $x \in \mathbb{C}$, consider the absolutely convergent series

$$A(x) = \sum_{k=0}^{\infty} \binom{x}{k}^2 \binom{x+k}{k}^2. \tag{1}$$

If $x = n \in \mathbb{Z}_{\geq 0}$, this series terminates at $k = n$ and agrees with the well-known Apéry numbers $A(n)$ for $\zeta(3)$ [5, 35]. Let

$$f(\tau) = \sum_{n \geq 1} a_n q^n \in S_k(\Gamma_1(N)), \quad q = e^{2\pi i \tau},$$

be a cusp form of weight k and level N, and

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$$L(f,s) := \sum_{n\geq 1} \frac{a_n}{n^s}$$

be the L-function for f defined for Re s large. Following Deligne, we say that $L(f, j)$ is a *critical L-value* if $j \in \{1, 2, \ldots, k-1\}$. For a beautiful exposition concerning the importance of these numbers, see [22]. Zagier [40, (44)] recently showed that the interpolated Apéry numbers (1) are related to the critical L-value of a modular form of weight 4. Specifically, he proved the following intriguing identity:

$$A(-\tfrac{1}{2}) = \frac{16}{\pi^2} L(f,2), \tag{2}$$

where

$$f(\tau) = \eta(2\tau)^4 \eta(4\tau)^4 = \sum_{n\geq 1} \alpha_n q^n \tag{3}$$

is the unique normalized Hecke eigenform in $S_4(\Gamma_0(8))$ and $\eta(\tau)$ is the Dedekind eta function. We note that, expressing the left-hand side as a hypergeometric series, the identity (2) was previously established by Rogers, Wan and Zucker [29]. The evaluation (2) can be seen as a continuous counterpart to the congruence

$$A(\tfrac{p-1}{2}) \equiv \alpha_p \pmod{p}, \tag{4}$$

which holds for primes $p > 2$ and was established by Beukers [9], who further conjectured that the congruence (4) actually holds modulo p^2. This supercongruence was later proven by Ahlgren and Ono [2] using Gaussian hypergeometric series.

Zagier indicates that Golyshev predicted an evaluation of the form (2) based on motivic considerations and the connection of the Apéry numbers with the double covering of a related family of K3 surfaces. Here, we do not touch on these geometric considerations (see [40, Section 7] for further details), but only note that Golyshev's prediction further relies on the Tate conjecture, which remains open in the required generality. Identity (2), and similar ones to be explored in this paper, might therefore serve as evidence supporting the motivic philosophy and the Tate conjecture.

The goal of this paper is to extend Zagier's evaluation (2) in two directions. Firstly, in Sect. 2, we consider the six sporadic sequences that Zagier [39] obtained as integral solutions to Apéry-like second order recurrences. Based on numerical experiments, we observe that each of these sequences $C_*(n)$ appears to satisfy congruences like (4) connecting them with the Fourier coefficients of a modular form $f_*(\tau)$ of weight 3. For three of these sequences these congruences were shown by Stienstra and Beukers [34], while the other three congruences do not appear to have been recorded before. We prove two of these new cases, one using a general result of Verrill [36] and the other via p-adic analysis and comparison with another case. Our main objective is to show that in each case there is a version of Zagier's evaluation (2). For $x \in \mathbb{C}$, there is a natural interpolation $C_*(x)$ of each sequence and the value $C_*(-1/2)$ can in five of the six cases be expressed as $\frac{\alpha}{\pi^2} L(f_*, 2)$ for $\alpha \in \{6, 8, 12, 16\}$. In the remaining case, $C_*(x)$ has a pole at $x = -1/2$. Remarkably, the residue of that pole equals $\frac{6}{\pi^2}L(f_*, 1)$.

Secondly, Brown [13] recently introduced cellular integrals generalizing the linear forms used in Apéry's proof of the irrationality of $\zeta(3)$ as well as many other constructions related to the irrationality of zeta values. These are linear forms in multiple zeta values and their leading coefficients $A_\sigma(n)$ are generalizations of the Apéry numbers. McCarthy and the authors [27] proved that, for a certain infinite family of these cellular integrals, the leading coefficients $A_\sigma(n)$ satisfy congruences like (4) with Fourier coefficients of modular forms $f_k(\tau)$ of odd weight $k \geq 3$. In Sect. 3, we review these facts and prove an analogue of Zagier's evaluation (2) for all of these sequences. Finally, in Sect. 4, we conclude with several directions for future study.

2 Zagier's Sporadic Sequences

2.1 The Congruences and L-Value Relations

In addition to $A(n)$, Apéry [5] introduced a second sequence which allowed him to reprove the irrationality of $\zeta(2)$. This sequence is the solution of the three-term recursion, for $(a, b, c) = (11, 3, -1)$,

$$(n+1)^2 u_{n+1} = (an^2 + an + b)u_n - cn^2 u_{n-1}, \tag{5}$$

with initial conditions $u_{-1} = 0$, $u_0 = 1$. Inspired by Beukers [10], Zagier [39] conducted a systematic search for parameters (a, b, c) which similarly result in integer solutions to the recurrence (5). After normalizing, and apart from degenerate cases, he discovered four hypergeometric, four Legendrian and six sporadic solutions. It remains an open question whether this list is complete. The six sporadic solutions are listed in Table 1. As in [39], we use the labels $\boldsymbol{A}$–$\boldsymbol{F}$ and index the sequences accordingly.

For each of these sequences, a binomial sum representation is known. For instance, if $(a, b, c) = (11, 3, -1)$, then

$$C_{\boldsymbol{D}}(n) = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}. \tag{6}$$

Following Zagier's approach for (1), we obtain an interpolation of a sporadic sequence by replacing the integer n in the binomial representation with a complex number x and extending the sum to all nonnegative integers k. Note that some care is needed for sequence $\boldsymbol{C}$ (see Example 2 in Sect. 2.4). The resulting interpolations are recorded in Table 1. We note that this construction depends on the binomial sum which is neither unique nor easily obtained from the recursion (5). The fact that we

Table 1 Zagier's six sporadic sequences [39] and their interpolations

$*$	$C_*(n)$	$C_*(x)$
$\boldsymbol{A}$	$\sum_{k=0}^{n} \binom{n}{k}^3$	$\sum_{k\geq 0} \binom{x}{k}^3$
$\boldsymbol{B}$	$\sum_{k=0}^{\lfloor n/3 \rfloor} (-1)^k 3^{n-3k} \binom{n}{3k} \frac{(3k)!}{k!^3}$	$\sum_{k\geq 0} (-1)^k 3^{x-3k} \binom{x}{3k} \frac{(3k)!}{k!^3}$
$\boldsymbol{C}$	$\sum_{k=0}^{n} \binom{n}{k}^2 \binom{2k}{k}$	$\operatorname{Re} {}_3F_2\left[\begin{matrix} -x, -x, 1/2 \\ 1, 1 \end{matrix} \middle\| 4\right]$
$\boldsymbol{D}$	$\sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}$	$\sum_{k\geq 0} \binom{x}{k}^2 \binom{x+k}{k}$
$\boldsymbol{E}$	$\sum_{k=0}^{n} \binom{n}{k} \binom{2k}{k} \binom{2(n-k)}{n-k}$	$\sum_{k\geq 0} \binom{x}{k} \binom{2k}{k} \binom{2(x-k)}{x-k}$
$\boldsymbol{F}$	$\sum_{k=0}^{n} (-1)^k 8^{n-k} \binom{n}{k} C_{\boldsymbol{A}}(k)$	$\sum_{k\geq 0} (-1)^k 8^{x-k} \binom{x}{k} C_{\boldsymbol{A}}(k)$

Table 2 The weight 3, level N_* newforms f_* with their L-values

$*$	$f_*(\tau)$	N_*	$L(f_*, 2)$	α_*
$\boldsymbol{A}$	$\frac{\eta(4\tau)^5 \eta(8\tau)^5}{\eta(2\tau)^2 \eta(16\tau)^2}$	32	$\frac{\Gamma^2\left(\frac{1}{8}\right)\Gamma^2\left(\frac{3}{8}\right)}{64\sqrt{2}\pi}$	8
$\boldsymbol{B}$	$\eta(4\tau)^6$	16	$\frac{\Gamma^4\left(\frac{1}{4}\right)}{64\pi}$	8
$\boldsymbol{C}$	$\eta(2\tau)^3 \eta(6\tau)^3$	12	$\frac{\Gamma^6\left(\frac{1}{3}\right)}{2^{17/3}\pi^2}$	12
$\boldsymbol{D}$	$\eta(4\tau)^6$	16	$\frac{\Gamma^4\left(\frac{1}{4}\right)}{64\pi}$	16
$\boldsymbol{E}$	$\eta(\tau)^2 \eta(2\tau) \eta(4\tau) \eta(8\tau)^2$	8	$\frac{\Gamma^2\left(\frac{1}{8}\right)\Gamma^2\left(\frac{3}{8}\right)}{192\pi}$	6
$\boldsymbol{F}$	$q - 2q^2 + 3q^3 + \ldots$	24	$\frac{\Gamma\left(\frac{1}{24}\right)\Gamma\left(\frac{5}{24}\right)\Gamma\left(\frac{7}{24}\right)\Gamma\left(\frac{11}{24}\right)}{96\sqrt{6}\pi}$	6

can relate the value of these interpolations at $x = -1/2$ to critical L-values, as in Zagier's evaluation (2), indicates that our choices are natural. We offer some more comments on these interpolations in Sect. 2.4.

Our first main result is the following.

Theorem 1 *Let $C_*(n)$ be the sporadic sequence in Table 1 and $f_*(\tau) = \sum_{n\geq 1} \gamma_{n,*} q^n$ be the weight 3, level N_* newform listed in Table 2 where the label $*$ is $\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{C}$, $\boldsymbol{D}$ or $\boldsymbol{E}$. Then, for all primes $p > 2$,*

$$C_*\left(\tfrac{p-1}{2}\right) \equiv \gamma_{p,*} \pmod{p}. \tag{7}$$

We note that the congruences (7) hold modulo p^2 only for sequence $\boldsymbol{D}$ [1]. Theorem 1 is known to be true for sequences $\boldsymbol{C}$ and $\boldsymbol{D}$ by work of Stienstra and Beukers

[34], and we show in Sect. 2.2 that the congruences for sequence $\boldsymbol{A}$ can be deduced from their work. The other three cases, including $\boldsymbol{F}$, appear not to have been considered before. We also show in Sect. 2.2 that a general result of Verrill [36] can be used to prove the modular congruences of Theorem 1 for sequences $\boldsymbol{C}$ and $\boldsymbol{E}$. As she points out with sequence $\boldsymbol{A}$, the same approach does not apply in the other cases. Verrill indicates that the modular congruences for sequence $\boldsymbol{A}$ can be explained by Atkin-Swinnerton-Dyer congruences [25, Section 5.8]. We expect that similar ideas can be applied to the case $\boldsymbol{F}$, for which we have numerically observed that Theorem 1 holds as well.

For our second main result, we have the following analogues of Zagier's evaluation (2).

Theorem 2 *Let $C_*(x)$ be the interpolated sequence in Table 1 and $f_*(\tau)$ be the weight 3, level N_* newform listed in Table 2 where the label $*$ is $\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{C}$, $\boldsymbol{D}$ or $\boldsymbol{F}$. Then*

$$C_*(-\tfrac{1}{2}) = \frac{\alpha_*}{\pi^2} L(f_*, 2). \tag{8}$$

For sequence $\boldsymbol{E}$,

$$\operatorname*{res}_{x=-1/2} C_{\boldsymbol{E}}(x) = \frac{6}{\pi^2} L(f_{\boldsymbol{E}}, 1). \tag{9}$$

We prove Theorem 2 in Sect. 2.3. The proof for sequence $\boldsymbol{F}$, using a modular parametrization from [14], is due to Wadim Zudilin. We note from Table 2 that α_* divides N_* in all cases except $\boldsymbol{E}$. It is natural to wonder if a uniform explanation can be given for this observation.

Finally, we note that for sequence $\boldsymbol{E}$, (9) can be written in terms of $L(f_{\boldsymbol{E}}, 2)$ by virtue of the relation

$$L(f_{\boldsymbol{E}}, 1) = \frac{\sqrt{2}}{\pi} L(f_{\boldsymbol{E}}, 2). \tag{10}$$

This is an instance of a general principle, briefly discussed at the end of Sect. 3, which implies that the normalized critical L-values of $f_{\boldsymbol{E}}(\tau)$ are algebraic multiples of each other.

2.2 *Proof of Theorem 1*

Zagier showed that each of the sporadic sequences $C_*(n)$ in Table 1 has a modular parametrization, that is, there exists a modular function $x(\tau)$ such that

$$y(\tau) := \sum_{n=0}^{\infty} C(n) x(\tau)^n \tag{11}$$

is a modular form of weight 1. In cases $\boldsymbol{C}$ and $\boldsymbol{E}$, these are connected to the corresponding modular form $f_*(\tau)$ in Table 2 in such a way that we can apply a general result of Verrill [36] to prove the modular congruences claimed in Theorem 1. This general result is an extension of Beukers' proof [9], which we revisit in Example 1, of the congruences (4) for the Apéry numbers.

Theorem 3 ([36, Theorem 1.1]) *Let $y(\tau)$ be a modular form of weight k and $x(\tau)$ a modular function of level N, and define $C(n)$ by (11). Suppose that, for some integers M and a_d,*

$$y \frac{q}{x} \frac{\mathrm{d}x}{\mathrm{d}q} = \sum_{d|M} a_d f(d\tau),$$

where $f(\tau) = \sum \gamma_n q^n$ is a weight $k+2$, level N Hecke eigenform with character χ. Then,

$$C(mp^r) - \gamma_p C(mp^{r-1}) + \chi(p) p^{k+1} C(mp^{r-2}) \equiv 0 \pmod{p^r},$$

for any prime $p \nmid NM$ and integers m, r. In particular, if $C(1) = 1$, then

$$C(p) \equiv \gamma_p \pmod{p}.$$

In the next example, we apply Theorem 3 to deduce the congruences (4) for the Apéry numbers $A(n)$ (see also [36, Section 2.1]).

Example 1 As shown in [9], the Apéry numbers $A(n)$ have the modular parametrization (11) with

$$x(\tau) = \frac{\eta(\tau)^{12}\eta(6\tau)^{12}}{\eta(2\tau)^{12}\eta(3\tau)^{12}}, \quad y(\tau) = \frac{\eta(2\tau)^7\eta(3\tau)^7}{\eta(\tau)^5\eta(6\tau)^5}.$$

Observe that, defining $\tilde{x}(\tau)$ and $\tilde{y}(\tau)$ by

$$\tilde{x}(\tau)^2 = x(2\tau), \quad \tilde{y}(\tau) = \tilde{x}(\tau)y(2\tau),$$

we have from (11) that

$$\tilde{y}(\tau) = \sum_{\substack{n=0 \\ n \text{ odd}}}^{\infty} A(\tfrac{n-1}{2})\tilde{x}(\tau)^n.$$

It then follows from

$$\tilde{y} \frac{q}{\tilde{x}} \frac{\mathrm{d}\tilde{x}}{\mathrm{d}q} = f(\tau) - 9f(3\tau),$$

where $f(\tau)$ is given by (3), and Theorem 3 that the congruences (4) hold for primes $p > 3$. This is the proof given in [9], which is generalized to Theorem 3 in [36].

We now proceed with the proof of Theorem 1.

Proof (*of Theorem* 1) We first recall that the cases $\boldsymbol{C}$ and $\boldsymbol{D}$ were already proved in [34]. To alternatively deduce case $\boldsymbol{C}$ from Theorem 3, we note that $C_{\boldsymbol{C}}(n)$ has the modular parametrization (11) with (see [39])

$$x(\tau) = \frac{\eta(\tau)^4\eta(6\tau)^8}{\eta(2\tau)^8\eta(3\tau)^4}, \quad y(\tau) = \frac{\eta(2\tau)^6\eta(3\tau)}{\eta(\tau)^3\eta(6\tau)^2}.$$

Defining $\tilde{x}(\tau)$ and $\tilde{y}(\tau)$ from $x(\tau)$ and $y(\tau)$ as in Example 1, it then follows from

$$\tilde{y}\frac{q}{\tilde{x}}\frac{\mathrm{d}\tilde{x}}{\mathrm{d}q} = f_{\boldsymbol{C}}(\tau)$$

and Theorem 3 that the congruences (7) hold for sequence $\boldsymbol{C}$.

Similarly, it is shown in [39] that $C_{\boldsymbol{E}}(n)$ has the modular parametrization (11) with

$$x(\tau) = \frac{\eta(\tau)^4\eta(4\tau)^2\eta(8\tau)^4}{\eta(2\tau)^{10}}, \quad y(\tau) = \frac{\eta(2\tau)^{10}}{\eta(\tau)^4\eta(4\tau)^4}.$$

Again, defining $\tilde{x}(\tau)$ and $\tilde{y}(\tau)$ as in Example 1, it follows from

$$\tilde{y}\frac{q}{\tilde{x}}\frac{\mathrm{d}\tilde{x}}{\mathrm{d}q} = f_{\boldsymbol{E}}(\tau) + 2f_{\boldsymbol{E}}(2\tau)$$

and Theorem 3 that the congruences (7) hold for sequence $\boldsymbol{E}$. We now claim that

$$C_{\boldsymbol{A}}(\tfrac{p-1}{2}) \equiv \gamma_{p,\boldsymbol{A}} \pmod{p}, \tag{12}$$

where $\gamma_{p,\boldsymbol{A}}$ is the pth Fourier coefficient of $f_{\boldsymbol{A}}(\tau)$. To see this, note that (see [34]) for primes $p > 2$,

$$(-1)^{(p-1)/2}C_{\boldsymbol{A}}(\tfrac{p-1}{2}) \equiv \gamma_{p,\boldsymbol{E}} \pmod{p}, \tag{13}$$

(this congruence is recorded in [36, (4.55)] with the sign missing) where $\gamma_{p,\boldsymbol{E}}$ is the pth Fourier coefficient of $f_{\boldsymbol{E}}(\tau)$. Now, observe the relation

$$(-1)^{(n-1)/2}\gamma_{n,\boldsymbol{A}} = \gamma_{n,\boldsymbol{E}} + 2\gamma_{n/2,\boldsymbol{E}}$$

for all integers $n \geq 1$. In particular, for odd n, $\gamma_{n,\boldsymbol{E}} = (-1)^{(n-1)/2}\gamma_{n,\boldsymbol{A}}$. Thus, (13) is equivalent to (12). We note that (13) provides a quick alternative proof of the congruences for sequence $\boldsymbol{E}$ by showing that

$$C_{\boldsymbol{E}}(\tfrac{p-1}{2}) \equiv (-1)^{(p-1)/2}C_{\boldsymbol{A}}(\tfrac{p-1}{2}) \pmod{p}.$$

This congruence can be deduced directly from the binomial sums recorded in Table 1 and the fact that the congruences hold termwise.

Finally, let us prove the congruences for sequence $\boldsymbol{B}$. Expressing the defining binomial sum hypergeometrically, we have

$$C_{\boldsymbol{B}}(\tfrac{p-1}{2}) = 3^{(p-1)/2}{}_3F_2\left[\begin{matrix}\frac{1-p}{6}, \frac{3-p}{6}, \frac{5-p}{6}\\ 1, 1\end{matrix}\middle| 1\right].$$

Because the hypergeometric series is a finite sum (one of the top parameters is a negative integer), it follows that

$$C_{\boldsymbol{B}}(\tfrac{p-1}{2}) \equiv 3^{(p-1)/2}{}_3F_2\left[\begin{matrix}\frac{1-p}{6}, \frac{3-p}{6}, \frac{5-p}{6}\\ 1-\frac{p}{6}, 1-\frac{p}{3}\end{matrix}\middle| 1\right] \pmod{p}.$$

By specializing Watson's identity (see, for instance, [4, Theorem 3.5.5(i)]), we find that this hypergeometric sum has the closed form evaluation

$${}_3F_2\left[\begin{matrix}\frac{1-p}{6}, \frac{3-p}{6}, \frac{5-p}{6}\\ 1-\frac{p}{6}, 1-\frac{p}{3}\end{matrix}\middle| 1\right] = \left(\frac{\Gamma(\frac{1}{2})\Gamma(1-\frac{p}{6})}{\Gamma(\frac{7-p}{12})\Gamma(\frac{11-p}{12})}\right)^2. \tag{14}$$

If $p \equiv 3 \pmod 4$, then $p \equiv 7, 11 \pmod{12}$ and we see that the right-hand side of (14) is zero, so that $C_{\boldsymbol{B}}(\frac{p-1}{2})$ vanishes modulo p. Suppose that $p \equiv 1 \pmod 4$. With some care, we are able to write

$$\frac{\Gamma(\frac{1}{2})\Gamma(1-\frac{p}{6})}{\Gamma(\frac{7-p}{12})\Gamma(\frac{11-p}{12})} \equiv \frac{\Gamma_p(\frac{1}{2})\Gamma_p(1-\frac{p}{6})}{\Gamma_p(\frac{7-p}{12})\Gamma_p(\frac{11-p}{12})} \equiv -\frac{\Gamma_p(\frac{1}{2})}{\Gamma_p(\frac{7}{12})\Gamma_p(\frac{11}{12})} \pmod{p},$$

where Γ_p is Morita's p-adic gamma function (see, for instance, [15, 11.6] or [21, IV.2]). Since $\Gamma_p(1/2)^2 = (-1)^{(p+1)/2}$, it follows that, if $p \equiv 1 \pmod 4$, then

$$C_{\boldsymbol{B}}(\tfrac{p-1}{2}) \equiv -\frac{3^{(p-1)/2}}{\Gamma_p(\frac{7}{12})^2\Gamma_p(\frac{11}{12})^2} \equiv -3^{(p-1)/2}\Gamma_p(\tfrac{1}{12})^2\Gamma_p(\tfrac{5}{12})^2 \pmod{p},$$

where we used the p-adic version of the reflection formula for the final congruence. On the other hand, it follows from the p-adic Gauss–Legendre multiplication formula (see, for instance, [15, 11.6.14] or [21, p. 91]) that, for primes $p \equiv 1 \pmod 4$,

$$\Gamma_p(\tfrac{1}{12})^2\Gamma_p(\tfrac{5}{12})^2 = (\tfrac{3}{p})\Gamma_p(\tfrac{1}{4})^4.$$

Since $3^{(p-1)/2} \equiv (\frac{3}{p}) \pmod p$, we conclude that, modulo p,

$$C_{\boldsymbol{B}}(\tfrac{p-1}{2}) \equiv \begin{cases} -\Gamma_p(\frac{1}{4})^4, & \text{if } p \equiv 1 \pmod 4,\\ 0, & \text{if } p \equiv 3 \pmod 4.\end{cases}$$

Comparing with the congruences established for sequence $\boldsymbol{D}$ in [34, (13.4)], we arrive at

$$C_{\boldsymbol{B}}(\tfrac{p-1}{2}) \equiv C_{\boldsymbol{D}}(\tfrac{p-1}{2}) \pmod{p}, \tag{15}$$

which implies the claimed congruences for sequence $\boldsymbol{B}$.

2.3 Proof of Theorem 2

This section is devoted to proving Theorem 2. We first prove case $\boldsymbol{D}$ in detail, then briefly indicate how to establish cases $\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{C}$ and $\boldsymbol{E}$. We conclude with a sketch of case $\boldsymbol{F}$. We note that the relation of the hypergeometric series, which arise for sequences $\boldsymbol{A}$, $\boldsymbol{C}$, $\boldsymbol{D}$, and the corresponding L-values already appears in [42].

Proof (*of Theorem* 2) We first claim that

$$C_{\boldsymbol{D}}(-\tfrac{1}{2}) = \frac{16}{\pi^2} L(f_{\boldsymbol{D}}, 2). \tag{16}$$

Expressing the defining binomial sum hypergeometrically, we have

$$C_{\boldsymbol{D}}(x) = {}_3F_2\left[\left.\begin{matrix} -x, -x, x+1 \\ 1, 1 \end{matrix}\right| 1\right],$$

so that, in particular,

$$C_{\boldsymbol{D}}(-\tfrac{1}{2}) = {}_3F_2\left[\left.\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix}\right| 1\right].$$

We could evaluate the right-hand side using hypergeometric identities (such as, in this case, [4, Theorem 3.5.5]). Instead, here and in subsequent cases, we find it more fitting to the overall theme to employ modular parametrizations. As such, applying Clausen's identity (see, for instance, [12, Proposition 5.6])

$${}_3F_2\left[\left.\begin{matrix} \frac{1}{2}, s, 1-s \\ 1, 1 \end{matrix}\right| 4x(1-x)\right] = {}_2F_1\left[\left.\begin{matrix} s, 1-s \\ 1 \end{matrix}\right| x\right]^2, \tag{17}$$

with $s = 1/2$ and the modular parametrization (see [11], [38, p.63] or [40, (37)])

$${}_2F_1\left[\left.\begin{matrix} \frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix}\right| \lambda(\tau)\right] = \theta_3(\tau)^2, \tag{18}$$

where $\theta_2(\tau) = \sum_{n\in\mathbb{Z}+1/2} q^{n^2/2}$, $\theta_3(\tau) = \sum_{n\in\mathbb{Z}} q^{n^2/2}$ and $\lambda(\tau) = \left(\frac{\theta_2(\tau)}{\theta_3(\tau)}\right)^4$, we find that

$$C_{\boldsymbol{D}}(-\tfrac{1}{2}) = {}_2F_1\left[\begin{matrix}\frac{1}{2}, \frac{1}{2} \\ 1\end{matrix}\middle|\frac{1}{2}\right]^2 = \left(\frac{\Gamma^2(\frac{1}{4})}{2\pi^{3/2}}\right)^2, \tag{19}$$

upon taking $\tau = i$, in which case $\lambda(i) = \frac{1}{2}$ and $\theta_3(i)^2 = \frac{\Gamma^2(1/4)}{2\pi^{3/2}}$. On the other hand, it is shown by Rogers, Wan and Zucker [29] that

$$L(f_{\boldsymbol{D}}, 2) = \frac{\Gamma^4(\frac{1}{4})}{64\pi}.$$

In light of (19), this proves (16). Next, we claim that

$$C_{\boldsymbol{A}}(-\tfrac{1}{2}) = \frac{8}{\pi^2} L(f_{\boldsymbol{A}}, 2). \tag{20}$$

Proceeding as above, we find that

$$C_{\boldsymbol{A}}(-\tfrac{1}{2}) = {}_3F_2\left[\begin{matrix}\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1\end{matrix}\middle|-1\right].$$

Employing (17) and the modular parametrization, we obtain

$$C_{\boldsymbol{A}}(-\tfrac{1}{2}) = {}_2F_1\left[\begin{matrix}\frac{1}{2}, \frac{1}{2} \\ 1\end{matrix}\middle|\frac{1-\sqrt{2}}{2}\right]^2 = \theta_3\left(1 + i\sqrt{2}\right)^4 = \frac{\Gamma^2(\frac{1}{8})\Gamma^2(\frac{3}{8})}{8\sqrt{2}\pi^3}. \tag{21}$$

Again, up to the factor $8/\pi^2$, this matches the corresponding L-value evaluation [29]

$$L(f_{\boldsymbol{A}}, 2) = \frac{\Gamma^2(\frac{1}{8})\Gamma^2(\frac{3}{8})}{64\sqrt{2}\pi}.$$

This proves (20). Now, in order to see

$$C_{\boldsymbol{B}}(-\tfrac{1}{2}) = \frac{8}{\pi^2} L(f_{\boldsymbol{B}}, 2), \tag{22}$$

we begin with

$$C_{\boldsymbol{B}}(x) = 3^x {}_3F_2\left[\begin{matrix}-\frac{x}{3}, -\frac{x-1}{3}, -\frac{x-2}{3} \\ 1, 1\end{matrix}\middle|1\right]$$

and hence

$$C_{\boldsymbol{B}}(-\tfrac{1}{2}) = 3^{-1/2} {}_3F_2\left[\begin{matrix}\frac{1}{6}, \frac{1}{2}, \frac{5}{6} \\ 1, 1\end{matrix}\middle|1\right].$$

Let $j(\tau)$ denote Klein's modular function. By [12, Theorem 5.7], we have

$$ {}_3F_2\left[\begin{matrix}\frac{1}{6},\frac{1}{2},\frac{5}{6}\\1,1\end{matrix}\middle|\frac{1728}{j(\tau)}\right]=\sqrt{1-\lambda(\tau)(1-\lambda(\tau))}\;{}_2F_1\left[\begin{matrix}\frac{1}{2},\frac{1}{2}\\1\end{matrix}\middle|\lambda(\tau)\right]^2, $$

which specialized to $\tau = i$, and combined with (18), yields

$$ C_{\boldsymbol{B}}(-\tfrac{1}{2})=3^{-1/2}{}_3F_2\left[\begin{matrix}\frac{1}{6},\frac{1}{2},\frac{5}{6}\\1,1\end{matrix}\middle|1\right]=\frac{1}{2}\theta_3(i)^4=\frac{\Gamma^4(\frac{1}{4})}{8\pi^3}. $$

Up to the factor $8/\pi^2$, this equals the L-value evaluation [29]

$$ L(f_{\boldsymbol{B}},2)=\frac{\Gamma^4(\frac{1}{4})}{64\pi}. $$

Thus, (22) follows. To prove

$$ C_{\boldsymbol{C}}(-\tfrac{1}{2})=\frac{12}{\pi^2}L(f_{\boldsymbol{C}},2), \tag{23} $$

we first observe

$$ C_{\boldsymbol{C}}(-\tfrac{1}{2})=\operatorname{Re}{}_3F_2\left[\begin{matrix}\frac{1}{2},\frac{1}{2},\frac{1}{2}\\1,1\end{matrix}\middle|4\right]. $$

Employing (17) and the modular parametrization, we obtain

$$ {}_3F_2\left[\begin{matrix}\frac{1}{2},\frac{1}{2},\frac{1}{2}\\1,1\end{matrix}\middle|4\right]={}_2F_1\left[\begin{matrix}\frac{1}{2},\frac{1}{2}\\1\end{matrix}\middle|\frac{1-i\sqrt{3}}{2}\right]^2=\theta_3\left(-\frac{1-i\sqrt{3}}{2}\right)^4=\frac{\left(3-i\sqrt{3}\right)\Gamma^6(\frac{1}{3})}{2^{11/3}\pi^4}. $$

Up to the factor $12/\pi^2$, the real part of this equals the L-value evaluation [29]

$$ L(f_{\boldsymbol{C}},2)=\frac{\Gamma^6(\frac{1}{3})}{2^{17/3}\pi^2}. $$

This yields (23). Next, to deduce

$$ \operatorname*{res}_{x=-1/2}C_{\boldsymbol{E}}(x)=\frac{6}{\pi^2}L(f_{\boldsymbol{E}},1), \tag{24} $$

we start with

$$ C_{\boldsymbol{E}}(x)=\binom{2x}{x}{}_3F_2\left[\begin{matrix}-x,-x,\frac{1}{2}\\\frac{1}{2}-x,1\end{matrix}\middle|-1\right] $$

and hence

$$\operatorname*{res}_{x=-1/2} C_{\boldsymbol{E}}(x) = \frac{1}{2\pi} {}_3F_2\left[\begin{matrix}\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1\end{matrix}\middle| -1\right] = \frac{\Gamma^2(\frac{1}{8})\Gamma^2(\frac{3}{8})}{16\sqrt{2}\pi^4},$$

where the second equality is a consequence of (21). Up to the factor $6/\pi^2$, this equals

$$L(f_{\boldsymbol{E}}, 1) = \frac{\Gamma^2(\frac{1}{8})\Gamma^2(\frac{3}{8})}{96\sqrt{2}\pi^2},$$

which follows from (10) and the value for $L(f_{\boldsymbol{E}}, 2)$ obtained in [29]. This proves (24). Finally, we claim that (see also [37, 41])

$$C_{\boldsymbol{F}}(-\tfrac{1}{2}) = \frac{6}{\pi^2} L(f_{\boldsymbol{F}}, 2) = \frac{\Gamma(\frac{1}{24})\Gamma(\frac{5}{24})\Gamma(\frac{7}{24})\Gamma(\frac{11}{24})}{16\sqrt{6}\pi^3}. \tag{25}$$

To begin with, note that

$$C_{\boldsymbol{F}}(-\tfrac{1}{2}) = \frac{1}{\sqrt{8}} \sum_{k=0}^{\infty} 2^{-5k} \binom{2k}{k} C_{\boldsymbol{A}}(k) = \frac{1}{\sqrt{8}} g\left(\frac{1}{32}\right),$$

where

$$g(z) = \sum_{k=0}^{\infty} z^k \binom{2k}{k} \sum_{j=0}^{k} \binom{k}{j}^3.$$

In [14, Theorem 2.1], the modular parametrization

$$g\left(\frac{x(\tau)}{(1-x(\tau))^2}\right) = \frac{1}{6}(6E_2(6\tau) + 3E_2(3\tau) - 2E_2(2\tau) - E_2(\tau)),$$

with

$$x(\tau) = \left(\frac{\eta(\tau)\eta(6\tau)}{\eta(2\tau)\eta(3\tau)}\right)^{12}, \quad E_2(\tau) = 1 - 24\sum_{n=1}^{\infty} \frac{nq^n}{1-q^n},$$

is obtained. Specializing this parametrization at $\tau = \tau_0 = i/\sqrt{6}$, we obtain the desired value $g(1/32)$. It then is a standard application of the Chowla–Selberg formula [31] to show that

$$3E_2(3\tau_0) - E_2(\tau_0) = 6E_2(6\tau_0) - 2E_2(2\tau_0) = \frac{\sqrt{3}\Gamma(\frac{1}{24})\Gamma(\frac{5}{24})\Gamma(\frac{7}{24})\Gamma(\frac{11}{24})}{8\pi^3},$$

which implies

$$C_{\boldsymbol{F}}(-\tfrac{1}{2}) = \frac{\Gamma(\frac{1}{24})\Gamma(\frac{5}{24})\Gamma(\frac{7}{24})\Gamma(\frac{11}{24})}{16\sqrt{6}\pi^3}. \tag{26}$$

That the right-hand side equals the claimed L-value then follows from work of Damerell [17] because $L(f_F, s)$ can be viewed as a Hecke L-series on the field $\mathbb{Q}(\sqrt{-6})$ (see also [7, 30]).

2.4 Interpolating the Sporadic Sequences

Zagier's interpolated series (1) is absolutely convergent for all $x \in \mathbb{C}$ (as a consequence of (30)) and defines a holomorphic function satisfying the symmetry $A(x) = A(-x-1)$. Zagier shows the somewhat surprising fact that $A(x)$ does not satisfy the same recurrence as the Apéry numbers, but instead the inhomogeneous functional equation

$$P(x, S_x)A(x) = \frac{8}{\pi^2}(2x+3)\sin^2(\pi x) \tag{27}$$

for all complex x, where

$$P(x, S_x) = (x+2)^3 S_x^2 - (2x+3)(17x^2+51x+39)S_x + (x+1)^3 \tag{28}$$

is Apéry's recurrence operator, and S_x denotes the (forward) shift operator in x, meaning that $S_x f(x) = f(x+1)$.

Remark 1 Let us illustrate how one can algorithmically derive and prove (27). Let $D(x,k)$ be the summand in the sum defining $A(x)$. Creative telescoping applied to $D(x,k)$ determines the operator $P(x, S_x)$ given in (28) as well as a rational function $R(x,k)$ such that

$$P(x, S_x)D(x,k) = (1 - S_k)R(x,k)D(x,k). \tag{29}$$

It follows that

$$P(x, S_x)\sum_{k=0}^{K-1} D(x,k) = R(x,0)D(x,0) - R(x,K)D(x,K) = -R(x,K)D(x,K),$$

and it remains to compute the limit of the right-hand side as $K \to \infty$. Using basic properties of the gamma function, as done in [40], one obtains

$$D(x,k) = \left[\frac{\sin(\pi x)}{\pi k}\right]^2 + O\left(\frac{1}{k^3}\right), \quad k \to \infty, \tag{30}$$

from which we deduce that $-R(x,K)D(x,K)$ approaches $8(2x+3)\sin^2(\pi x)/\pi^2$ as $K \to \infty$. The following lines of Mathematica code use Koutschan's Mathematica package `HolonomicFunctions` [23] to perform all of these computations automatically:

```
Dxk = Binomial[x,k]^2 Binomial[x+k,k]^2
{{P}, {R}} = CreativeTelescoping[Dxk, S[k]-1, {S[x]}]
{R} = OrePolynomialListCoefficients[R]
Limit[-R Dxk, k->Infinity, Assumptions->Element[k,Integers]]
```

Remark 2 We note that the sum in (1) actually has natural boundaries, meaning that the range of summation can be extended from nonnegative integers to all integers without changing the sum. The reason is that the summand vanishes for all $x \in \mathbb{C}$ if k is a negative integer. More specifically, if k is a negative integer, then $\binom{x+k}{k} = 0$ for all $x \in \mathbb{C}\backslash\{-k-1, -k-2, \ldots, 1, 0\}$, while $\binom{x}{k} = 0$ for all $x \in \mathbb{C}\backslash\{-1, -2, \ldots, k\}$. For more details on binomial coefficients with negative integer entries, we refer to [18, 26].

Somewhat unexpectedly, there are marked differences when considering the interpolations of the sporadic sequences given in Table 1. For illustration, consider sequence $\boldsymbol{D}$ with interpolation

$$C_{\boldsymbol{D}}(x) = \sum_{k=0}^{\infty} \binom{x}{k}^2 \binom{x+k}{k}. \tag{31}$$

In this case, we find that, as $k \to \infty$,

$$\binom{x}{k}^2 \binom{x+k}{k} \sim \frac{\Gamma(x+1)}{k^x} \left[\frac{\sin(\pi x)}{\pi k}\right]^2,$$

which implies that the series (31) converges if $\operatorname{Re} x > -1$ but diverges if $\operatorname{Re} x < -1$. Moreover, proceeding as in the case of the Apéry numbers $A(n)$, it follows that $C_{\boldsymbol{D}}(x)$ satisfies the homogeneous functional equation

$$[(x+2)^2 S_x^2 - (11x^2 + 33x + 25)S_x - (x+1)^2]C_{\boldsymbol{D}}(x) = 0$$

for all complex x with $\operatorname{Re} x > -1$. This is recurrence (5) with $(a, b, c) = (11, 3, -1)$.

The situation is similar for our interpolations of the sequences $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{E}$. In each case, the defining series (see Table 1) converges if $\operatorname{Re} x > -1$ and one finds, as in the case of sequence $\boldsymbol{D}$, that the interpolation satisfies the recurrence (5) for the appropriate choice of (a, b, c).

Example 2 Some care is required for sequence $\boldsymbol{C}$, which has the binomial sum representation

$$C_{\boldsymbol{C}}(n) = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{2k}{k}.$$

In this case, letting n be a complex variable and extending the summation over all nonnegative integers k never yields a convergent sum (unless n is a nonnegative integer, in which case the sum is a finite one). However, the binomial sum can be expressed hypergeometrically as

$$C_{\boldsymbol{C}}(n) = {}_3F_2\left[\begin{matrix} -n, -n, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| 4\right]. \tag{32}$$

For integers $n \geq 0$, this hypergeometric series is a finite sum. For other values of n, we can make sense of the hypergeometric function (32) by replacing 4 with a complex argument z (the series converges for $|z| < 1$) and analytic continuation to $z = 4$. As usual, the principal branch of the hypergeometric function is chosen by cutting from $z = 1$ to $z = \infty$ on the real axis. As a consequence, there is a choice to approach $z = 4$ from either above or below the real axis, and the two resulting values are complex conjugates of each other. We avoid this ambiguity, as well as complex values, by defining

$$C_{\boldsymbol{C}}(x) = \operatorname{Re} {}_3F_2\left[\begin{matrix} -x, -x, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| 4\right].$$

That this is a sensible choice of interpolation is supported by Theorem 2.

Example 3 For sequence $\boldsymbol{F}$, let us consider the interpolation

$$C_{\boldsymbol{F}}(x) = \sum_{k=0}^{\infty} (-1)^k 8^{x-k} \binom{x}{k} C_{\boldsymbol{A}}(k), \tag{33}$$

where $C_{\boldsymbol{A}}(n)$ are the Franel numbers

$$C_{\boldsymbol{A}}(n) = \sum_{k=0}^{n} \binom{n}{k}^3 = \frac{2\sqrt{3}}{\pi} \frac{2^{3n}}{3n} \left(1 + O\left(\frac{1}{n}\right)\right).$$

It follows that, as $k \to \infty$,

$$(-1)^k 8^{x-k} \binom{x}{k} C_{\boldsymbol{A}}(k) = \frac{2}{\pi\sqrt{3}} \frac{8^x}{\Gamma(-x)} \frac{1}{k^{x+2}} \left(1 + O\left(\frac{1}{k}\right)\right),$$

from which we deduce that, once more, the series (33) converges if $\operatorname{Re} x > -1$. Consequently, we expect that the truncation

$$C_{\boldsymbol{F}}(x; N) = \sum_{k=0}^{N} (-1)^k 8^{x-k} \binom{x}{k} C_{\boldsymbol{A}}(k),$$

as $N \to \infty$, has an asymptotic expansion of the form

$$C_{\boldsymbol{F}}(x;N) = C_{\boldsymbol{F}}(x) + \frac{b_1(x)}{N^{x+1}} + \frac{b_2(x)}{N^{x+2}} + \ldots$$

Using this assumption, we can speed up the convergence of $C_{\boldsymbol{F}}(-1/2;N)$ by considering the sequence $c_n = C_{\boldsymbol{F}}(-1/2;n^2)$ and approximating its limit via the differences $(S_n-1)^m n^m c_n/m!$ for suitable choices of m and n. This allows us to compute $C_{\boldsymbol{F}}(-1/2)$ to, say, 50 decimal places. Namely,

$$C_{\boldsymbol{F}}(-\tfrac{1}{2}) = 0.50546201971732600605200405322714025998512901481742\ldots$$

This allowed us to numerically discover (8) for sequence $\boldsymbol{F}$. For comparison, summing the first 100, 000 terms of the series only produces three correct digits.

3 Cellular Integrals

Recently, Brown [13] introduced a program where period integrals on the moduli space $\mathcal{M}_{0,N}$ of curves of genus 0 with N marked points play a central role in understanding irrationality proofs of values of the Riemann zeta function. The idea is to associate a rational function f_σ and a differential $(N-3)$-form ω_σ to a given permutation $\sigma = \sigma_N$ on $\{1,2,\ldots,N\}$. Consider the cellular integral

$$I_\sigma(n) := \int_{S_N} f_\sigma^n \, \omega_\sigma,$$

where

$$S_N = \{(t_1,\ldots,t_{N-3}) \in \mathbb{R}^{N-3} : 0 < t_1 < \ldots < t_{N-3} < 1\}.$$

By [13, Corollary 8.2], $I_\sigma(n)$ is a $\mathbb{Q}$-linear combination of multiple zeta values of weight less than or equal to $N-3$. Suppose that this linear combination is of the form $A_{\sigma_N}(n)\zeta_\sigma(N-3)$, with $A_{\sigma_N}(n) \in \mathbb{Q}$, plus a combination of multiple zeta values of weight less than $N-3$. We then say that $A_\sigma(n) = A_{\sigma_N}(n)$ is the *leading coefficient* of the cellular integral $I_\sigma(n)$. For example, if $N=5$, then $\sigma_5 = (1,3,5,2,4)$ is the unique convergent permutation, $I_{\sigma_5}(n)$ recovers Beukers' integral for $\zeta(2)$ [8] and the leading coefficients $A_{\sigma_5}(n)$ are the Apéry numbers $C_{\boldsymbol{D}}(n)$ in (6).

In [27], an explicit family σ_N of convergent configurations for odd $N \geq 5$ is constructed such that the leading coefficients $A_{\sigma_N}(n)$ are powers of the Apéry numbers $C_{\boldsymbol{D}}(n)$, that is,

$$A_{\sigma_N}(n) = C_{\boldsymbol{D}}(n)^{(N-3)/2}. \tag{34}$$

The first main result in [27] extends Theorem 1 for sequence $\boldsymbol{D}$ to a supercongruence for all odd weights greater than or equal to 3. Specifically, for odd $k = N-2 \geq 3$, consider the binary theta series

$$f_k(\tau) = \frac{1}{4} \sum_{(n,m)\in\mathbb{Z}^2} (-1)^{m(k-1)/2}(n-im)^{k-1} q^{n^2+m^2} =: \sum_{n\geq 1} \gamma_k(n) q^n. \tag{35}$$

Theorem 4 ([27, Theorem 1.1]) *For each odd integer $N \geq 5$, let $A_{\sigma_N}(n)$ and $f_k(\tau)$ be as in (34) and (35), respectively. Then, for all primes $p \geq 5$,*

$$A_{\sigma_N}(\tfrac{p-1}{2}) \equiv \gamma_k(p) \pmod{p^2}. \tag{36}$$

Using the interpolation (31) for $C_{\boldsymbol{D}}(n)$ and (34), we have the following analogue of (2) for all odd $N \geq 5$.

Theorem 5 *Let $N \geq 5$ be an odd positive integer, $k = N-2$ and $f_k(\tau)$ be as in* (35). *Then,*

$$A_{\sigma_N}(-\tfrac{1}{2}) = \frac{\alpha_k}{\pi^{k-1}} L(f_k, k-1), \tag{37}$$

where α_k is an explicit rational number given as follows:

$$\alpha_k = 2^{(k+1)/2}(k-2) \begin{cases} 2/r_{(k-1)/2}, & \text{if } k \equiv 1 \pmod 4, \\ 1/s_{(k-1)/2}, & \text{if } k \equiv 3 \pmod 4. \end{cases} \tag{38}$$

Here, r_n is defined by $r_2 = 1/5$, $r_3 = 0$ and

$$(2n+1)(n-3)r_n = 3\sum_{k=2}^{n-2} r_k r_{n-k} \tag{39}$$

for $n \geq 4$, and s_n is defined by $s_1 = 1/4$, $s_2 = 11/80$, $s_3 = 1/32$ and the same recursion (39) *for $n \geq 4$.*

Proof (*of Theorem* 5) Since $f_3(\tau) = \eta(4\tau)^6$, the case $N = 5$ is (16). Thus, we assume $N > 5$. As a consequence of (19) and (34), we have

$$A_{\sigma_N}(-\tfrac{1}{2}) = \left(\frac{\Gamma^2(\frac{1}{4})}{2\pi^{3/2}}\right)^{N-3} = \left(\frac{\sqrt{2}\omega}{\pi}\right)^{k-1}, \tag{40}$$

where

$$\omega = 2\int_0^1 \frac{\mathrm{d}x}{\sqrt{1-x^4}} = \frac{\Gamma^2(\frac{1}{4})}{2\sqrt{2\pi}}$$

is the lemniscate constant. On the other hand, it follows from the representation (35) that

$$L(f_k, k-1) = \frac{1}{4} \sum_{(n,m)\neq(0,0)} (-1)^{m(k-1)/2} \frac{(n-im)^{k-1}}{(n^2+m^2)^{k-1}}$$
$$= \frac{1}{4} \sum_{(n,m)\neq(0,0)} (-1)^{m(k-1)/2} \frac{1}{(n+im)^{k-1}}.$$

In other words, these L-values are values of the Eisenstein series

$$G_\ell(\tau) = \sum_{(n,m)\neq(0,0)} \frac{1}{(n+m\tau)^\ell}$$

of even weight ℓ. Specifically, since

$$2G_\ell(2\tau) - G_\ell(\tau) = \sum_{(n,m)\neq(0,0)} \frac{(-1)^m}{(n+m\tau)^\ell},$$

we have

$$L(f_k, k-1) = \frac{1}{4} \begin{cases} G_{k-1}(i), & \text{if } k \equiv 1 \pmod 4, \\ 2G_{k-1}(2i) - G_{k-1}(i), & \text{if } k \equiv 3 \pmod 4. \end{cases}$$

We note that, if $k \equiv 3 \pmod 4$, then $G_{k-1}(i) = 0$ because, writing $k = 4\ell + 3$,

$$G_{k-1}(i) = \sum_{(n,m)\neq(0,0)} \frac{1}{(n+mi)^{4\ell+2}}$$
$$= \sum_{(n,m)\neq(0,0)} \frac{1}{i^{4\ell+2}(m-ni)^{4\ell+2}} = -G_{k-1}(i).$$

For $n \geq 4$, we have (see [6, Theorem 1.13])

$$(4n^2-1)(n-3)G_{2n} = 3\sum_{k=2}^{n-2}(2k-1)(2n-2k-1)G_{2k}G_{2(n-k)},$$

which, upon setting $H_k = (2k-1)G_{2k}$, takes the simplified form

$$(2n+1)(n-3)H_n = 3\sum_{k=2}^{n-2} H_k H_{n-k}. \tag{41}$$

In terms of the functions H_k, we have

$$L(f_k, k-1) = \frac{1}{4(k-2)} \begin{cases} H_{2\ell}(i), & \text{if } k = 4\ell+1, \\ 2H_{2\ell+1}(2i), & \text{if } k = 4\ell+3. \end{cases}$$

Note that the required values of $H_k(\tau)$ at $\tau = i$ and $\tau = 2i$ are determined by the recursive relation (41) once we know the initial cases $k = 2$ and $k = 3$. It is shown, for instance, in [24, Theorem 6] that

$$H_2(i) = 3G_4(i) = \frac{\omega^4}{5},$$

and our earlier discussion implies $H_3(i) = 5G_6(i) = 0$. Similarly, one shows that

$$H_2(2i) = 3G_4(2i) = \frac{11\omega^4}{80}, \quad H_3(2i) = 5G_6(2i) = \frac{\omega^6}{32}.$$

In light of these initial values, the recurrence (41) implies that, for $n \geq 2$, the values $H_n(i)$ and $H_n(2i)$ are rational multiples of ω^{2n}. Moreover, the rational factors are given by the sequences r_n and s_n:

$$r_n = \frac{H_n(i)}{\omega^{2n}}, \quad s_n = \frac{H_n(2i)}{\omega^{2n}}.$$

Thus,

$$L(f_k, k-1) = \frac{\omega^{k-1}}{4(k-2)} \begin{cases} r_{2\ell}, & \text{if } k = 4\ell + 1, \\ 2s_{2\ell+1}, & \text{if } k = 4\ell + 3, \end{cases}$$

and the claim then follows from comparison with (40).

Remark 3 Let us indicate that the rational numbers featuring in Theorem 5 are arithmetically interesting in their own right, and analogous to Bernoulli numbers. The values $G_{4\ell}(i)$ were first explicitly evaluated by Hurwitz [20] (see [24] for a modern account), who showed that

$$G_{4\ell}(i) = \sum_{(n,m)\neq(0,0)} \frac{1}{(n+im)^{4\ell}} = \frac{(2\omega)^{4\ell}}{(4\ell)!} E_\ell, \tag{42}$$

where the E_ℓ are positive rational numbers characterized by $E_1 = 1/10$ and the recurrence

$$E_n = \frac{3}{(2n-3)(16n^2-1)} \sum_{k=1}^{n-1} (4k-1)(4n-4k-1) \binom{4n}{4k} E_k E_{n-k}.$$

In terms of the numbers r_n defined in Theorem 5, we have

$$E_n = \frac{(4n)!}{2^{4n}} \frac{r_{2n}}{4n-1}.$$

Equation (42), defining the Hurwitz numbers E_ℓ, can be seen as an analog of

$$\sum_{n\neq 0}\frac{1}{n^{2\ell}}=\frac{(2\pi)^{2\ell}}{(2\ell)!}B_\ell$$

characterizing the Bernoulli numbers B_ℓ. In other words, in the theory of Gaussian integers the Hurwitz numbers E_ℓ play a role comparable to that played by the Bernoulli numbers for the usual integers. That this analogy extends much further, including to the theorem of von Staudt–Clausen, is beautifully demonstrated by Hurwitz [20].

Example 4 Let us make the case $N=7$ of Theorem 5 explicit. The leading coefficients $A_{\sigma_7}(n)$ are the squares of the Apéry numbers $C_{\boldsymbol{D}}(n)$ and the modular form $f_5(\tau)$ can alternatively be expressed as

$$f_5(\tau)=\eta(\tau)^4\eta(2\tau)^2\eta(4\tau)^4.$$

The Zagier-type L-value evaluation proven in Theorem 5 is

$$A_{\sigma_7}(-\tfrac{1}{2})=\frac{240}{\pi^2}L(f_5,4).$$

It is observed in [29] that this and many other L-values are naturally expressed in terms of integrals of the complete elliptic integral K; for instance,

$$L(f_5,4)=\frac{1}{30}\int_0^1 K'(k)^3\mathrm{d}k=\frac{1}{9}\int_0^1 K(k)^3\mathrm{d}k.$$

Example 5 The values of the first several α_k in Theorem 5 are $\alpha_3=16$, $\alpha_5=240$, $\alpha_7=2560$, $\alpha_9=33600$, $\alpha_{11}=491520$, $\alpha_{13}=6864000$ and $\alpha_{15}=\frac{1022361600}{11}$.

Let $L^*(f,s)=(2\pi)^{-s}\Gamma(s)L(f,s)$ be the normalized L-function for f. It follows from the work of Eichler, Shimura and Manin on period polynomials (for example, see [33]) that the critical L-values $L^*(f,s)$ for odd s (as well as those for even s) are algebraic multiples of each other. Moreover, if f has odd weight k, then by virtue of the functional equation all critical L-values $L^*(f,s)$ are algebraic multiples of each other. In particular, it follows that (37) can be rewritten as

$$A_{\sigma_N}(-\tfrac{1}{2})=\beta_k\frac{L(f_k,2)}{\pi^2}$$

for some algebraic numbers β_k. In fact, it appears that the β_k's are rational numbers.

Example 6 Numerically, the first several values of β_k are $\beta_3=16$, $\beta_5=48$, $\beta_7=4$, $\beta_9=14$, $\beta_{11}=\frac{1}{33}$, $\beta_{13}=\frac{11}{18}$, $\beta_{15}=\frac{1}{33156}$. These values, as well as the relations indicated in Example 7, may in principle be rigorously obtained using, for instance, Rankin's method [32].

Example 7 As indicated above, all critical L-values $L^*(f_k, s)$ are algebraic multiples of each other. In fact, numerical computations suggest that all critical L-values are rationally related. The first few cases are:

$$\begin{aligned}
L(f_5,4) &= \frac{2\pi}{5}L(f_5,3) = \frac{\pi^2}{5}L(f_5,2) = \frac{\pi^3}{6}L(f_5,1),\\
L(f_7,6) &= \frac{3\pi}{10}L(f_7,5) = \frac{3\pi^2}{40}L(f_7,4) = \frac{\pi^3}{80}L(f_7,3) = \frac{\pi^4}{640}L(f_7,2)\\
&= \frac{\pi^5}{3840}L(f_7,1),\\
L(f_9,8) &= \frac{3\pi}{10}L(f_9,7) = \frac{3\pi^2}{35}L(f_9,6) = \frac{4\pi^3}{175}L(f_9,5) = \frac{\pi^4}{175}L(f_9,4)\\
&= \frac{\pi^5}{700}L(f_9,3) = \frac{\pi^6}{2400}L(f_9,2) = \frac{\pi^7}{5040}L(f_9,1).
\end{aligned}$$

We thank Yifan Yang for pointing out that one can prove the relation

$$L(f_5,4) = \frac{\pi^2}{5}L(f_5,2)$$

using Theorem 2.3 in [19].

4 Outlook

There are numerous directions for future study. First, motivated by Beukers' and Zagier's numerical investigation of (5), Almkvist, Zudilin [3] and Cooper [16] searched for parameters (a,b,c,d) such that the three-term relation

$$(n+1)^3 u_{n+1} = (2n+1)(an^2+an+b)u_n - n(cn^2+d)u_{n-1}, \tag{43}$$

with initial conditions $u_{-1}=0$, $u_0=1$, produces only integer solutions. For $(a,b,c,d)=(17,5,1,0)$, we obtain the Apéry numbers $A(n)$. In total, there are nine sporadic cases for (43). It is not currently known if each of these cases has an interpolated version which is related (similar to (2)) to the critical L-value of a modular form of weight 4. Second, we echo the lament in [28] concerning the lack of algorithmic approaches in directly proving congruences, such as (15), between binomial sums. Third, can one extend the results in [19] to verify the cases in Example 7 and, more generally, find an explicit formula for the ratio $L(f_k,k-1)/L(f_k,2)$ in terms of a rational number and a power of π? Fourth, in the context of Sect. 3, a supercongruence (akin to (36)) has been proven in [27] between the leading coefficient

$$A_{\sigma_8}(n) = \sum_{\substack{k_1,k_2,k_3,k_4=0\\k_1+k_2=k_3+k_4}}^{n} \prod_{i=1}^{4} \binom{n}{k_i}\binom{n+k_i}{k_i}$$

and $\eta(2\tau)^{12}$, the unique newform in $S_6(\Gamma_0(4))$. Does there exist a version of Theorem 5 in this case? Fifth, Zudilin [42] recently considered periods of certain instances of rigid Calabi–Yau manifolds, which are expressed in terms of hypergeometric functions. In these instances, he conjecturally indicated a relation between special bases of the hypergeometric differential equations and all critical L-values of the corresponding modular forms (these relations include those that we observed during the proof of Theorem 2). From our present perspective of interpolations of sequences, can one similarly engage all of the critical L-values? Finally, it would be highly desirable to have a more conceptual understanding of the connection between these (and potentially other) interpolations and L-values.

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Towards a Symbolic Summation Theory for Unspecified Sequences

Peter Paule and Carsten Schneider

Abstract The article addresses the problem whether indefinite double sums involving a generic sequence can be simplified in terms of indefinite single sums. Depending on the structure of the double sum, the proposed summation machinery may provide such a simplification without exceptions. If it fails, it may suggest a more advanced simplification introducing in addition a single nested sum where the summand has to satisfy a particular constraint. More precisely, an explicitly given parameterized telescoping equation must hold. Restricting to the case that the arising unspecified sequences are specialized to the class of indefinite nested sums defined over hypergeometric, multi-basic or mixed hypergeometric products, it can be shown that this constraint is not only sufficient but also necessary.

1 Introduction

Over recent years the second named author succeeded in developing a difference field (resp. ring) theory which allows to treat within a common algorithmic framework summation problems with elements from algebraically specified domains as well as problems involving concrete sequences which are analytically specified (e.g., from quantum field theory, combinatorics, number theory, and special functions). In this article we establish a new algebraic/algorithmic connection between this setting and summation problems involving generic sequences. We feel there is a high application potential for this connection. One future domain for algorithmic discovery (as described below) might be identities involving elliptic functions and modular forms.

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In the course of a project devoted to an algorithmic revival of MacMahon's partition analysis, Andrews and Paule showed in [5] that a variant of partition analysis can be applied also for simplification of multiple combinatorial sums. Starting with the pioneering work of Abramov [3, 4], Gosper[7], Karr [8, 9], and Zeilberger [24], significant progress has been made. In particular, in the context of summation in difference fields and, more generally, difference rings [19, 21, 22] Schneider has developed substantial extensions and generalizations [15, 17, 18, 20] of Karr's seminal work. Owing to such an algorithmic machinery, the summation problems treated in [5] can nowadays be done in a jiffy with Schneider's `Sigma` package [16].

Nevertheless, the present article connects to [5] in various ways. First, it also considers a class of summation identities related to the celebrated Calkin sum which is the case $\ell = 3$ of

$$C_\ell(n) := \sum_{k=0}^{n} \left(\sum_{j=0}^{k} \binom{n}{j} \right)^{\ell}.$$

More generally, we will focus also on the truncated versions

$$C_\ell(a, n) := \sum_{k=0}^{a} \left(\sum_{j=0}^{k} \binom{n}{j} \right)^{\ell}.$$

And second, similarly to [5] presenting a "non-standard" variation of the method of partition analysis, we present "non-standard" variations of difference field summation techniques.

The first "non-standard" ingredient is the aspect of "generic" summation in difference fields and rings. First pioneering steps in this direction were made by Kauers and Schneider; see [10, 11].

To illustrate the generic aspect, consider the problem of simplifying the sums

$$C_1(a, n) = \sum_{k=0}^{a} \sum_{j=0}^{k} \binom{n}{j} \quad \text{and} \quad C_1(n) = \sum_{k=0}^{n} \sum_{j=0}^{k} \binom{n}{j}.$$

A rewriting of $C_1(a, n)$ is obtained by specializing $Y_k = 1$ and $X_j = \binom{n}{j}$ in the generic summation relation

$$\sum_{k=0}^{a} \left(\sum_{j=0}^{k} X_j \right) Y_k = \left(\sum_{k=0}^{a} Y_k \right) \left(\sum_{j=0}^{a} X_j \right) + \sum_{k=0}^{a} Y_k X_k - \sum_{k=0}^{a} X_k \left(\sum_{j=0}^{k} Y_j \right). \tag{1}$$

Pictorially, (1) corresponds to summing over a square shaped grid in two different ways; see Fig. 1.

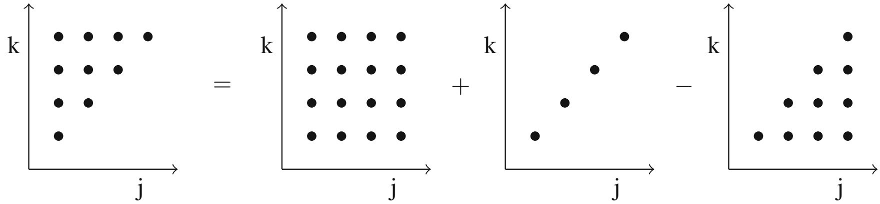

Fig. 1 Summing over a rectangular grid in two different ways

Specializing (1) as proposed results in

$$\begin{aligned} C_1(a,n) =&(a+1)\sum_{j=0}^{a}\binom{n}{j}+\sum_{k=0}^{a}\binom{n}{k}-\sum_{k=0}^{a}\binom{n}{k}(k+1)\\ =&(a+1)\sum_{k=0}^{a}\binom{n}{k}-\sum_{k=0}^{a}k\binom{n}{k}. \end{aligned}$$

This means that the application of (1) indeed results in a simplification: the original double sum is expressed in terms of single sums. Specializing $a=n$ the single sums in turn simplify further by the binomial theorem:

$$\sum_{k=0}^{n}k\binom{n}{k}=n\sum_{k=1}^{n}\binom{n-1}{k-1}=n\sum_{k=0}^{n-1}\binom{n-1}{k}=n\,2^{n-1}.$$

This yields

$$C_1(n)=C_1(n,n)=(n+1)2^n-n\,2^{n-1}=2^{n-1}(n+2).$$

We remark that the generic formula (1) can be obtained with the `Sigma` package[1]:

In[1]:= **<< Sigma.m**

Sigma - A summation package by Carsten Schneider © RISC-JKU

In[2]:= **mySum1 = SigmaSum[Y[k]SigmaSum[X[j], {j, 0, k}], {k, 0, a}]**

Out[2]= $\sum_{k=0}^{a}\Big(\sum_{j=0}^{k}\mathtt{X[j]}\Big)\mathtt{Y[k]}$

In[3]:= **res1 = SigmaReduce[mySum1, XList → {X, Y}, XWeight → {2, 1}, SimplifyByExt → MinDepth, SimpleSumRepresentation → True]**

Out[3]= $-\sum_{i=0}^{a}\Big(\sum_{j=0}^{i}\mathtt{Y[j]}\Big)\mathtt{X[i]}+\Big(\sum_{i=0}^{a}\mathtt{X[i]}\Big)\Big(\sum_{i=0}^{a}\mathtt{Y[i]}\Big)+\sum_{i=0}^{a}\mathtt{X[i]Y[i]}$

[1]Freely available with password request at http://www.risc.jku.at/research/combinat/software/Sigma/.

Remark 1.1 Applying `SigmaReduce` with the option **XList → {X, Y}** one activates the summation algorithms given in [11, 18] by telling `Sigma` that $X[j](=X_j)$ and $Y[k](=Y_k)$ are generic sequences. With the option `SimplifyByExt→MinDepth` the underlying algorithms try to simplify the sum In[2] so that the nested depth (i.e., the number of nested sum quantifiers) is minimized. Moreover, the option `SimpleSumRepresentation→True` implies that the found sum representations have only denominators, if possible, that are linear. For this particular instance, the underlying algorithm would detect that the input expression cannot be simplified further if X and Y are considered as equally complicated. However, using in addition the option **XWeight → {2, 1}** one tells `Sigma` that $X[k]$ is counted as a more nested expression than $Y[k]$. This extra information will finally produce the output given in Out[3] by introducing the sum $\sum_{i=0}^{a}\big(\sum_{j=0}^{i}Y[j]\big)X[i]$ which is considered as simpler than the sum In[2].

Next we apply the same strategy to

$$C_2(a,n)=\sum_{k=0}^{a}\left(\sum_{j=0}^{k}\binom{n}{j}\right)^2 \quad \text{and} \quad C_2(n)=\sum_{k=0}^{n}\left(\sum_{j=0}^{k}\binom{n}{j}\right)^2.$$

A generic formula for this situation is obtained from (1) by replacing Y_k with $Y_k\sum_{j=0}^{k}X_j$, and by rewriting the resulting right-hand side by using (1) together with some manipulation. Doing this by hand already becomes quite tedious; so we use `Sigma` to carry out this task automatically:

In[4]:= $\mathbf{mySum2}=\sum_{k=0}^{a}\Big(\sum_{j=0}^{k}\mathbf{X[j]}\Big)^2\mathbf{Y[k]};$

In[5]:= **res2 = SigmaReduce[mySum2, XList → {X, Y}, XWeight → {2, 1},**
SimplifyByExt → DepthNumberDegree, SimpleSumRepresentation → True]

Out[5]= $$-2\sum_{i=0}^{a}\Big(\sum_{j=0}^{i}X[j]\Big)\Big(\sum_{j=0}^{i}Y[j]\Big)X[i]+2\sum_{i=0}^{a}\Big(\sum_{j=0}^{i}X[j]\Big)X[i]Y[i] +\sum_{i=0}^{a}\Big(\sum_{j=0}^{i}Y[j]\Big)X[i]^2+\Big(\sum_{i=0}^{a}X[i]\Big)^2\Big(\sum_{i=0}^{a}Y[i]\Big)-\sum_{i=0}^{a}X[i]^2Y[i]$$

Remark 1.2 If we execute `SigmaReduce` with the same options as described in Remark 1.1, we would fail for this input sum: there is no alternative expression in terms of nested sums where the nesting depth is simpler – even with the assumption that $X[k]$ is considered as more nested than $Y[k]$.[2] However, inserting the extra option **SimplifyByExt → DepthNumberDegree** one aims at a simplification where the degree of the most complicated sum $\sum_{j=0}^{k}X[j]$ in In[4] is minimized; in addition, extra sums with lower nesting depth will be used (exploiting the fact that $Y[j]$ is less nested than $X[j]$) whenever such a degree reduction can be performed. This simplification

[2]If a simpler expression exists, `Sigma` would find it with the same options as described in Remark 1.1.

strategy can be set up by combining the enhanced telescoping algorithms from [15, Section 5] with [17] to make `Sigma` compute Out[5] as an alternative presentation of

$$\sum_{k=0}^{a} Y_k \left(\sum_{j=0}^{k} X_j\right)^2. \tag{2}$$

Specializing $Y_k = 1$ and $X_j = \binom{n}{j}$ in this generic relation Out[5] gives

$$C_2(a,n) = (a+1)\left(\sum_{k=0}^{a}\binom{n}{k}\right)^2 - 2\sum_{k=0}^{a} k\binom{n}{k}\sum_{j=0}^{k}\binom{n}{j} + \sum_{k=0}^{a} k\binom{n}{k}^2. \tag{3}$$

The specialization $a = n$ is treated algorithmically in Sect. 3.2 resulting in the presentation (35) for $C_2(n)$.

The paper is organized as follows. After introducing the basic notions and constructions for setting up summation problems in terms of generic sequences in Sect. 2, in Sect. 3 we explain the basic simplification machinery to reduce double sums to expressions in terms of single nested sums. In Sect. 4 we reformulate this simplification methodology in the setting of abstract difference rings, and in Sect. 5 we connect these ideas with the ring of sequences utilizing an advanced difference ring theory; further supporting tools and notions (like $R\Pi\Sigma$-rings) can be found in Sect. 8 of the Appendix. Putting everything together will enable us to show that the suggested simplification strategy forms a complete algorithm for inputs that are given in terms of indefinite nested sums defined over hypergeometric products, multibasic products and their mixed versions. In Sect. 6 we give further details how this simplification engine is implemented in the package `Sigma` and elaborate various concrete examples. In Sect. 7 the paper concludes by giving some pointers to future research.

2 Generic Sequences and Sums

We want to model sequences and sums generically. To this end we introduce a set X of indeterminates indexed over $\mathbb{Z}$ together with the ring of multivariate polynomials in these symbols over $\mathbb{K}$,[3]

$$X := \{X_j\}_{j\in\mathbb{Z}} \text{ and } \mathbb{K}_X := \mathbb{K}[X]. \tag{4}$$

It will be convenient to consider bilateral sequences $f : \mathbb{Z} \to \mathbb{K}_X$, $j \mapsto f(j)$. The set of bilateral sequences is denoted by $\mathbb{K}_X^{\mathbb{Z}}$. In the following we only speak about "sequences"; whether a sequence is bilateral or not will be always clear from the context.

[3] $\mathbb{K}$ is a field of characteristic 0.

Convention 2.1 We fix k as a "generic" symbol which in this article we overload with three different meanings which will be always clear from the context:

- As in Sect. 1, k can stand for an integer; i.e., $k \in \mathbb{Z}$.
- It stands for the bilateral sequence $k : \mathbb{Z} \to \mathbb{K}_X$, $j \mapsto j$.
- More generally, k stands for a generic variable, respectively index; i.e., for a sequence $P = (P(j))_{j \in \mathbb{Z}} \in \mathbb{K}_X^{\mathbb{Z}}$ we alternatively write $P(k)$ $(= P)$; see Example 2.6.

In particular, the latter meaning arises in generic sequences and sums defined in Definitions 2.2 and 2.5, respectively.

Definition 2.2 (*generic sequences*) The symbol X_k *with generic index* k and its shifted versions X_{k+l}, $l \in \mathbb{Z}$, denote bilateral sequences in $\mathbb{K}_X^{\mathbb{Z}}$ defined as $X_{k+l} : \mathbb{Z} \to \mathbb{K}_X$, $j \mapsto X_{j+l}$. The *set of all such generic sequences* is denoted by the symbol "$\{X_k\}$"; i.e., $\{X_k\} := \{X_{k+l}\}_{l \in \mathbb{Z}}$.

The ring $\mathbb{K}_X[k, \{X_k\}]$ of polynomials in k and in generic sequences from $\{X_k\}$ is a subring of the ring of sequences $\mathbb{K}_X^{\mathbb{Z}}$ with the usual (component-wise) plus and times.

Example 2.3 $P(k) = k^2 X_0 X_{k-1} X_{k+1} - k X_{-3} X_k^2 + X_3 - 2 \in \mathbb{K}_X[k, \{X_k\}]$ represents the sequence $(p(j))_{j \in \mathbb{Z}}$,

$$P(k) : \mathbb{Z} \to \mathbb{K}_X,\ j \mapsto p(j) = j^2 X_0 X_{j-1} X_{j+1} - j X_{-3} X_j^2 + X_3 - 2.$$

Lemma 2.4 *Let $P(k) \in \mathbb{K}_X[k, \{X_k\}]$ be such that*

$$P(j) = 0 \text{ for all } j \geq \mu$$

for some $\mu \in \mathbb{Z}_{\geq 0}$. Then $P(k) = 0$, the zero sequence.

Proof The statement is obvious if one views $P(k)$ as a polynomial in k over the integral domain $\mathbb{K}_X[\{X_k\}]$. □

Definition 2.5 (*generic sums*) Given $P(k) \in \mathbb{K}_X^{\mathbb{Z}}$, for $a, b \in \mathbb{Z}$ the *generic sum* $\sum_{l=a}^{k+b} P(l)$ denotes a sequence in $\mathbb{K}_X^{\mathbb{Z}}$ defined as

$$\sum_{l=a}^{k+b} P(l) : \mathbb{Z} \to \mathbb{K}_X,\ j \mapsto \begin{cases} \sum_{l=a}^{j+b} P(l), & \text{if } a \leq j + b \\ 0, & \text{otherwise.} \end{cases} \tag{5}$$

Example 2.6 For any $P(k) \in \mathbb{K}_X^{\mathbb{Z}}$ and

$$(f_P(k))_{k \in \mathbb{Z}} := \sum_{l=0}^{k} P(l) - \sum_{l=0}^{k-1} P(l)$$

one has

$$f_P(j) = \begin{cases} P(j), & \text{if } j \geq 0 \\ 0, & \text{otherwise.} \end{cases}$$

In other words, in the context of generic sequences and sums,

$$\sum_{l=0}^{k} P(l) - \sum_{l=0}^{k-1} P(l) \neq P(k). \tag{6}$$

This leads us to introducing an equivalence relation "≡" such that in situations as in Example 2.6,

$$\left[\sum_{l=0}^{k} P(l)\right] - \left[\sum_{l=0}^{k-1} P(l)\right] \equiv [P(k)], \tag{7}$$

where we write $[f]$ for the equivalence class of a sequence $f \in \mathbb{K}_X^{\mathbb{Z}}$.

Definition 2.7 For $f = (f(j))_{j\in\mathbb{Z}}, g = (g(j))_{j\in\mathbb{Z}} \in \mathbb{K}_X^{\mathbb{Z}}$ define

$$f \equiv g \;:\Leftrightarrow\; \exists\lambda \in \mathbb{Z} : f(j) = g(j) \text{ for all } j \geq \lambda.$$

Obviously this introduces an equivalence relation on $\mathbb{K}_X^{\mathbb{Z}}$. Equivalence classes are denoted by $[f]$, the set of equivalence classes by $\mathrm{Seq}(\mathbb{K}_X)$; i.e.,

$$\mathrm{Seq}(\mathbb{K}_X) = \{[f] : f \in \mathbb{K}_X^{\mathbb{Z}}\}.$$

Clearly, $\mathrm{Seq}(\mathbb{K}_X)$ forms a commutative ring with 1, which is defined by extending the usual (componentwise) sequence operations plus and times in an obvious way by $[f] + [g] := [f + g]$ and $[f][g] := [fg]$.

The shift operator

$$S : \mathrm{Seq}(\mathbb{K}_X) \to \mathrm{Seq}(\mathbb{K}_X), [f] \mapsto S[f] := [Sf] \tag{8}$$

where $Sf = (f(j+1))_{j\in\mathbb{Z}}$ if $f = (f(j))_{j\in\mathbb{Z}}$, is a ring automorphism, a property which is inherited from the shift operator on sequences from $\mathbb{K}_X^{\mathbb{Z}}$. For $f(k) = (f(j))_{j\in\mathbb{Z}} \in \mathbb{K}_X^{\mathbb{Z}}$ and $m \in \mathbb{Z}$ we often write $f(k+m)$ instead of $S^m f(k) = (f(j+m))_{j\in\mathbb{Z}}$.

Convention. If things are clear from the context, for equivalence classes from $\mathrm{Seq}(\mathbb{K}_X)$ we will simply write f instead of $[f]$. Nevertheless, we will continue to use "≡" to express equality between equivalence classes. For example, instead of (7) we write,

$$\sum_{l=0}^{k} P(l) - \sum_{l=0}^{k-1} P(l) \equiv P(k). \tag{9}$$

In the same spirit, given $f(k) \in \mathbb{K}_X^{\mathbb{Z}}$ and $m \in \mathbb{Z}$, we will write

$$f(k+m) \text{ instead of } [f(k+m)],$$

provided that the meaning $f(k+m) \in \mathrm{Seq}(\mathbb{K}_X)$ is clear from the context.

Summation methods often rely on coefficient comparison. To apply this technique one usually exploits algebraic independence; for instance, equivalence classes $[f]$ of generic sums like $f = \sum_{l=0}^{k} X_l \in \mathbb{K}_X^{\mathbb{Z}}$ are algebraically independent over $(\mathbb{K}_X[k, \{X_k\}], \equiv)$.[4] Slightly more generally, we prove the following

Lemma 2.8 *Let* $P(k) \in \mathbb{K}_X[k]\backslash\{0\}$. *Then*

$$\left[\sum_{l=0}^{k} P(l)X_l\right] \textit{ is transcendental over } (\mathbb{K}_X[k, \{X_k\}], \equiv).$$

Proof For $F(k) := \sum_{l=0}^{k} P(l)X_l \in \mathbb{K}_X^{\mathbb{Z}}$ suppose that

$$0 \equiv q_0(k) + q_1(k)F(k) + \cdots + q_d(k)F(k)^d \tag{10}$$

for polynomials $q_i(k) \in \mathbb{K}_X[k, \{X_k\}]$ with $q_d(k) \not\equiv 0$.[5] Let $d \geq 1$ be the minimal degree such that a relation like (10) holds. Denoting the sequence on the right side of (10) by $(f(j))_{j\in\mathbb{Z}}$, we have that there is a $k_0 \in \mathbb{Z}$ such that

$$f(j) = 0 \text{ for all } j \geq k_0.$$

Define

$$l_0 := \max\{l \in \mathbb{Z} : X_l \text{ divides some monomial of some } q_i(k)\},$$

and set

$$j_0 := \max\{0, k_0, l_0 + 1\}.$$

Then

$$\begin{aligned} 0 = &\text{ coefficient of } X_{j_0}^d \text{ in } f(j_0) = q_d(j_0)P(j_0)^d,\\ 0 = &\text{ coefficient of } X_{j_0}^d \text{ in } f(j_0+1) = q_d(j_0+1)P(j_0+1)^d,\\ &\text{etc.} \end{aligned}$$

Since $P(k) \in \mathbb{K}_X[k]$ has at most finitely many integer roots (if any), there is a $\mu \in \mathbb{Z}_{\geq 0}$ such that

$$q_d(j) = 0 \text{ for all } j \geq \mu.$$

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[4] The quotient ring of $\mathbb{K}_X[k, \{X_k\}]$ subject to the equivalence relation $\equiv$; this ring is a subring of $\mathrm{Seq}(\mathbb{K}_X)$.

[5] This means that $q_d(k)$ is not equivalent to the 0-sequence $(\ldots, 0, 0, 0, \ldots) \in \mathbb{K}_X^{\mathbb{Z}}$.

Consequently, $q_d(k) \equiv 0$, a contradiction to $q_d(k) \not\equiv 0$. Therefore $d = 0$, and the statement follows from Lemma 2.4. □

3 The Basic Simplification

In the following, instead of considering sums like (2), we will restrict to a slightly less general class of sums by setting $Y_j = 1$ for all $j \geq 0$, i.e., we will explore for $p = 1, 2$ the sums

$$\sum_{j=0}^{a}\left(\sum_{l=0}^{j} X_l\right)^p \tag{11}$$

involving the generic sequence X_k. Obviously, for fixed p this sum can be viewed as a sequence $s(a) = (s(a))_{a\in\mathbb{Z}} \in \mathbb{K}_X^{\mathbb{Z}}$.[6] So, more precisely, we will investigate if and how sequences from $\mathbb{K}_X^{\mathbb{Z}}$ given by such sum expressions can be simplified in terms of "simpler" generic sums.

3.1 Simplifications by Sum Extensions

We start to look at the case $p = 1$ of (11), respectively $C_1(a, n)$, by considering the following problem.

Given a generic sum $F(k) = \sum_{l=0}^{k} X_l \in \mathbb{K}_X^{\mathbb{Z}}$; *find* $G(k) \in \mathbb{K}_X^{\mathbb{Z}}$, "*as simple as possible*", such that

$$G(k+1) - G(k) \equiv F(k+1). \tag{12}$$

Trivially,

$$G(k) = \sum_{j=0}^{k} F(j) \in \mathbb{K}_X^{\mathbb{Z}} \tag{13}$$

is always a solution to (12). So the problem splits into two parts: (a) to specify a concrete meaning of "as simple as possible", and (b) to compute solutions which meet this specification.

For part (a), for the given problem we start by considering solutions of the form

$$G(k) = G_0(k) + G_1(k)F(k) \tag{14}$$

with $G_j(k) \in \mathbb{K}_X[k, \{X_k\}]$ to be determined, the latter task being part (b) of the problem.

[6] Note that $s(a) = 0$ if $a < 0$.

In practice the specifications given to settle part (a) of the problem are motivated by the context of the problem, but also driven by theory. For instance, here Lemma 2.8 implies that there is no solution $G(k) \in \mathbb{K}_X[k, \{X_k\}]$ to the telescoping equation (12). In this sense,[7] the ansatz in (14) is the best possible we can achieve.

To execute part (b) of the problem we proceed by coefficient comparison. To this end, we substitute the ansatz (14) into (12) to obtain:

$$\begin{aligned}(G_1(k+1) - G_1(k))F(k) + G_0(k+1) - G_0(k) + G_1(k+1)X_{k+1}\\ \equiv F(k) + X_{k+1}.\end{aligned} \tag{15}$$

Owing to Lemma 2.8 we can do coefficient comparison with respect to powers of $F(k)$ and obtain,

$$G_1(k+1) - G_1(k) \equiv 1.$$

It is straightforward to verify that

$$G_1(k) = k + d, \text{ with } d \in \mathbb{K}_X \text{ arbitrary},$$

describes all the solutions in $\mathbb{K}_X[k, \{X_k\}] = \mathbb{K}_X[\{X_k\}][k]$. To keep things simple we set $d = 0$, and substituting $G_1(k) = k$ into (15) yields

$$G_0(k+1) - G_0(k) \equiv -kX_{k+1}. \tag{16}$$

Using a similar idea as used in the proof of Lemma 2.8 reveals that (16) admits no solution $G_0(k) \in \mathbb{K}_X[k, \{X_k\}]$. So we are led to relax our specification of "simple" and— in view of (13)— set G_0 to the trivial solution of (16); i.e., to the generic sum

$$G_0(k) = -\sum_{j=0}^{k} jX_j + F(k) \left(\equiv -\sum_{j=0}^{k}(j-1)X_j\right).$$

Putting things together,

$$G(k) = G_0(k) + G_1(k)F(k) = -\sum_{j=0}^{k} jX_j + (k+1)F(k) \in \mathbb{K}_X^{\mathbb{Z}} \tag{17}$$

is a solution of (12).

Finally, we convert (12) into the form of a summation identity. Passing from the generic sequence variable k to concrete integers $k \in \mathbb{Z}$, using (17) we can easily verify that for all $k \geq 0$,[8]

[7]By difference ring theory (see Lemma 4.13 below) the exponent with which $F(k)$ can appear in $G(k)$ is at most 2. As it turns out, exponent 1 suffices here to obtain a solution of the desired form.

[8]Note that $F(-1) = 0$ by definition of a generic sum.

$$\begin{aligned}G(k) - G(k-1) &= -kX_k + (k+1)F(k) - kF(k-1)\\ &= -kX_k + (k+1)(F(k-1) + X_k) - kF(k-1)\\ &= X_k + F(k-1) = F(k).\end{aligned}$$

Summing this telescoping relation over k from 0 to $a \in \mathbb{Z}$, $a \geq 0$, produces[9]

$$\begin{aligned}\sum_{k=0}^{a}\sum_{j=0}^{k} X_j &= \sum_{k=0}^{a} F(k) = G(a) - G(-1) = G(a)\\ &= -\sum_{j=0}^{a} jX_j + (a+1)F(a) = -\sum_{j=0}^{a} jX_j + (a+1)\sum_{j=0}^{a} X_j.\end{aligned}$$

Finally, observe that the generic sequence X_k can be replaced by any concrete sequence $(\bar{X}_k)_{k\geq 0}$ with $\bar{X}_k \in \mathbb{K}$ yielding the identity

$$\sum_{k=0}^{a}\sum_{j=0}^{k} \bar{X}_j = -\sum_{j=0}^{a} j\bar{X}_j + (a+1)\sum_{j=0}^{a} \bar{X}_j. \tag{18}$$

With `Sigma` this can be obtained automatically. Namely, the package allows one to activate the desired mechanism by entering the sum

In[6]:= $\mathbf{mySum = \sum_{k=0}^{a}\sum_{j=0}^{k} X[j];}$

and executing the function call

In[7]:= **SigmaReduce[mySum, XList → {X}, SimpleSumRepresentation → True]**

Out[7]= $(a+1)\sum_{i=0}^{a} X_i - \sum_{i=0}^{a} iX_i.$

3.2 *Simplifications by Introducing Constraints and Sum Extensions*

Next, in view of the sum

$$\sum_{k=0}^{a} k\binom{n}{k}\sum_{j=0}^{k}\binom{n}{j},$$

arising in the presentation (3) for $C_2(a,n)$, we look at the following problem.

Given a generic sum $F(k) = k\, X_k \sum_{j=0}^{k} X_j \in \mathbb{K}_X^{\mathbb{Z}}$; *find* $G(k) \in \mathbb{K}_X^{\mathbb{Z}}$, *as simple as possible*, such that

[9]According to (17): $G(-1) = 0$.

$$G(k+1) - G(k) \equiv F(k+1). \tag{19}$$

This time we start by considering solutions of the form

$$G(k) = G_0(k) + G_1(k)S(k) + G_2(k)S(k)^2 \tag{20}$$

with $S(k) := \sum_{j=0}^{k} X_j$, and where we again try to find the coefficients $G_j(k)$ of polynomial form such that $G_j(k) \in \mathbb{K}_X[k, \{X_k\}]$.

To this end, we again proceed by coefficient comparison; i.e., we substitute the ansatz (20) into (19) to obtain:

$$\begin{aligned}(G_2(k+1) - G_2(k))\, S(k)^2 + \big(G_1(k+1) - G_1(k) + 2G_2(k+1)X_{k+1}\big)\, S(k) \quad &(21)\\ + G_0(k+1) - G_0(k) + G_1(k+1)X_{k+1} + G_2(k+1)X_{k+1}^2&\\ \equiv (k+1)X_{k+1}S(k) + (k+1)X_{k+1}^2. \quad &(22)\end{aligned}$$

Owing to Lemma 2.8 we again can do coefficient comparison. With respect to $S(k)^2$ we obtain,

$$G_2(k+1) - G_2(k) \equiv 0. \tag{23}$$

This has $G_2(k) = c$, $c \in \mathbb{K}_X$ arbitrary, as the general solution in $\mathbb{K}_X[k, \{X_k\}] = \mathbb{K}_X[\{X_k\}][k]$.

Coefficient comparison with respect to $S(k)$ in (21) gives

$$G_1(k+1) - G_1(k) \equiv (k+1-2c)X_{k+1}. \tag{24}$$

In order to proceed, we suppose that the generic sequence $Y_k \in \mathbb{K}_X^{\mathbb{Z}}$ is a solution to (24) and set $G_1(k) := Y_k$.

Finally, coefficient comparison with respect to $S(k)^0$ in (21) gives

$$G_0(k+1) - G_0(k) \equiv (k+1-c)X_{k+1}^2 - Y_{k+1}X_{k+1}. \tag{25}$$

Similarly to the situation in Eq. (16) we relax our specification of "simple" and set G_0 to the trivial solution of (25); i.e., to the generic sum

$$G_0(k) = \sum_{j=0}^{k} (j-c)X_j^2 - \sum_{j=0}^{k} X_j Y_j.$$

Combining all these ingredients yields the solution

$$G(k) = c\,\Big(\sum_{j=0}^{k} X_j\Big)^2 + Y_k \sum_{j=0}^{k} X_j + \sum_{j=0}^{k}(-cX_j^2 + jX_j^2 - X_jY_j) \in \mathbb{K}_X^{\mathbb{Z}}, \tag{26}$$

under the assumption that

$$Y_k \in \mathbb{K}_X^{\mathbb{Z}} \text{ and } c \in \mathbb{K}_X \text{ are chosen so that (24) holds.} \tag{27}$$

Finally, as in Sect. 3.1 we convert (19) into a summation identity. Passing from the generic sequence variable k to concrete integers $k \in \mathbb{Z}$, using (26) we can easily verify that telescoping yields for all integers $a \geq 0$,

$$\sum_{k=0}^{a} k\, X_k \sum_{j=0}^{k} X_j = c\,\Big(\sum_{j=0}^{a} X_j\Big)^2 - c\sum_{j=0}^{a} X_j^2 - \sum_{j=0}^{a} X_j Y_j + Y_a \sum_{j=0}^{a} X_j + \sum_{j=0}^{a} j X_j^2 \tag{28}$$

under the constraint that the sequence values $Y_k \in \mathbb{K}_X$ and $c \in \mathbb{K}_X$ are chosen such

$$Y_{k+1} - Y_k = (k + 1 - 2c)X_{k+1} \text{ for all } k \geq 0. \tag{29}$$

Using Sigma this solution strategy can be automatically applied to the sum

In[8]:= $\mathbf{mySum} = \sum_{\mathbf{k=0}}^{\mathbf{a}} \mathbf{k\,X[k]} \sum_{\mathbf{j=0}}^{\mathbf{k}} \mathbf{X[j]};$

with the procedure call[10]

In[9]:= **{closedForm, constraint} = SigmaReduce[mySum, XList → {X}, ExtractConstraints → {Y}, SimpleSumRepresentation → False, RefinedForwardShift → False]**

Out[9]= $\{c\,(\sum_{i=0}^{a} X[i])^2 + Y[a] \sum_{i=0}^{a} X[i] + \sum_{i=0}^{a} (-c X[i]^2 + i X[i]^2 - X[i] Y[i]),$
$\{Y[a+1] - Y[a] = (1+a) X[a+1] - 2\,c\,X[a+1]\}\}$

This yields the identity (26) with the constraint (29).

To produce the output in exactly the same form as in identity (28), one can use the option `SimpleSumRepresentation→True` to the derived result:

In[10]:= **SigmaReduce[closedForm, a, XList → {X, Y}, SimpleSumRepresentation → True]**

Out[10]= $c(\sum_{i=0}^{a} X[i])^2 - c \sum_{i=0}^{a} X[i]^2 - \sum_{i=0}^{a} X[i] Y[i] + (\sum_{i=0}^{a} X[i]) Y[a] + \sum_{i=0}^{a} i X[i]^2$

Further details on the calculation steps in the setting of difference rings will be given in Sect. 6.1.

As a consequence, one can now fabricate specialized identities with the following strategy. Choose a concrete sequence $\bar{X}_k \in \mathbb{K}$ such that one finds a "nice" solution $\bar{Y}_k \in \mathbb{K}$ and $c \in \mathbb{K}$ for

[10] By using the option `RefinedForwardShift→False`, Sigma follows the calculation steps carried out above. Without this option a more complicated (but more efficient) strategy is used that produces a slight variation of the output.

$$\bar{Y}_{k+1} - \bar{Y}_k = (1+k)\bar{X}_{k+1} - c\,2\bar{X}_{k+1}. \tag{30}$$

This will yield the specialized identity

$$\sum_{k=0}^{a} k\,\bar{X}_k \sum_{j=0}^{k} \bar{X}_j = c\,\Big(\sum_{j=0}^{a} \bar{X}_j\Big)^2 - c\sum_{j=0}^{a} \bar{X}_j^2 - \sum_{j=0}^{a} \bar{X}_j\bar{Y}_j + \bar{Y}_a \sum_{j=0}^{a} \bar{X}_j + \sum_{j=0}^{a} j\bar{X}_j^2. \tag{31}$$

Example 3.1 Taking $\bar{X}_k = \binom{n}{k}$ in (31) leads to solving

$$\bar{Y}_{k+1} - \bar{Y}_k = (k+1-2c)\binom{n}{k+1} \text{ for all } k \geq 0 \tag{32}$$

which can be done by `Sigma` as follows:

In[11]:= **ParameterizedTelescoping[{(k + 1)SigmaBinomial[n, k + 1], −2SigmaBinomial[n, k + 1]}, k]**

Out[11]= $\{\{1, \frac{n}{4}, -\frac{1}{2}(k+1)\binom{n}{k+1}\}\}$

The output Out[11] means that as a solution to (32) we have

$$\bar{Y}_k = -\frac{1}{2}(k+1)\binom{n}{k+1} = -\frac{1}{2}\binom{n}{k}(n-k) \text{ and } c = \frac{n}{4}.$$

Remark. Alternatively, one can use the RISC package `fastZeil` [13] by

In[12]:= **<< RISC‘fastZeil‘**

Fast Zeilberger Package version 3.61 written by Peter Paule, Markus Schorn, and Axel Riese ©RISC-JKU

In[13]:= **Gosper[Binomial[n, k + 1], k, 1]**

Out[13]= $(-2-2k+n)\text{Binomial}[n,1+k] == \Delta_k[(1+k)\text{Binomial}[n,1+k]]$

In[13] calls an extended version of Gosper's algorithm. In the given example the last entry "1" asks the procedure to compute - in case it exists - a polynomial $p_1(n)k + p_0(n)$ of order 1 in k such that the polynomial times the summand $\binom{n}{k+1}$ telescopes. In Out[13] this polynomial is determined to be $(-2)k + n - 2$; $(\Delta_k f)(k) = f(k+1) - f(k)$ is the forward difference operator.

This turns (31) into

$$\sum_{k=0}^{a} k\binom{n}{k}\sum_{j=0}^{k}\binom{n}{j} = \frac{n}{4}\Big(\sum_{j=0}^{a}\binom{n}{j}\Big)^2 + \frac{n}{4}\sum_{j=0}^{a}\binom{n}{j}^2 + \frac{1}{2}\sum_{j=0}^{a} j\binom{n}{j}^2 - \frac{n-a}{2}\binom{n}{a}\sum_{j=0}^{a}\binom{n}{j}. \tag{33}$$

For $a = n$ we have, using $\sum_{j=0}^{m}\binom{a}{j}\binom{b}{m-j} = \binom{a+b}{m}$ and $\binom{n}{j} = \frac{n}{j}\binom{n-1}{j-1} = \frac{n}{j}\binom{n-1}{n-j}$,

$$\sum_{k=0}^{n} k\binom{n}{k}\sum_{j=0}^{k}\binom{n}{j} = \frac{n}{4}\,2^{2n} + \frac{n}{4}\binom{2n}{n} + \frac{n}{2}\binom{2n-1}{n} = n\,4^{n-1} + n\binom{2n-1}{n}.$$

Finally, substituting (33) into Eq. (3) yields,

$$C_2(a,n) = \Big(a + 1 - \frac{n}{2}\Big)\left(\sum_{j=0}^{a}\binom{n}{j}\right)^2 - \frac{n}{2}\sum_{j=0}^{a}\binom{n}{j}^2 + (n-a)\binom{n}{a}\sum_{j=0}^{a}\binom{n}{j}. \tag{34}$$

Similarly to before, for $a = n$ this simplifies to

$$C_2(n) = C_2(n,n) = \Big(\frac{n}{2} + 1\Big)\,2^{2n} - \frac{n}{2}\binom{2n}{n} = (n+2)2^{2n-1} - n\binom{2n-1}{n}. \tag{35}$$

Example 3.2 Taking $\bar{X}_k = H_k := \sum_{i=1}^{k}\frac{1}{i}$ in (31) leads to solving

$$\bar{Y}_{k+1} - \bar{Y}_k = (k+1-2c)H_{k+1} \text{ for all } k \geq 0.$$

The solution

$$\bar{Y}_k = \frac{1}{4}\big(-k^2 + 2k(k+1)H_k + k - 5\big) \text{ and } c = 0$$

turns (31) into

$$\begin{aligned}\sum_{k=0}^{a} k\,H_k\sum_{j=0}^{k} H_j =& \frac{1}{4}\big(-5 + a - a^2 + 2a(a+1)H_a\big)\sum_{j=0}^{a} H_j + \sum_{j=0}^{a} j\,H_j^2\\ &- \sum_{j=0}^{a}\frac{1}{4}\big(-5 + j - j^2 + 2j(1+j)H_j\big)H_j\\ &\overset{\texttt{Sigma}}{=} -\tfrac{(2a+1)(5a^2+5a-6)}{18}H_a + \tfrac{a(20a^2+3a-59)}{108} + \tfrac{a(a+1)(a+2)}{3}H_a^2.\end{aligned}$$

The second equality is obtained by applying `SigmaReduce` to the specialized expression. Here the underlying difference ring theory [22] is utilized in order to return an expression in terms of sums which are algebraically independent among each other.

Example 3.3 Taking $\bar{X}_k = \binom{n}{k}^2$ in (31) leads to solving

$$\bar{Y}_{k+1} - \bar{Y}_k = (k+1-2c)\binom{n}{k+1}^2 \text{ for all } k \geq 0.$$

The solution

$$\bar{Y}_k = -\frac{(n-k)^2}{2n}\binom{n}{k}^2 \text{ and } c = \frac{n}{4}$$

turns (31) into

$$\begin{aligned}\sum_{k=0}^{a} k\binom{n}{k}^2 \sum_{j=0}^{k}\binom{n}{j}^2 &= -\frac{\binom{n}{a}^2}{n}\frac{1}{2}(-a+n)^2\sum_{j=0}^{a}\binom{n}{j}^2 + \frac{1}{4}n\Big(\sum_{j=0}^{a}\binom{n}{j}^2\Big)^2\\ &\quad -\frac{1}{4}n\sum_{j=0}^{a}\binom{n}{j}^4 + \sum_{j=0}^{a} j\binom{n}{j}^4 - \sum_{j=0}^{a} -\frac{\binom{n}{j}^4(-j+n)^2}{2n}\\ &\overset{\texttt{Sigma}}{=} \frac{-a^2+2an-n^2}{2n}\binom{n}{a}^2\sum_{i=0}^{a}\binom{n}{i}^2\\ &\quad + \frac{1}{2n}\sum_{i=0}^{a} i^2\binom{n}{i}^4 + \frac{n}{4}\Big(\sum_{i=0}^{a}\binom{n}{i}^2\Big)^2 + \frac{n}{4}\sum_{i=0}^{a}\binom{n}{i}^4\end{aligned}$$

which holds for all $a, n \in \mathbb{Z}_{\geq 0}$ with $n \neq 0$.

4 A Reformulation in Abstract Difference Rings

In the following we plan to gain more insight into when the double sums under consideration can be simplified to single sums. So far, we showed that the double sum on the left-hand side of (31) in terms of a sequence $(\bar{X}_k)_{k\geq 0}$ with $\bar{X}_k \in \mathbb{K}$ can be simplified to the right-hand side of (31) in terms of single nested sums provided that for $c \in \mathbb{K}$ and $\bar{Y}_k \in \mathbb{K}$ the parameterized telescoping equation (30) holds. In the following we will show that for certain classes of sequences $\bar{X}_k$ and $\bar{Y}_k$ the constraint (30) is not only sufficient but also necessary; see Theorem 5.7 below. In order to accomplish this task, we will utilize new results of difference ring theory [12, 19, 21, 22]; compare also [23]. To warm up, we first rephrase the constructions of the previous sections in the difference ring setting.

Definition 4.1 A *difference ring (resp. field)* $(\mathbb{A}, \sigma)$ is a ring (resp. field) $\mathbb{A}$ equipped with a ring (resp. field) automorphism $\sigma : \mathbb{A} \to \mathbb{A}$.

In fact, in Sect. 2 we introduced the difference ring $(\text{Seq}(\mathbb{K}_X), S)$ where $\text{Seq}(\mathbb{K}_X)$ is the ring of (equivalent) sequences equipped with the ring automorphism defined in (8). In addition, we considered the subring $\mathbb{A}_1 := (\mathbb{K}_X[k, \{X_k\}], \equiv)$ of $\text{Seq}(\mathbb{K}_X)$. Since $\mathbb{A}_1$ is closed under S, the restricted version of S to $\mathbb{A}_1$ forms a ring automorphism. In short, we obtain the difference ring $(\mathbb{A}_1, S)$ which is a subdifference ring of $(\text{Seq}(\mathbb{K}_X), S)$.

Definition 4.2 A difference ring $(\mathbb{A}', \sigma')$ is called a *subdifference ring* of $(\mathbb{A}, \sigma)$ if $\mathbb{A}'$ is a subring of $\mathbb{A}$ and $\sigma'(a) = \sigma(a)$ for all $a \in \mathbb{A}'$. Conversely, $(\mathbb{A}, \sigma)$ is called a *difference ring extension* of $(\mathbb{A}', \sigma')$. Since σ' agrees with σ on $\mathbb{A}'$, we usually do not distinguish anymore between them.

Further, by Lemma 2.8 the sequence $\sum_{l=0}^{k} X_l \in \mathrm{Seq}(\mathbb{K}_X)$ is transcendental over $\mathbb{A}_1$. Thus the smallest subring of $\mathrm{Seq}(\mathbb{K}_X)$ that contains $\mathbb{A}_1$ and $\sum_{l=0}^{k} X_l$ forms a polynomial ring which we denote by

$$\mathbb{A}_2 := \mathbb{K}_X[k, \{X_k\}]\left[\sum_{l=0}^{k} X_l\right]. \tag{36}$$

Then using the fact that

$$S\sum_{l=0}^{k} X_l \equiv \sum_{l=0}^{k+1} X_l \equiv \sum_{l=0}^{k} X_l + X_{l+1} \tag{37}$$

holds with $X_{l+1} \in \mathbb{K}_X[k, \{X_k\}]$ it follows that $\mathbb{A}_2$ is closed under S and thus $(\mathbb{A}_2, S)$ is a subdifference ring of $(\mathrm{Seq}(\mathbb{K}_X), S)$. Summarizing, we obtain the following chain of difference ring extensions:

$$(\mathbb{K}_X, S) \leq (\mathbb{A}_1, S) \leq (\mathbb{A}_2, S) \leq (\mathrm{Seq}(\mathbb{K}_X), S)$$

where $(\mathbb{K}_X, S)$ is the trivial difference ring with $S(f) \equiv f$ for all $f \in \mathbb{K}_X$, i.e., the elements in $\mathbb{K}_X$ are precisely the constant sequences.

In the light of these constructions, we can reformulate the problem in Sect. 3.2 within the difference ring $(\mathbb{A}_2, S)$ as follows: Given the sequence $F(k) = k\, X_k \sum_{j=0}^{k} X_j \in \mathbb{A}_2$, find a sequence $G(k) \in \mathbb{A}_2$ or in a suitable subring of $\mathrm{Seq}(\mathbb{K}_X)$ such that

$$G(k+1) - G(k) \equiv F(k).$$

Here we found out that we can choose (26) with $Y_k \in \mathrm{Seq}(\mathbb{K}_X)$ and $c \in \mathbb{K}_X$ which satisfies the constraint (27). Thus specializing X_k to concrete sequences $(\bar{X}_k)_{k\geq 0}$ with $\bar{X}_k \in \mathbb{K}$ such that there is a nice sequence $(\bar{Y}_k)_{k\geq 0}$ with $\bar{Y}_k \in \mathbb{K}$ that satisfies property (30) for some $c \in \mathbb{K}$ will lead to the simplification (31).

In the following we denote by $\mathrm{Seq}(\mathbb{K})$ the subset of all sequences of $\mathrm{Seq}(\mathbb{K}_X)$ whose entries are from $\mathbb{K}$. Then it follows that $\mathrm{Seq}(\mathbb{K})$ is a subring of $\mathrm{Seq}(\mathbb{K}_X)$ and that $S : \mathrm{Seq}(\mathbb{K}_X) \to \mathrm{Seq}(\mathbb{K}_X)$ restricted to $\mathrm{Seq}(\mathbb{K})$ forms a ring automorphism. Thus $(\mathrm{Seq}(\mathbb{K}), S)$ forms a subdifference ring of $(\mathrm{Seq}(\mathbb{K}_X), S)$. Sometimes $(\mathrm{Seq}(\mathbb{K}), S)$ is also called the *difference ring of sequences*.

Remark 4.3 Usually, the difference ring $(\mathrm{Seq}(\mathbb{K}), S)$ is defined by starting with the commutative ring $\mathbb{K}^{\mathbb{Z}_{\geq 0}}$ with 1 and defining the equivalence relation

$$f \equiv g \;:\Leftrightarrow\; \exists \lambda \in \mathbb{Z}_{\geq 0} : f(j) = g(j) \text{ for all } j \geq \lambda$$

for $f=(f(j))_{j\geq 0}, g=(g(j))_{j\geq 0}\in\mathbb{K}^{\mathbb{Z}_{\geq 0}}$; compare [14]. It is easily seen that the set of equivalence classes $[f]$ with $f\in\mathbb{K}^{\mathbb{Z}_{\geq 0}}$ forms a commutative ring with 1 which is isomorphic to $\mathrm{Seq}(\mathbb{K})$. In a nutshell, we can either choose $(a_n)_{n\in\mathbb{Z}_{\geq 0}}$ or $(a_n)_{n\in\mathbb{Z}}$ in order to describe the equivalence classes of $\mathrm{Seq}(\mathbb{K})$.

Subsequently, we will pursue a more general and ambitious goal. Namely, we will show that our new method produces constraints given in terms of parameterized telescoping equations that provide not only sufficient but also necessary conditions in order to simplify a nested sum in terms of generic sequences to an expression in terms of single nested sums over the given summand objects. In order to derive this extra insight, we will consider not an arbitrary specialization of X_k, Y_k to general sequences $(\bar{X}_k)_{k\geq 0}, (\bar{Y}_k)_{k\geq 0}\in\mathrm{Seq}(\mathbb{K})$ but only to those sequences that can be generated by expressions in terms of indefinite nested sums defined over products. Typical examples are, e.g., the left- and right-hand sides of (33), and (34); for a more precise definition we refer to Definition 5.3 below. With this restriction, we will then utilize Schneider's newly established difference ring results [12, 19, 21, 22] to show that (31) is the only possible simplification of a double sum in terms of single sums.

In Schneider's difference ring approach sequences are represented by elements from a ring $\mathbb{A}$ which is given either by certain rational function field extensions, polynomial ring extensions or by polynomial ring extensions factored out by certain ideals. In addition, a so-called evaluation function $\mathrm{ev}:\mathbb{A}\times\mathbb{Z}_{\geq 0}\to\mathbb{K}$ accompanies this ring construction that links the generators (variables) of the ring to the sequence interpretation. We will not give a full account on all the construction aspects [21, 22], but will emphasize only the key steps that are relevant for our considerations below. Further details can be found in the Appendix 8 below.

Example 4.4 Consider the rational function field $\mathbb{A}=\mathbb{K}(k)$ in the variable k. Then we define the *evaluation function* $\mathrm{ev}:\mathbb{A}\times\mathbb{Z}_{\geq 0}\to\mathbb{K}$ by

$$\mathrm{ev}(\tfrac{p}{q},i)=\begin{cases}0 & \text{if } q(i)=0\\ \frac{p(i)}{q(i)} & \text{if } q(i)\neq 0;\end{cases} \tag{38}$$

where $p,q\in\mathbb{K}[k]$ are polynomials with $q\neq 0$; here $p(i), q(i)$ are the usual evaluations of polynomials at $i\in\mathbb{Z}_{\geq 0}$. Note that here we introduce yet another meaning of k, different from those introduced in Convention 2.1: k is an algebraic variable (indeterminate) that produces the rational function field $\mathbb{K}(k)$. E.g., $f=1+k+k^2$ in this context is considered as a polynomial in the variable k with integer coefficients and $s=(\mathrm{ev}(f,i))_{i\geq 0}\in\mathrm{Seq}(\mathbb{K})$ provides us with the corresponding sequence interpretation. With our earlier notations from Convention 2.1 we could simply write $P(k)=1+k+k^2$ to abbreviate the same sequence s.

Besides such a ring $\mathbb{A}$, also a ring automorphism $\sigma:\mathbb{A}\to\mathbb{A}$ is introduced which scopes the shift behavior accordingly: for any $x\in\mathbb{A}$ we will take care that

$$(\mathrm{ev}(\sigma(x),i))_{i\geq 0}\equiv(\mathrm{ev}(x,i+1))_{i\geq 0}=(\mathrm{ev}(x,i))_{i\geq 1} \tag{39}$$

holds. In addition, the construction is carried out so that the *set of constants*[11]

$$\mathrm{const}(\mathbb{A},\sigma)=\{c\in\mathbb{A}|\,\sigma(c)=c\}$$

of the difference ring $(\mathbb{A},\sigma)$ equals precisely the field $\mathbb{K}$ in which the sequences are evaluated. All these properties hold, for instance, for the ground field $\mathbb{A}=\mathbb{K}(k)$ given in Example 4.4.

Example 4.5 Consider for instance the sequence $(\bar{X}_i)_{i\geq 0}$ with $\bar{X}_0=0$ and $\bar{X}_i=\frac{1}{i}$ for $i\geq 1$. Then we can choose the rational function $x:=\frac{1}{k}\in\mathbb{A}$. In particular, we get (39). Further, we have $\mathbb{K}=\mathrm{const}(\mathbb{K}(k),\sigma)$.

In the following we will reconsider the calculation steps of Sect. 3 within such abstract difference rings. In this context we will consider X_k not as a generic sequence, but as a sequence $(\bar{X}_i)_{i\geq 0}\in\mathrm{Seq}(\mathbb{K})$ which can be modeled by an element $x\in\mathbb{A}$ of a given difference ring $(\mathbb{A},\sigma)$ with $\mathbb{K}=\mathrm{const}(\mathbb{A},\sigma)$.

Definition 4.6 Let $(\mathbb{A},\sigma)$ be a difference ring with constant field $\mathbb{K}$ and equipped with an *evaluation function* ev satisfying (39). We say that a *sequence* $\bar{X}_k\in\mathbb{K}$ *is modeled by* $x\in\mathbb{A}$ if $\bar{X}_k=\mathrm{ev}(x,k)$ for all k from a certain point on.

In particular, $\bar{X}_{k+i}$ with $i\in\mathbb{Z}$ is then modeled by $\sigma^i(x)\in\mathbb{A}$. What we understand by "modeled by" has been illustrated also in the Example 4.5.

Remark 4.7 Note that the generic aspect is moved from a generic sequence X_k to a "generic" difference ring $(\mathbb{A},\sigma)$ and choosing an $x\in\mathbb{A}$ from this ring $\mathbb{A}$. This change of paradigm will be very useful in Sect. 5 in order to show that the found simplifications are optimal in the sequence world.

Next we explain how to adjoin the formal sum[12]

$$\sum_{i=0}^{k}\bar{X}_i \tag{40}$$

to such an arbitrary ring $\mathbb{A}$ with the shift behavior

$$\sum_{i=0}^{k+1}\bar{X}_i\equiv\sum_{i=0}^{k}\bar{X}_i+\bar{X}_{k+1}. \tag{41}$$

To this end, we introduce a new variable s being transcendental over $\mathbb{A}$ and consider the polynomial ring $\mathbb{A}[s]$. More precisely, using the fixed element $x\in\mathbb{A}$, we define

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[11]Note that $\mathrm{const}(\mathbb{A},\sigma)$ in general is a subring of $\mathbb{A}$.

[12]Note that $\mathbb{K}\subseteq\mathbb{K}_X$ and thus the evaluation of a sum has been defined already in (5).

$$\operatorname{ev}(s,i) := \sum_{j=1}^{i} \operatorname{ev}(x,j) = \sum_{j=1}^{i} \bar{X}_j \tag{42}$$

in order to give s the sequence meaning of our sum (40). More precisely, we extend this definition of s to $\mathbb{A}[s]$ by

$$\operatorname{ev}\left(\sum_{l=0}^{d} f_l\, s^l, i\right) = \sum_{l=0}^{d} \operatorname{ev}(f_l, i)\operatorname{ev}(s,i)^l \tag{43}$$

for any polynomial $\sum_{l=0}^{d} f_l\, s^l \in \mathbb{A}[s]$ with $f_l \in \mathbb{A}$.

Finally, we extend also the automorphism $\sigma : \mathbb{A} \to \mathbb{A}$ to $\sigma' : \mathbb{A}[s] \to \mathbb{A}[s]$ with $\sigma'(h) = \sigma(h)$ for all $h \in \mathbb{A}$ and

$$\sigma'(s) = s + \sigma(x). \tag{44}$$

Note that to define the shift operator, we again used the fixed element $x \in \mathbb{A}$. More precisely, there is exactly one such automorphism where for $f = \sum_{l=0}^{d} f_l\, s^l$ we obtain the map

$$\sigma'(f) = \sum_{l=0}^{d} \sigma(f_l)(s + \sigma(x))^l;$$

since σ and σ' agree on $\mathbb{A}$, we do not distinguish them anymore. In particular, by our construction it follows that

$$(\operatorname{ev}(\sigma(f), i))_{i\geq 0} \equiv (\operatorname{ev}(f, i+1))_{i\geq 0} = (\operatorname{ev}(f, i))_{i\geq 1}$$

for all $f \in \mathbb{A}[s]$.

Summarizing, we constructed a difference ring extension $(\mathbb{A}[s], \sigma)$ of $(\mathbb{A}, \sigma)$ where s models the sum (40): ev provides the sequence representation and σ describes the corresponding shift behavior.

Note that this abstract construction can be turned to concrete applications.

Example 4.8 We specialize $(\mathbb{A}, \sigma)$ to $\mathbb{A} = \mathbb{K}(k)$ and $\sigma(k) = k + 1$. Starting with this ring, we want to model the harmonic numbers $H_k = \sum_{i=1}^{k} \bar{X}_i$ with $\bar{X}_i = \frac{1}{i}$. Thus we set $x := \frac{1}{k}$ and follow the above construction, i.e., we take the difference ring extension $(\mathbb{A}[s], \sigma)$ of $(\mathbb{A}, \sigma)$ with s being transcendental over $\mathbb{A}$ and with $\sigma(s) = s + \beta$ where $\beta := \sigma(x) = \frac{1}{k+1}$. Further, we extend ev from $\mathbb{A}$ to $\mathbb{A}[s]$ by (42) and (43). For $f = k\, s$ this yields, e.g., $\operatorname{ev}(f, i) = i\, H_i$ for $i \geq 0$. Moreover, we obtain $\operatorname{ev}(\sigma(f), i) = \operatorname{ev}((i+1)H_{i+1}, i) = \operatorname{ev}(i\, H_i, i+1)$ for all $i \geq 0$. In a nutshell, we have rephrased the sequence of harmonic numbers H_k by s in $\mathbb{A}[s]$ where ev provides the sequence representation and σ describes the corresponding shift behavior.

We emphasize that this elementary construction is still too naive for our subsequent considerations. Namely, a key feature will be that

$$\mathrm{const}(\mathbb{A}[s], \sigma) = \mathrm{const}(\mathbb{A}, \sigma) \tag{45}$$

holds. Together with our earlier assumption that $\mathrm{const}(\mathbb{A}, \sigma) = \mathbb{K}$ holds, this will imply that in $(\mathbb{A}[s], \sigma)$ the set of constants is precisely $\mathbb{K}$. We install this special construction in the form of a definition.

Definition 4.9 Let $(\mathbb{A}[s], \sigma)$ be a difference ring extension of $(\mathbb{A}, \sigma)$ with s being transcendental over $\mathbb{A}$ and $\sigma(s) = s + \beta$ for some $\beta \in \mathbb{A}$. Then this extension is called a *Σ-extension* if (45) holds.

In the following we will rely heavily on the following result [21, Thm. 2.12]; for the field version see [8].

Theorem 4.10 *Let $(\mathbb{A}, \sigma)$ be a difference ring with constant field $\mathbb{K}$ and let $(\mathbb{A}[s], \sigma)$ be a difference ring extension of $(\mathbb{A}, \sigma)$ with s being transcendental over $\mathbb{A}$ and with $\sigma(s) = s + \beta$ where $\beta \in \mathbb{A}$. Then this is a Σ-extension (i.e.,* $\mathrm{const}(\mathbb{A}[s], \sigma) = \mathrm{const}(\mathbb{A}, \sigma)$*) iff there is no $g \in \mathbb{A}$ with $\sigma(g) = g + \beta$.*

Remark 4.11 Consider the difference ring extension $(\mathbb{A}_2, S)$ of $(\mathbb{A}_1, S)$ with (36) and (37). By Lemma 2.8 $\mathbb{A}_2$ is a polynomial ring over the coefficient domain $\mathbb{A}_1$. One can show that $\mathrm{const}(\mathbb{A}_2, S) = \mathrm{const}(\mathbb{A}_1, S) = \mathbb{K}_X$ which implies that $(\mathbb{A}_2, S)$ is a Σ-extension of $(\mathbb{A}_1, S)$. By Theorem 4.10[13] this implies that the generic sum $\sum_{i=0}^{k} X_k$ cannot be simplified via telescoping in the difference ring $(\mathbb{A}_1, S)$. However, specializing X_k to a particular sequence $(\bar{X}_k)_{k\geq 0}$, the situation might be different.

Let us turn back to our generic construction: we are given an arbitrary difference ring $(\mathbb{A}, \sigma)$ in which we choose $x \in \mathbb{A}$ which models the desired sequence $\bar{X}_k$. Suppose that there exists[14] a $g \in \mathbb{A}$ such that $\sigma(g) = g + \sigma(x)$ holds. In this case one can model the sum (40) having the shift-behavior as in (41) by g with $\sigma(g) = g + \beta$. In other words, the double sum on the left-hand side of (18) turns into a single sum in $(\mathbb{A}, \sigma)$. In the following we will ignore this degenerated case and assume that such a g does not exist.

More precisely, we suppose that we are given a difference ring $(\mathbb{A}, \sigma)$ with constant field $\mathbb{K}$ with the following properties:

1. $\mathrm{const}(\mathbb{A}, \sigma) = \mathbb{K}$;
2. there is a $k \in \mathbb{A}$ with $\sigma(k) = k + 1$;
3. the sequence $\bar{X}_k \in \mathbb{K}$ for $k \geq 0$ can be modeled by an $x \in \mathbb{A}$;
4. there is no $g \in \mathbb{A}$ with $\sigma(g) = g + \sigma(x)$, i.e., we cannot represent the sum (40) in $(\mathbb{A}, \sigma)$.

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[13] In the theorem we require that the set of constants form a field. However, if $\mathrm{const}(\mathbb{A}[s], \sigma) = \mathrm{const}(\mathbb{A}, \sigma)$, to prove the non-existence of a telescoping solution one does not need to assume that $\mathrm{const}(\mathbb{A}, \sigma)$ is a field.

[14] In `Sigma` the existence can be decided constructively by efficient telescoping algorithms [17, 20] provided that $(\mathbb{A}, \sigma)$ is a simple $R\Pi\Sigma$-ring; see Appendix 8.

The third assumption together with Theorem 4.10 implies that one can construct the Σ-extension $(\mathbb{A}[s], \sigma)$ of $(\mathbb{A}, \sigma)$ with $\sigma(s) = s + \sigma(x)$. This means that $\mathbb{A}[s]$ is a polynomial ring and $\text{const}(\mathbb{A}[s], \sigma) = \mathbb{K}$.

Example 4.12 Consider our concrete difference ring extension $(\mathbb{A}[s], \sigma)$ of $(\mathbb{A}, \sigma)$ from Example 4.5 with $\mathbb{A} = \mathbb{K}(k)$ and $\sigma(s) = s + \beta$ with $\beta = \frac{1}{k+1}$. Using `Sigma` (or, e.g., Abramov's or Gosper's algorithms [3, 7, 13]), one can verify that there is no $g \in \mathbb{K}(k)$ with $\sigma(g) = g + \beta$. Hence by Theorem 4.10 our extension is a Σ-extension.

Within such a difference ring setting the telescoping problem in Sect. 3.2 can be rephrased as follows.

Given $(\mathbb{A}[s], \sigma)$ with the properties (1)–(4) from above and $f = k\,x\,s \in \mathbb{A}[s]$.
Find a $g \in \mathbb{A}[s]$ such that

$$\sigma(g) - g = \sigma(f) \tag{46}$$

holds (note: $\sigma(f) = (k+1)\sigma(x)(s + \sigma(x))$).

Now we repeat the calculation steps of Sect. 3.2 within this (more abstract) difference ring exploiting the following extra insight [21, Lemma 7.2].

Lemma 4.13 *Let* $(\mathbb{A}[s], \sigma)$ *be a* Σ*-extension of* $(\mathbb{A}, \sigma)$ *and* $f, g \in \mathbb{A}[s]$ *with* $\sigma(g) - g = f$. *Then* $\deg(g) \leq \deg(f) + 1$.

Thus any solution $g \in \mathbb{A}[s]$ of (46) must have the form

$$g = g_0 + g_1\,s + g_2\,s^2;$$

compare (14). Plugging g into (46) we get

$$\sigma(g_2)(s+\sigma(x))^2 + \sigma(g_1\,s + g_0) - \big[g_2\,s^2 + g_1\,s + g_0\big] = (k+1)\,\sigma(x)(s + \sigma(x)).$$

The polynomials on the left- and right-hand sides agree if they agree coefficient-wise. Thus comparing coefficients with respect to s^2, it follows that $\sigma(g_2) = g_2$ which implies that $g_2 \in \mathbb{K}$. Thus we take an undetermined parameter $c \in \mathbb{K}$ and set $g_2 := c$. Using this information we get

$$\begin{aligned}\big[\sigma(g_1)(s+\sigma(x)) + \sigma(g_0)\big] - \big[g_1\,s + g_0\big]& \\ = (k+1)\sigma(x)(s+\sigma(x)) + c\big[&-\sigma(x)^2 - 2\sigma(x)\,s\big].\end{aligned} \tag{47}$$

Again by coefficient comparison with respect to s we obtain the constraint

$$\sigma(g_1) - g_1 = (1 + k - 2c)\sigma(x); \tag{48}$$

compare with (24). Now suppose we find a $c \in \mathbb{K}$ and a $y \in \mathbb{A}$ such that

$$\sigma(y) - y = (1 + k)\sigma(x) - 2\,c\sigma(x) \tag{49}$$

holds. Consequently, we get the general solution $g_1 = y + d$ of (48) for some undetermined constant $d \in \mathbb{K}$. Plugging the solution into (47) yields

$$\sigma(g_0) - g_0 = (k + 1 - c)\sigma(x)^2 - \sigma(x)\sigma(y) - d\,\sigma(x); \tag{50}$$

this is equivalent to (25) when $d = 0$. At this point two scenarios may happen.

Case 1. We find a $g_0 \in \mathbb{A}$ and $d \in \mathbb{K}$ such that (50) holds. Then combining the derived sub-results provides the solution

$$g = c\,s^2 + (y + d)\,s + g_0. \tag{51}$$

Case 2. We do not find a $g_0 \in \mathbb{A}$ and $d \in \mathbb{K}$ such that (50) holds. Then we can construct the polynomial ring $\mathbb{A}[s][t]$ and extend the automorphism σ from $\mathbb{A}[s]$ to $\mathbb{A}[s][t]$ subject to the relation

$$\sigma(t) = t + \Big(\sigma(x)^2 - c\sigma(x)^2 + k\sigma(x)^2 - \sigma(x)\sigma(y)\Big). \tag{52}$$

By Theorem 4.10 it follows that this extension is a Σ-extension. Namely, we have $\mathrm{const}(\mathbb{A}[s][t], \sigma) = \mathbb{K}$. This, in particular, implies the solution $g_0 = t$ and $d = 0$ for (50). Finally, in this case, combining the obtained representations of the coefficients produces the solution

$$g = c\,s^2 + y\,s + t \tag{53}$$

within the difference ring $(\mathbb{A}[s][t], \sigma)$ where $c \in \mathbb{K}$ and y are a solution of (49); compare with (26).

The previous considerations can be summarized as follows.

Theorem 4.14 *Let $(\mathbb{A}, \sigma)$ be a difference ring with constant field $\mathbb{K}$ and with $k \in \mathbb{A}$ where $\sigma(k) = k + 1$. Let $(\mathbb{A}[s], \sigma)$ be a Σ-extension of $(\mathbb{A}, \sigma)$ with $\sigma(s) = s + \sigma(x)$ for some $x \in \mathbb{A}$. Then the following holds.*

(1) There is a $g \in \mathbb{A}[s]$ with $\sigma(g) - g = \sigma(k\,x\,s)$ iff the following two statements hold:

(a) there is a $y \in \mathbb{A}$ and $c \in \mathbb{K}$ with (49),
(b) and there is a $g_0 \in \mathbb{A}$ and $d \in \mathbb{K}$ with (50) (where c is the one from part (a)).

If (a) and (b) hold, we get the solution g as given in (51).

(2) There is a Σ-extension $(\mathbb{A}[s][t], \sigma)$ of $(\mathbb{A}[s], \sigma)$ with $\sigma(t) - t \in \mathbb{A}$ together with a $g \in \mathbb{A}[s][t] \setminus \mathbb{A}[s]$ with $\sigma(g) - g = \sigma(k\,x\,s)$ iff the following two statements hold:

(a) there is a $y \in \mathbb{A}$ and $c \in \mathbb{K}$ with (49),

(b) there is no $g_0 \in \mathbb{A}$ *and* $d \in \mathbb{K}$ *with* (50) *(where c is the one from part (a)).*

If (a) and (b) hold, we get the solution g as given in (53) *with* (52).

Part 2 of the theorem describes the situation where one can adjoin a Σ-extension with the generator t in order to gain a parameterized telescoping solution for (50). Using the following extra insight from difference ring theory, we can generalize this situation if one allows a tower of single nested Σ-extensions.

Theorem 4.15 *Let* $(\mathbb{A}, \sigma)$ *be a difference ring with constant field* $\mathbb{K}$ *and with* $k \in \mathbb{A}$ *where* $\sigma(k) = k + 1$. *Let* $(\mathbb{A}[s], \sigma)$ *be a* Σ*-extension of* $(\mathbb{A}, \sigma)$ *such that* $\sigma(s) = s + \sigma(x)$ *for some* $x \in \mathbb{A}$. *Then there is a tower of* Σ*-extensions* $(\mathbb{A}[s][t_1]\dots[t_e], \sigma)$ *of* $(\mathbb{A}[s], \sigma)$ *with* $\sigma(t_i) - t_i \in \mathbb{A}$ *for* $1 \le i \le e$ *together with a* $g \in \mathbb{A}[s][t_1, \dots, t_e] \setminus \mathbb{A}[s]$ *with* $\sigma(g) - g = \sigma(k\,x\,s)$ *iff the following two statements hold:*

(a) there is a $y \in \mathbb{A}$ *and* $c \in \mathbb{K}$ *with* (49)*,*
(b) there is no g_0 *and* $d \in \mathbb{K}$ *with* (50) *(where c is the one from part (a)).*

If (a) and (b) hold, we obtain the solution g as given in (53) *with* (52) *(i.e.,* $e := 1$ *and* $t_1 := t$*).*

Proof If statements (a) and (b) hold, we can take (52) and get the solution g as given in (53). What remains to show is the other direction. Suppose that there is a tower of Σ-extensions $(\mathbb{A}[s][t_1]\dots[t_e], \sigma)$ of $(\mathbb{A}, \sigma)$ with $\beta_i = \sigma(t_i) - t_i \in \mathbb{A}$ for $1 \le i \le e$. Assume further that there is a $g \in \mathbb{A}[s][t_1, \dots, t_e] \setminus \mathbb{A}[s]$ with $\sigma(g) - g = \sigma(k\,x\,s)$. By [2, Prop. 1] it follows that

$$g = g' + \kappa_1\, t_1 + \dots + \kappa_e\, t_e \tag{54}$$

for some $g' \in \mathbb{A}[s]$ and $(\kappa_1, \dots, \kappa_e) \in \mathbb{K}^e \setminus \{(0, \dots, 0)\}$. Take the polynomial ring $\mathbb{A}[s][t]$ and extend σ from $\mathbb{A}[s]$ to $\mathbb{A}[s][t]$ subject to the relation $\sigma(t) = t + h$ with $h := \kappa_1\, \beta_1 + \dots + \kappa_e\, \beta_e$. By construction we have that

$$\sigma(g' + t) - (g' + t) = \sigma(g') - g' + \kappa_1\, \beta_1 + \dots + \kappa_e\, \beta_e = \sigma(g) - g = \sigma(k\,x\,s). \tag{55}$$

Now suppose that $(\mathbb{A}[s][t], \sigma)$ is not a Σ-extension of $(\mathbb{A}[s], \sigma)$. Then there is a $\gamma \in \mathbb{A}[s]$ with $\sigma(\gamma) - \gamma = \kappa_1\, \beta_1 + \dots + \kappa_e\, \beta_e$. Let j be maximal such that κ_j is non-zero. Then we conclude that $\sigma(\gamma') - \gamma' = \beta_j$ with

$$\gamma' := \frac{1}{\kappa_j}(\gamma - \kappa_1\, t_1 - \dots - \kappa_{j-1}\, t_{j-1}) \in \mathbb{A}[s][t_1]\dots[t_{j-1}]$$

which implies that $(\mathbb{A}[s][t_1]\dots[t_j], \sigma)$ is not a Σ-extension of $(\mathbb{A}[s][t_1]\dots[t_{j-1}], \sigma)$ by Theorem 4.10; a contradiction. Thus $(\mathbb{A}[s][t], \sigma)$ is a Σ-extension of $(\mathbb{A}[s], \sigma)$. Together with (55) we can apply part 2 of Theorem 4.14. This concludes the proof. □

5 A Refinement to the Class of Indefinite Nested Sums Over Mixed (Q–)Hypergeometric Products

In Theorems 4.14 and 4.15 we established criteria for the simplification of our double sum in the setting of difference rings. More precisely, we assumed that we are given a Σ-extension $(\mathbb{A}[s], \sigma)$ of $(\mathbb{A}, \sigma)$ with $\sigma(s) = s + \sigma(x)$ for some fixed $x \in \mathbb{A}$ and derived criteria when one can find a $g \in \mathbb{A}[s]$ or in an appropriate Σ-extension such that g solves the telescoping equation (46) with $f = k\,x\,s$. In the following we will transfer this result from the difference ring $(\mathbb{A}[s], \sigma)$ to the ring of sequences $(\text{Seq}(\mathbb{K}), S)$. To this end, we assume that we are given a ring embedding, i.e., an injective ring homomorphism τ from $\mathbb{A}$ into $\text{Seq}(\mathbb{K})$ with the additional property that $\tau(\sigma(f)) \equiv S(\tau(f))$ holds for all $f \in \mathbb{A}$, i.e., we require that the diagram

$$\begin{array}{ccc} \mathbb{A} & \xrightarrow{\sigma} & \mathbb{A} \\ \downarrow{\scriptstyle \tau} & & \downarrow{\scriptstyle \tau} \\ \text{Seq}(\mathbb{K}) & \xrightarrow{S} & \text{Seq}(\mathbb{K}) \end{array}$$

commutes. In addition, we assume naturally that $\tau(c) \equiv (c)_{n\geq 0}$ holds for all $c \in \mathbb{K}$. Such a map τ is also called a $\mathbb{K}$-*embedding* (it is called a $\mathbb{K}$-*homomorphism* if the injectivity of τ is dropped). Note that for such a $\mathbb{K}$-embedding it follows that $\tau(\mathbb{A})$ is a subring of $\text{Seq}(\mathbb{K})$ and S restricted to $\tau(\mathbb{A})$ forms a ring automorphism. Note that $(\mathbb{A}, \sigma)$ and $(\tau(\mathbb{A}), S)$ are the same up to renaming of the elements by τ.

Example 5.1 Consider the difference field $(\mathbb{K}(k), \sigma)$ from Example 4.4 with the evaluation function $\text{ev} : \mathbb{K}(k) \times \mathbb{Z}_{\geq 0} \to \mathbb{K}$ as in (38). Then we can define the map $\tau : \mathbb{K}(k) \to \text{Seq}(\mathbb{K})$ with $\tau(f) = (\text{ev}(f, i))_{i\geq 0}$ for $f \in \mathbb{K}(k)$. One can easily see that τ is a ring homomorphism and with (39) it follows that τ is a $\mathbb{K}$-homomorphism. Finally, $\tau(f) \equiv 0$ implies that $f = 0$ since the numerator and denominator of f can have only finitely many roots. Consequently, τ is a $\mathbb{K}$-embedding. The subdifference ring $(\tau(\mathbb{K}(k)), S)$ of $(\text{Seq}(\mathbb{K}), S)$ is also called the *difference ring of rational sequences*.

Example 5.2 Consider the Σ-extension $(\mathbb{K}(k)[s], \sigma)$ of $(\mathbb{K}(k), \sigma)$ from Example 4.12 (see also Example 4.4) with the corresponding evaluation function $\text{ev} : \mathbb{K}(k)[s] \times \mathbb{Z}_{\geq 0} \to \mathbb{K}$ that models the harmonic numbers H_k with s. Then using similar arguments as in Example 5.1 we conclude that $\tau : \mathbb{K}(k)[s] \to \text{Seq}(\mathbb{K})$ defined by $\tau(f) = (\text{ev}(f, i))_{i\geq 0}$ for $f \in \mathbb{K}(k)[s]$ is a $\mathbb{K}$-homomorphism. By difference ring theory [22] it follows that τ is injective, and thus τ is a $\mathbb{K}$-embedding.

More generally, we succeeded in such a construction in [22] not only for the harmonic numbers H_k as elaborated in Example 5.2 but for the general class of sequences that can be given in terms of nested sums over hypergeometric/q-hypergeometric/mixed-hypergeometric products.

Definition 5.3 Let $\mathbb{K} = \mathbb{K}'(q_1, \ldots, q_v)$ be a rational function field where $\mathbb{K}'$ is a field of characteristic 0. A product $\prod_{j=l}^{k} f(j, q_1^j, \ldots, q_v^j)$, $l \in \mathbb{Z}_{\geq 0}$, is called *mixed-multibasic hypergeometric* [6] (in short *mixed hypergeometric*) in k over $\mathbb{K}$ if $f(y, z_1, \ldots, z_v)$ is an element from the rational function field $\mathbb{K}(y, z_1, \ldots, z_v)$ where the numerator and denominator of $f(j, q_1^j, \ldots, q_v^j)$ are nonzero for all $j \in \mathbb{Z}$ with $j \geq l$. Such a product is evaluated to a sequence following the rule

$$\prod_{j=l}^{k} f(j, q_1^j, \ldots, q_v^j) : \mathbb{Z} \to \mathbb{K}, m \mapsto \begin{cases} \prod_{j=l}^{m} f(j, q_1^j, \ldots, q_v^j), & \text{if } l \leq m \\ 1, & \text{otherwise.} \end{cases}$$

Further, such a product is called *q-hypergeometric* if f is free of y, $v = 1$ and $q_1 = q$, i.e., $f \in \mathbb{K}(z_1)$ with $\mathbb{K} = \mathbb{K}'(q)$. It is called *hypergeometric* if $v = 0$, i.e., $f \in \mathbb{K}(y)$ with $\mathbb{K} = \mathbb{K}'$.

An *expression in terms of nested sums over hypergeometric/q-hypergeometric/mixed hypergeometric products in k over* $\mathbb{K}$ is composed recursively by the three operations $(+, -, \cdot)$ with

- elements from the rational function field $\mathbb{K}(k)$,
- hypergeometric/q-hypergeometric/mixed hypergeometric products in k over $\mathbb{K}$,
- and sums of the form $\sum_{j=l}^{k} f(j)$ with $l \in \mathbb{Z}_{\geq 0}$ where $f(j)$ is an expression in terms of nested sums over hypergeometric/q-hypergeometric/mixed hypergeometric products in j over $\mathbb{K}$; here it is assumed that the evaluation[15] of $f(j)|_{j \mapsto \lambda}$ for all $\lambda \in \mathbb{Z}$ with $\lambda \geq l$ does not introduce any poles.

Given such an expression $F(k)$ the evaluation $F(k)|_{k \mapsto \lambda}$ might be only defined for all $\lambda \geq l$ for some $l \in \mathbb{Z}_{\geq 0}$. In order to obtain an evaluation for all $\lambda \in \mathbb{Z}_{\geq 0}$, we set $F(k)|_{k \mapsto \lambda} = 0$ for $\lambda = 0, \ldots, l - 1$. Similarly to Definition 2.5 we will give such products and sums defined over such products two different meanings. They form expressions that evaluate to sequences as introduced above, or they are just shorthand notations for the underlying sequences $(F(k)|_{k \mapsto \lambda})_{\lambda \geq 0}$. The meaning (expression or sequence) of such sums or products will be always clear from the context. E.g., the harmonic numbers H_n or the left- and right-hand sides of (33) and (34) are either expressions in terms of indefinite nested sums over hypergeometric products in a over $\mathbb{K} = \mathbb{Q}(n)$ or they are shorthand notations for sequences in $\mathbb{K}$.

In general, as the sum $H_k \in \text{Seq}(\mathbb{K})$ can be rephrased in the difference ring $(\mathbb{K}(k)[s], \sigma)$ given in Example 5.2, we can represent nested sums as defined in Definition 5.3 in a particular class of difference rings called *simple* $R\Pi\Sigma$*-rings*; for their definition we refer to the Appendix 8. At this point we want to emphasize only the following crucial properties [12, 22] of simple $R\Pi\Sigma$-rings that enable one to treat the above class of nested sums in full generality.

[15] Note that $\mathbb{K} \subseteq \mathbb{K}_X$ and thus the evaluation of a sum has been defined already in (5).

Theorem 5.4 *Let $\bar{X}_k(=\bar{X}(k)) \in \mathrm{Seq}(\mathbb{K})$ be a sequence given in terms of nested sums over hypergeometric (resp. q-hypergeometric or mixed hypergeometric) products where $\mathbb{K}$ is algebraically closed.*[16] *Then the following holds.*

(1) There is a simple $R\Pi\Sigma$-ring $(\mathbb{A}, \sigma)$ with constant field $\mathbb{K}$ equipped with a $\mathbb{K}$-embedding $\tau : \mathbb{A} \to \mathrm{Seq}(\mathbb{K})$ and with $x \in \mathbb{A}$ such that $\tau(x) \equiv \bar{X}_k$ holds.

Moreover, for this τ one has:

(2a) For any $h \in \mathbb{A}$ there is a sequence $H(k)$ expressible in terms of nested sums over hypergeometric (resp. q-hypergeometric or mixed hypergeometric) products with $\tau(h) \equiv H(k)$.

(2b) If the difference ring extension $(\mathbb{A}[s], \sigma)$ of $(\mathbb{A}, \sigma)$ with s being transcendental over $\mathbb{A}$ and $\sigma(s) = s + \sigma(x)$, x as in part (1), forms a Σ-extension, then the difference ring homomorphism $\tau' : \mathbb{A}[s] \to \mathrm{Seq}(\mathbb{K})$ defined by $\tau'|_{\mathbb{A}} = \tau$ and $\tau'(s) \equiv \sum_{k=0}^{n} \bar{X}_k$ forms a $\mathbb{K}$-embedding.[17]

In particular, the simple $R\Pi\Sigma$-ring $(\mathbb{A}, \sigma)$ with f and the embedding τ can be computed explicitly; for further details see Appendix 8.

Note that part (1) implies that a finite number of nested sums over hypergeometric, q-hypergeometric or mixed hypergeometric can be always formalized in a simple $R\Pi\Sigma$-ring, and part (2a) states that any element in such a ring can be reinterpreted as such a sum or product. This representation justifies the following definition.

Definition 5.5 A sub-difference ring $(\mathbb{S}, S)$ of $(\mathrm{Seq}(\mathbb{K}), S)$ is called a *product-sum sequence ring*, if there is a simple $R\Pi\Sigma$-ring $(\mathbb{A}, \sigma)$ with constant field $\mathbb{K}$ together with a $\mathbb{K}$-embedding $\tau : \mathbb{A} \to \mathrm{Seq}(\mathbb{K})$ with $\tau(\mathbb{A}) = \mathbb{S}$.

Now let us reconsider our difference ring calculations of Sect. 4 within such a product-sum sequence ring $(\mathbb{S}, S)$ where $\bar{X}_k$ stands for a sequence that is given in terms of nested sums over products. According to Theorem 5.4, this means that there is a simple $R\Pi\Sigma$-ring $(\mathbb{A}, \sigma)$ with constant field $\mathbb{K}$ equipped with a $\mathbb{K}$-embedding $\tau : \mathbb{A} \to \mathrm{Seq}(\mathbb{K})$ and with an $x \in \mathbb{A}$ such that $\tau(x) \equiv \bar{X}_k$ holds. Suppose the decision procedure implemented in `Sigma` tells us (as above in Example 4.12) that there is no $g \in \mathbb{A}$ such that $\sigma(g) = g + \sigma(x)$ holds. Note that this implies that there is no sequence $G(k) \in \tau(\mathbb{A})$ expressible in terms of nested sums with $G(k+1) - G(k) \equiv \bar{X}_{k+1}$ or equivalently it follows that

$$\sum_{i=0}^{k} \bar{X}_i \notin \tau(\mathbb{A}).$$

Furthermore, we conclude by part (2b) of Theorem 5.4 that we can extend the $\mathbb{K}$-embedding τ from $\mathbb{A}$ to $\mathbb{A}[s]$ with $\tau(s) \equiv \sum_{i=0}^{k} \bar{X}_k$. From this it can be derived that

[16] Algorithmically, one starts with a base field K (like $\mathbb{Q}$ or $\mathbb{Q}(n)$) and constructs —if necessary— a finite algebraic extension of it such that statement (1) is true.

[17] This means that $\tau(\sum_{i=0}^{r} f_i s^i) \equiv \sum_{i=0}^{r} \tau(f_i)\big(\big(\sum_{k=0}^{n} \bar{X}_k\big)^i\big)_{n \geq 0}$ for $f_0, \ldots, f_r \in \mathbb{A}$.

$(\mathbb{A}[s], \sigma)$ and $(\tau(\mathbb{A}[s]), S)$ are isomorphic, i.e., the difference rings are the same up to renaming of the objects using τ.

With this background we restart our calculations to obtain a solution g of the telescoping equation

$$\sigma(g) - g = (k+1)\,\sigma(x\,s) = (k+1)\sigma(x)(s+\sigma(x)). \tag{56}$$

In the first major step we assumed that we can find a $c \in \mathbb{K}$ and a $y \in \mathbb{A}$ such that (49) holds. Now let $\bar{Y}_k$ be the sequence in terms of nested sums with $\tau(y) \equiv \bar{Y}_k \in \tau(\mathbb{A})$. Then by construction it follows that (30) holds for $\bar{Y}_k$ and c.

We proceed with our calculations by entering in the already worked out case distinction.

Case 1. We can compute a $d \in \mathbb{K}$ and $g_0 \in \mathbb{A}$ with (50). Then for the sequence $G_0(k)$ with $\tau(g_0) = G_0(k)$ in terms of nested sums we obtain

$$G_0(k+1) - G_0(k) \equiv \bar{X}_{k+1}^2 - c\bar{X}_{k+1}^2 + k\bar{X}_{k+1}^2 - \bar{X}_{k+1}\bar{Y}_{k+1} - d\,\bar{X}_{k+1}. \tag{57}$$

Further, the $g \in \mathbb{A}[s]$ with (51) is a solution of (56) under the assumption that $c \in \mathbb{K}$ and y are a solution of (49). This implies that

$$S(\tau(g)) - \tau(g) \equiv \tau((k+1)\,\sigma(x)\,(s+\sigma(x)) \equiv ((k+1)\,\bar{X}_{k+1}\,(\sum_{i=0}^{k}\bar{X}_i + \bar{X}_{k+1}))_{k\geq 0}.$$

By construction, we obtain $\tau(g) \equiv G(k) \in \tau(\mathbb{A}[s])$ with $G(k) = c\left(\sum_{i=0}^{k}\bar{X}_i\right)^2 + (\bar{Y}_k + d)\sum_{i=0}^{k}\bar{X}_i + G_0(k)$, and thus $G(k)$ is a solution of

$$G(k+1) - G(k) \equiv (k+1)\,\bar{X}_{k+1}\Big(\sum_{j=0}^{k}\bar{X}_j + \bar{X}_{k+1}\Big) \tag{58}$$

under the constraint that (30) holds for $\bar{Y}_k$ and $c \in \mathbb{K}$. Passing from the generic sequence variable k to concrete integers $k \in \mathbb{Z}$, using (58) we can check that telescoping yields

$$\sum_{k=0}^{a} k\,\bar{X}_k \sum_{j=0}^{k}\bar{X}_j = G(a) - G(-1) = c\Big(\sum_{i=0}^{a}\bar{X}_i\Big)^2 + (\bar{Y}_a + d)\sum_{i=0}^{a}\bar{X}_i + G_0(a) - G_0(-1). \tag{59}$$

Case 2. There does not exist a $d \in \mathbb{K}$ and $g_0 \in \mathbb{A}$ with (50). By Theorem 5.4 we can extend the $\mathbb{K}$-embedding from $\mathbb{A}[s]$ to $\mathbb{A}[s][t]$ with $\tau(t) \equiv G_0(k)$ where

$$G_0(k) = \sum_{i=0}^{k}(-c\bar{X}_i^2 + i\bar{X}_i^2 - \bar{X}_i\bar{Y}_i). \tag{60}$$

In particular, we conclude that $G_0(k) \notin \tau(\mathbb{A})$. Moreover, the solution (53) of (56) yields the solution (26) of (58) under the constraint that (30) holds for $\bar{Y}_k$ and $c \in \mathbb{K}$. Finally, we arrive at our simplification given in (31).

In Theorem 4.14 of Sect. 4 we summarized the considerations leading to cases (1) and (2). Before we can reformulate these cases in the context of sequences, we collect some key properties indicated already above.

Lemma 5.6 *Let* $(\mathbb{A}, \sigma)$ *be a simple* $R\Pi\Sigma$*-ring (see Definition 8.2) with constant field* $\mathbb{K}$*, and let* $\tau : \mathbb{A} \to \mathrm{Seq}(\mathbb{K})$ *be a* $\mathbb{K}$*-embedding. Set* $\mathbb{S} = \tau(\mathbb{A})$ *and let* $f \in \mathbb{A}$ *with* $\tau(f) \equiv F = (F(k))_{k\geq 0} \in \mathbb{S}$ *and define* $\bar{S} := (\sum_{j=0}^{k} F(j))_{k\geq 0} \in \mathrm{Seq}(\mathbb{K})$*. Then the following statements are equivalent.*

(1) There is a Σ*-extension* $(\mathbb{A}[s], \sigma)$ *of* $(\mathbb{A}, \sigma)$ *with* $\sigma(s) = s + \sigma(f)$*.*
(2) There is no $G \in \mathbb{S}$ *with* $S(G) - G \equiv S(F)$*.*
(3) $\mathbb{S}[\bar{S}]$ *forms a polynomial ring.*
(4) $\bar{S} \notin \mathbb{S}$*.*

Proof (1) $\Leftrightarrow$ (2): There is a Σ-extension $(\mathbb{A}[s], \sigma)$ of $(\mathbb{A}, \sigma)$ iff there is no $g \in \mathbb{A}$ with $\sigma(g) = g + \sigma(f)$ by Theorem 4.10. Since τ is a $\mathbb{K}$-embedding, the latter condition is equivalent to saying that there is no $G \in \tau(\mathbb{A})$ with $S(G) - G \equiv \tau(\sigma(f)) \equiv S(\tau(f)) \equiv S(F)$.
(1) $\Rightarrow$ (3): By part (2b) of Theorem 5.4 one can extend τ from $\mathbb{A}$ to $\mathbb{A}[s]$ by $\tau(s) \equiv S$. Since $\mathbb{A}[s]$ is a polynomial ring, $\mathbb{S}[\bar{S}]$ forms a polynomial ring.
(3) $\Rightarrow$ (4) holds trivially.
(4) $\Rightarrow$ (2): Suppose that there is a $G \in \mathbb{S}$ with $S(G) - G \equiv \tau(\sigma(f))$. Since $S(\bar{S}) \equiv \bar{S} + (F(k+1))_{k\geq 0} \equiv \bar{S} + (F(k))_{k\geq 1} \equiv \bar{S} + S(\tau(f)) \equiv \bar{S} + \tau(\sigma(f))$, we conclude that $S(\bar{S} - G) \equiv \bar{S} - G$ and thus $\bar{S} \equiv G + (c, c, c, \dots)$ for some $c \in \mathbb{K}$. Hence $\bar{S} \in \mathbb{S}$. □

With Lemma 5.6 and the above considerations the statements of part 1 of Theorems 4.14 and 4.15 (which is a slightly more general version of part 2 of Theorem 4.14) translate directly to the corresponding statements of the following Theorem 5.7.

Theorem 5.7 *Let* $(\mathbb{S}, S)$ *be a product-sum sequence ring containing the sequence* k *with* $S(k) = k + 1$*. Let* $\bar{X}_k \in \mathbb{S}$ *and suppose that* $\sum_{i=0}^{k} \bar{X}_i \notin \mathbb{S}$*. Then within the polynomial ring* $\mathbb{S}' := \mathbb{S}[\sum_{i=0}^{k} \bar{X}_i]$ *the following two statements hold:*

(1) $\sum_{k=0}^{a} k\, \bar{X}_k \sum_{i=0}^{k} \bar{X}_i \in \mathbb{S}'$ *iff*
   (a) there is a $\bar{Y}_k \in \mathbb{S}$ *and* $c \in \mathbb{K}$ *with (30),*
   (b) and there is a $G_0(k) \in \mathbb{S}$ *and* $d \in \mathbb{K}$ *with (57) (where* c *is the one from part (a)).*

   If (a) and (b) hold, we get the simplification given in (59).

(2) *Suppose that* $Z_a := \sum_{k=0}^{a} k\,\bar{X}_k \sum_{i=0}^{k} \bar{X}_i \notin \mathbb{S}'$. *Then the sequence* Z_a *can be given in terms of single nested sums whose summands are from* $\mathbb{S}$ *iff the following two statements hold:*

   (a) *there is a* $\bar{Y}_k \in \mathbb{S}$ *and* $c \in \mathbb{K}$ *with* (30),
   (b) *there is no* $G_0(k) \in \mathbb{S}$ *and* $d \in \mathbb{K}$ *with* (57) *(where* c *is the one from part (a)).*

   If (a) and (b) hold, we obtain the simplification (28).

6 Using the `Sigma` Package

6.1 The Symbolic Approach with `Sigma`

As already demonstrated in In[7] the difference ring machinery is activated in `Sigma` by executing the function call `SigmaReduce` to the given summation problem. If a generic sequence X_k arises within the summation problem, this information has to be passed to `SigmaReduce` with the option `XList`$\to \{X\}$. Then the generic sequence X_k and its shifted versions $\dots, X_{k-2}, X_{k-1}, X_k, X_{k+1}, X_{k+2}, \dots$ are represented by the variables $\dots, x_{-2}, x_{-1}, x_0, x_1, x_2, \dots$, respectively. Namely, as worked out in [10, 11] `Sigma` takes the field $\mathbb{G} = \mathbb{K}(\dots, x_{-2}, x_{-1}, x_0, x_1, x_2, \dots)$ with infinitely many variables and uses the field automorphism $\sigma : \mathbb{G} \to \mathbb{G}$ with $\sigma(x_i) = x_{i+1}$ for all $i \in \mathbb{Z}$ and $\sigma(c) = c$ for all $c \in \mathbb{K}$. The obtained difference field $(\mathbb{G}, \sigma)$ with $\mathrm{const}(\mathbb{G}, \sigma) = \mathbb{K}$ is also called the *difference field of free sequences*. In order to define the underlying evaluation function for $\mathbb{G}$, the constant field $\mathbb{K}$ has to be constructed accordingly. Here one takes the rational function field $\mathbb{K} = \mathbb{K}'(\dots, X_{-2}, X_{-1}, X_0, X_1, X_2, \dots)$ again with infinitely many variables where $\mathbb{K}'$ is a field of characteristic 0; note that $\mathbb{K}'_X$ (see our earlier Definition 4) and $\mathbb{K}$ are closely related: $\mathbb{K}'_X$ is the polynomial ring in the variables X_i with $i \in \mathbb{Z}$ and $\mathbb{K}$ is simply its quotient field. The evaluation function ev for $\mathbb{G}$ is provided with $\mathrm{ev}(x_i, j) = X_{i+j}$ for $i, j \in \mathbb{Z}$.

Usually, in generic summation problems as considered in this article, the summation input of `SigmaReduce` depends not only on generic sequences, but on generic sums (see Definition 2.5) and more generally, on nested sums and products defined over generic sequences. In this case, the input expression is represented accordingly with a tower of $R\Pi\Sigma$-extensions over $(\mathbb{G}, \sigma)$, see the Appendix 8, which leads to a difference ring $(\mathbb{A}, \sigma)$. This construction can be carried out automatically by the tools given in [19, 21, 22] in combination with the machinery described in [10, 11]. Finally, `Sigma` tries to simplify the given summation problem using the different telescoping algorithms from [17, 18, 20].

Calculation steps for Sect. 3.1: In order to tackle the sum on the left-hand side of (18) `Sigma` represents X_j by $x_0 \in \mathbb{G}$. By default the difference field extension $(\mathbb{G}(k), \sigma)$ of $(\mathbb{G}, \sigma)$ with $\sigma(k) = k + 1$ and $\mathrm{const}(\mathbb{G}(k), \sigma) = \mathbb{K}$ is adjoined automatically.

Furthermore, the Σ-extension $(\mathbb{G}(k)[s], \sigma)$ of $(\mathbb{G}(k), \sigma)$ with $\sigma(s) = s + x_1$ is constructed to model the generic sum $\sum_{j=0}^{k} X_j$ with $\sum_{j=0}^{k+1} X_j = \sum_{j=0}^{k} X_j + X_{k+1}$; internally Theorem 4.10 is applied to check that this is indeed a Σ-extension. As a consequence, we have that $\text{const}(\mathbb{G}(k)[s], \sigma) = \mathbb{K}$. Now exactly the steps from Sect. 3.1 with $f = \sigma(s) = s + x_1$ are carried out in this difference ring, and the expression (18) (with the options `SimpleSumRepresentation→True` and `SimplifyByExt→MinDepth` activated; see Remark 1.1 for further explanations) is returned.

Calculation steps for Sect. 3.2: The tactic of Sect. 3.1 fails for the double sum on the left-hand side of (28). But, using in addition the `Sigma`-option `Extract Constraints→` $\{Y\}$, as demonstrated in In[9], the new machinery introduced in Sect. 4 is activated. Internally, again the difference ring $(\mathbb{G}(k)[s], \sigma)$ with constant field $\mathbb{K}$ is constructed, and the computation steps are carried out with $\sigma(f) = (k+1)x_1(s + x_1)$ (instead of $\sigma(f) = (k+1)\sigma(x)(s + \sigma(x))$. They are precisely the same as in Sect. 4. In this process we produce the constraint

$$\sigma(g_1) - g_1 = (1 + k)x_1 - 2\,c\,x_1;$$

compare with (48). Since `Sigma` does not find a solution $g_1 \in \mathbb{G}(k)[s]$, it extends the underlying difference field $\mathbb{G}$ by the new variables $\dots, y_{-2}, y_{-1}, y_0, y_1, y_2, \dots$ and extends the automorphism σ with $\sigma(y_i) = y_{i+1}$ for all $i \in \mathbb{Z}$. Now we continue our calculation with $g_1 = y_i + d$ and a new variable c (i.e., we extend the constant field $\mathbb{K}$ by c) and obtain the constraint

$$\sigma(g_0) - g_0 = x_1^2 - cx_1^2 + kx_1^2 - x_1 y_1 - d\,x_1$$

of g_0; compare with (50). Since we do not find a $g_0 \in \mathbb{G}(k)(s)$ (with the updated $\mathbb{G}$ containing now also the variables y_i with $i \in \mathbb{Z}$ and the new constant c) and $d \in \mathbb{K}(c)$, we construct the Σ-extension $(\mathbb{G}(k)[s][t], \sigma)$ of $(\mathbb{G}(k)[s], \sigma)$ with

$$\sigma(t) = t + (x_1^2 - cx_1^2 + kx_1^2 - x_1 y_1).$$

This finally produces the solution $g = c\,s^2 + y_0\,s + t$. Reinterpreting this result in terms of the generic sequences X_k and Y_k produces the output Out[9].

Concerning this concrete summation problem the following remarks are relevant.

1. The output Out[9] provides the full information that is needed to apply Theorem 5.7 taking care of the two possible scenarios. Specializing X_k and Y_k (where Y_k and c are solutions of the constraint (30)) to concrete sequences in $(\mathbb{S}, S)$, it might happen that the found sum extension simplifies further in the given ring $\mathbb{S}$. This situation is covered by part (1) of Theorem 5.7. Otherwise, if the sum cannot be simplified in $\mathbb{S}$, part (2) of the Theorem 5.7 can be applied.
2. Fix a product-sum sequence ring $(\mathbb{S}, S)$. If $\sum_{j=0}^{k} \bar{X}_j \notin \mathbb{S}$, the output gives a full characterization when the sum $\sum_{k=0}^{a} \bar{X}_k \sum_{j=0}^{k} \bar{X}_j$ can be written as an expression

in terms of single nested sums; see Theorem 5.7 for further details. However, if we enter the special case $\sum_{j=0}^{k}\bar{X}_j\in\mathbb{S}$, then the result provides only a sufficient criterion to get such a simplification. Still the toolbox can be applied also in such a case as worked out in Example 3.2; there we chose $X_j=H_j$ for which the simplification $\sum_{j=0}^{k}\bar{X}_j=-n+(1+n)H_n$ is possible.

3. Specializing the identities in (18) to concrete sequences $\bar{X}_k$ often leads to further simplifications.

We considered the very special case of the input expression $\sum_{k=0}^{a}k\,X_k\sum_{i=0}^{k}X_i$. However, the proposed method works for any input sum $\sum_{k=0}^{a}f(k)$ where the summand $f(k)$ is built by a finite number of generic sequences, say $X, Y, \dots, Z$, and over nested sums over hypergeometric/q-hypergeometric/mixed hypergeometric products. A typical function call, for instance, is In[3]. Here the same ideas are applied as in Sect. 3 where instead of $\sum_{i=0}^{k}X_i$ the most nested sum (and among the most nested sums the one with highest degree) of the summand $f(k)$ is chosen. In particular, the following refinements can be activated.

1. In Sect. 3.2 we combined the telescoping algorithm from [20] with our new idea to extract constraints in form of parameterized telescoping equations and to encode these constraints in the output expression by using new generic sequences. Within `Sigma` also other enhanced telescoping strategies for simplification [15, 17, 20] can be combined with this new feature. For further details on the possible options we refer also to Remarks 1.1 and 1.2.
2. In Sect. 3.2 the most complicated sum occurs only linearly. As a consequence we run into three constraints given by step-wise coefficient comparison. Namely, for our ansatz (20) we get the constraint (23), which can always be treated, the constraint (24) where we introduced a generic sequence Y_k subject to the parameterized telescoping relation (29), and the constraint (25) which we could handle by the sum extension (60). More generally, if the most complicated sum occurs with degree $d>1$, one ends up with $d+2$ constraints. Some of them can be solved directly by `Sigma` within the given difference ring, but in general there will remain constraints which can only be treated by introducing a new generic sequence that must satisfy a certain parameterized telescoping equation. Activating the option `ExtractConstraints`$\to\{Y^{(1)},\dots,Y^{(l)}\}$, `SigmaReduce` is allowed to provide (if necessary) up to l constraints in form of parameterized telescoping equations, each one with a different generic sequence from $Y^{(1)},\dots,Y^{(l)}$. If not successful, i.e., if more than l generic sequences are needed, `Sigma` gives up and returns the input expression.

6.2 Discovery of Identities

We illustrate how the presented techniques can support the (re)discovery of numerous identities. We start with the generic sum

In[14]:= $\mathbf{mySum} = \sum_{k=0}^{a}\left(\sum_{j=0}^{k}\mathbf{X[j]}\right)^2;$

and obtain the following general simplification formula

In[15]:= **{closedForm, constraint} = SigmaReduce[mySum, XList → {X}, ExtractConstraints → {Y}, SimpleSumRepresentation → False, RefinedForwardShift → False]**

Out[15]= $\{(a+c)\left(\sum_{i=0}^{a}\texttt{X[i]}\right)^2+\sum_{i=0}^{a}\left(\texttt{X[i]}^2-c\texttt{X[i]}^2-i\texttt{X[i]}^2-\texttt{X[i]Y[i]}\right)+\texttt{Y[a]}\sum_{i=0}^{a}\texttt{X[i]},$
$\{\texttt{Y[a+1]}-\texttt{Y[a]}==-2a\texttt{X[a+1]}-2\,c\texttt{X[a+1]}\}\}$

The result can be simplified further to the form

In[16]:= **SigmaReduce[closedForm, a, XList → {X, Y}, SimpleSumRepresentation → True]**

Out[16]= $(a+c)\left(\sum_{i=0}^{a}\texttt{X[i]}\right)^2-c\sum_{i=0}^{a}\texttt{X[i]}^2-\sum_{i=0}^{a}\texttt{X[i]Y[i]}+\texttt{Y[a]}\sum_{i=0}^{a}\texttt{X[i]}+\sum_{i=0}^{a}\texttt{X[i]}^2-\sum_{i=0}^{a}i\texttt{X[i]}^2$

This means that the identity

$$\sum_{k=0}^{a}\Big(\sum_{j=0}^{k}\bar{X}_j\Big)^2=(a+c)\Big(\sum_{k=0}^{a}\bar{X}_k\Big)^2-c\sum_{k=0}^{a}\bar{X}_k^2-\sum_{k=0}^{a}\bar{X}_k\bar{Y}_k+\bar{Y}_a\sum_{k=0}^{a}\bar{X}_k+\sum_{k=0}^{a}\bar{X}_k^2-\sum_{k=0}^{a}k\bar{X}_k^2 \tag{61}$$

holds for any sequences $(\bar{X}_k)_{k\geq 0}$, $(\bar{Y}_k)_{k\geq 0}$ with $\bar{X}_k, \bar{Y}_k\in\mathbb{K}$ and $c\in\mathbb{K}$ if c and $\bar{Y}_k$ are a solution of the parameterized telescoping equation

$$\bar{Y}_{k+1}-\bar{Y}_k=-2k\bar{X}_{k+1}-2\,c\,\bar{X}_{k+1}. \tag{62}$$

Even more holds by a straightforward variant of Theorem 5.7: if one takes a product-sum sequence ring $(\mathbb{S}, S)$ and takes a sequence $\bar{X}_k$ which is in $\mathbb{S}$ but where the sequence of $\sum_{j=0}^{k}\bar{X}_j$ is not in $\mathbb{S}$, then the double sum on the left-hand side of (61) can be simplified to single nested sums defined over $\mathbb{S}$ if and only if there is a solution $c\in\mathbb{K}$ and $\bar{Y}_k$ in $\mathbb{S}$ of (62). In this case the right-hand side of (62) with the explicitly given c and $\bar{Y}_k$ produces such a simplification.

Example 6.1 $\bar{X}_k=\binom{n}{k}$: Plugging the solution $c=\frac{2-n}{2}$ and $\bar{Y}_k=\binom{n}{k}(-k+n)$ of (62) into (61) yields

$$\begin{aligned}\sum_{k=0}^{a}\Big(\sum_{j=0}^{k}\binom{n}{j}\Big)^2&=(-a+n)\binom{n}{a}\sum_{k=0}^{a}\binom{n}{k}+\Big(a+\frac{2-n}{2}\Big)\Big(\sum_{k=0}^{a}\binom{n}{k}\Big)^2\\&\quad+\sum_{k=0}^{a}\binom{n}{k}^2-\frac{2-n}{2}\sum_{k=0}^{a}\binom{n}{k}^2-\sum_{k=0}^{a}k\binom{n}{k}^2-\sum_{k=0}^{a}\binom{n}{k}^2(-k+n)\\&\stackrel{\texttt{Sigma}}{=}\binom{n}{a}(-a+n)\sum_{k=0}^{a}\binom{n}{k}+\frac{1}{2}(2+2a-n)\Big(\sum_{k=0}^{a}\binom{n}{k}\Big)^2-\frac{1}{2}n\sum_{k=0}^{a}\binom{n}{k}^2\end{aligned}$$

which is valid for all $a, n\in\mathbb{Z}_{\geq 0}$. Following the same tactic, we "discover" the identities

$$\sum_{k=0}^{a}\Big(\sum_{j=0}^{k}x^j\binom{n}{j}\Big)^2=-\frac{nx}{x+1}\sum_{k=0}^{a}x^{2k}\binom{n}{k}^2+\tfrac{(1+a+x+ax-nx)}{x+1}\Big(\sum_{k=0}^{a}x^k\binom{n}{k}\Big)^2$$
$$+\frac{x-1}{x+1}\sum_{k=0}^{a}kx^{2k}\binom{n}{k}^2-\frac{2x^{a+1}(a-n)}{x+1}\binom{n}{a}\sum_{k=0}^{a}x^k\binom{n}{k},$$
$$\sum_{k=0}^{a}\Big(\sum_{j=0}^{k}(-1)^j\binom{n}{j}\Big)^2=\frac{n}{2(2n-1)}\sum_{k=0}^{a}\binom{n}{k}^2-\frac{(2a-3n+2)(a-n)^2}{2n^2(2n-1)}\binom{n}{a}^2;$$

the first identity holds for $x\in\mathbb{K}\setminus\{-1\}$ and $a,n\in\mathbb{Z}_{\geq 0}$ and the second holds for $a,n\in\mathbb{Z}_{\geq 0}$ with $n\neq 0$. Furthermore we obtain

$$\sum_{k=0}^{a}\Big(\sum_{j=0}^{k}\frac{x^j}{\binom{n}{j}}\Big)^2=\frac{1+n+x}{x+1}\sum_{k=0}^{a}\frac{x^{2k}}{\binom{n}{k}^2}+\frac{x-1}{x+1}\sum_{k=0}^{a}\frac{kx^{2k}}{\binom{n}{k}^2}$$
$$+\frac{a-n+2x+ax}{x+1}\Big(\sum_{k=0}^{a}\frac{x^k}{\binom{n}{k}}\Big)^2-\frac{2(a+1)x^{a+1}}{(x+1)\binom{n}{a}}\sum_{k=0}^{a}\frac{x^k}{\binom{n}{k}},$$
$$\sum_{k=0}^{a}\Big(\sum_{j=0}^{k}\frac{(-1)^j}{\binom{n}{j}}\Big)^2=\tfrac{(n+1)^2(4an^2+22an+30a+3n^2+23n+38)}{2(n+2)^2(n+3)(2n+5)}+\tfrac{2(-1)^a(a+1)(a+2)(n+1)}{(n+2)^2(n+3)}\frac{1}{\binom{n}{a}}$$
$$+\frac{(a+1)^2(6+2a+n)}{2(n+2)^2(2n+5)}\frac{1}{\binom{n}{a}^2}+\frac{n+2}{2(2n+5)}\sum_{k=0}^{a}\frac{1}{\binom{n}{k}^2}$$

for all $x\in\mathbb{K}\setminus\{-1\}$ and $a,n\in\mathbb{Z}_{\geq 0}$ with $a\leq n$.

Similarly, for the generic double sum

In[17]:= $\mathbf{mySum}=\sum_{k=0}^{a}(-1)^k\Big(\sum_{j=0}^{k}X[j]\Big)^2;$

`Sigma` finds the general simplification

In[18]:= **{closedForm, constraint} = SigmaReduce[mySum, XList → {X}, ExtractConstraints → {Y}, SimpleSumRepresentation → False, RefinedForwardShift → False]**

Out[18]= $\{-\frac{1}{2}c\Big(\sum_{i=0}^{a}X[i]\Big)^2+\frac{1}{2}(-1)^a\Big(\sum_{i=0}^{a}X[i]\Big)^2+\frac{1}{2}\sum_{i=0}^{a}\big((-1)^iX[i]+cX[i]+Y[i]\big)X[i]-\frac{1}{2}Y[a]\sum_{i=0}^{a}X[i],$
$\{Y[a+1]-Y[a]==2(-1)^aX[a+1]-2\,cX[a+1]\}\}.$

where the result can be simplified further to

In[19]:= **SigmaReduce[closedForm, a, XList → {X, Y}, SimpleSumRepresentation → True]**

Out[19]= $\big(-\frac{c}{2}+\frac{1}{2}(-1)^a\big)\Big(\sum_{i=0}^{a}X[i]\Big)^2+\frac{1}{2}c\sum_{i=0}^{a}X[i]^2+\frac{1}{2}\sum_{i=0}^{a}(-1)^iX[i]^2+\frac{1}{2}\sum_{i=0}^{a}X[i]Y[i]-\frac{1}{2}Y[a]\sum_{i=0}^{a}X[i]$

This means that for any sequences $\bar{X}_k\in\mathbb{K}$, $\bar{Y}_k\in\mathbb{K}$ and $c\in\mathbb{K}$ with

$$\bar{Y}_{k+1}-\bar{Y}_k=2(-1)^k\bar{X}_{k+1}-2\,c\,\bar{X}_{k+1}, \tag{63}$$

we obtain the simplification

$$\sum_{k=0}^{a}(-1)^k\Big(\sum_{j=0}^{k}\bar{X}_j\Big)^2=\big(-\frac{c}{2}+\frac{1}{2}(-1)^a\big)\big(\sum_{k=0}^{a}\bar{X}_k\big)^2 \\ +\frac{1}{2}c\sum_{k=0}^{a}\bar{X}_k^2+\frac{1}{2}\sum_{k=0}^{a}(-1)^k\bar{X}_k^2+\frac{1}{2}\sum_{k=0}^{a}\bar{X}_k\bar{Y}_k-\frac{1}{2}\bar{Y}_a\sum_{k=0}^{a}\bar{X}_k. \tag{64}$$

In addition, by a slight modification of Theorem 5.7 we obtain the following stronger statement for any product-sum sequence ring $(\mathbb{S}, S)$ under the assumption that $\bar{X}_k$ is in $\mathbb{S}$, but $\sum_{j=0}^{k}\bar{X}_j$ is not in $\mathbb{S}$: the double sum can be simplified to single nested sums defined over $\mathbb{S}$ if and only if (64) holds and there are $\bar{Y}_k\in\mathbb{S}$ and $c\in\mathbb{K}$ with (63).

Again proceeding as above one can find, for instance, the following identities:

$$\sum_{k=0}^{a}(-1)^k\Big(\sum_{j=0}^{k}\binom{n}{j}\Big)^2=\frac{(-a+n)(-1)^a\binom{n}{a}}{n}\sum_{k=0}^{a}\binom{n}{k}+\frac{(-1)^a}{2}\Big(\sum_{k=0}^{a}\binom{n}{k}\Big)^2 \\ -\frac{1}{2}\sum_{k=0}^{a}(-1)^k\binom{n}{k}^2+\frac{1}{n}\sum_{k=0}^{a}(-1)^k k\binom{n}{k}^2,$$

$$\sum_{k=0}^{a}(-1)^k\Big(\sum_{j=0}^{k}(-1)^j\binom{n}{j}\Big)^2=\frac{1}{2}\sum_{k=0}^{a}(-1)^k\binom{n}{k}^2 \\ -\frac{1}{n}\sum_{k=0}^{a}(-1)^k k\binom{n}{k}^2+\frac{(-1)^a\binom{n}{a}^2(-a+n)^2}{2n^2},$$

$$\sum_{k=0}^{a}(-1)^k\Big(\sum_{j=0}^{k}\frac{1}{\binom{n}{j}}\Big)^2=\frac{(a+1)(-1)^a}{(n+2)\binom{n}{a}}\sum_{k=0}^{a}\frac{1}{\binom{n}{k}}+\frac{(-1)^a}{2}\Big(\sum_{k=0}^{a}\frac{1}{\binom{n}{k}}\Big)^2 \\ +\frac{n}{2(n+2)}\sum_{k=0}^{a}\frac{(-1)^k}{\binom{n}{k}^2}-\frac{1}{n+2}\sum_{k=0}^{a}\frac{(-1)^k k}{\binom{n}{k}^2},$$

$$\sum_{k=0}^{a}(-1)^k\Big(\sum_{j=0}^{k}\frac{(-1)^j}{\binom{n}{j}}\Big)^2=-\frac{n}{2(n+2)}\sum_{k=0}^{a}\frac{(-1)^k}{\binom{n}{k}^2}+\frac{1}{n+2}\sum_{k=0}^{a}\frac{(-1)^k k}{\binom{n}{k}^2} \\ +\frac{n+1}{n+2}\sum_{k=0}^{a}\frac{1}{\binom{n}{k}}+\frac{(a+1)(n+1)}{(n+2)^2\binom{n}{a}} \\ +\frac{(n+1)^2(-1)^a}{2(n+2)^2}+\frac{(a+1)^2(-1)^a}{2(n+2)^2\binom{n}{a}^2},$$

where the first two identities are valid for $a, n \in \mathbb{Z}$ and $n \neq 0$ and the last two identities are valid for $a, n \in \mathbb{Z}$ with $a \leq n$.

7 Conclusion

In this article, under the umbrella of algorithmic symbolic summation, we established new algebraic connections between summation problems involving generic sequences and difference field/ring theory taking special care of concrete sequences arising in contexts like analysis, combinatorics, number theory and special functions. We feel this is only the "first word" in view of the high potential for applications of various kinds. One future application domain is summation identities involving elliptic functions or modular forms. This will be especially interesting in upcoming calculations [1] emerging in renormalizable Quantum Field Theories. Another more concrete application domain is the area of q-identities involving q-hypergeometric series and sums. But already for $q = 1$ one can study aspects of *definite* summation. We plan to investigate these questions in forthcoming articles. For example, if we specialize our sums to definite versions by setting $a = n$ (and possibly consider the even or odd case), further simplifications can be achieved by `Sigma`. Typical examples are

$$\sum_{k=0}^{n}\Big(\sum_{j=0}^{k}\frac{1}{\binom{n}{j}}\Big)^2 = \frac{3(n+1)^3(n+2)}{4(2n+1)(2n+3)\binom{2n}{n}}\sum_{k=1}^{n}\frac{\binom{2k}{k}}{k} + 2^{-n-1}(n+1)\sum_{k=1}^{n}\frac{2^k}{k}$$
$$+ 2^{-2n-3}(n+1)^2(n+2)\Big(\sum_{k=1}^{n}\frac{2^k}{k}\Big)^2 + \frac{n^2+6n+6}{2(2n+3)},$$

$$\sum_{k=0}^{2n}(-1)^k\Big(\sum_{j=0}^{k}\frac{1}{\binom{2n}{j}}\Big)^2 = \frac{2^{-2n-2}(2n+1)(4n+3)}{n+1}\sum_{k=1}^{2n}\frac{2^k}{k}$$
$$+ 2^{-4n-3}(2n+1)^2\Big(\sum_{k=1}^{2n}\frac{2^k}{k}\Big)^2 + \frac{3n+2}{2(n+1)},$$

$$\sum_{k=0}^{2n}(-1)^k\Big(\sum_{j=0}^{k}\binom{2n}{j}\Big)^2 = 2^{4n-1},$$

where the first two identities are valid for $n \geq 0$ and the last identity holds for $n \geq 1$.

8 Appendix: Simple *RΠΣ*-Rings and Algorithmic Properties

For a given difference ring (resp. field) $(\mathbb{A}, \sigma)$, i.e., a ring (resp. field) $\mathbb{A}$ equipped with a ring (resp. field) automorphism $\sigma : \mathbb{A} \to \mathbb{A}$ the set of constants $\mathbb{K} := \mathrm{const}(\mathbb{A}, \sigma) = \{c \in \mathbb{A} \,|\, \sigma(c) = c\}$ forms a subring (resp. subfield) of $\mathbb{A}$. In this article we suppose that $\mathbb{A}$ contains the rational numbers $\mathbb{Q}$ as a subfield. Since $\sigma(1) = 1$, this implies that $\mathbb{Q} \subseteq \mathbb{K}$ always holds. Moreover, by construction we will take care that $\mathbb{K}$ will be always a field which will be called the constant field of $(\mathbb{A}, \sigma)$.

In the following we introduce the class of simple $R\Pi\Sigma$-rings that forms the fundament of Sigma's difference ring engine. Depending on the given input problem, the ground field is chosen accordingly among one of the following three difference fields.

Definition 8.1 We consider the following three difference fields $(\mathbb{F}, \sigma)$ with constant field $\mathbb{K}$.

(1) The *rational case*: $\mathbb{F} = \mathbb{K}(k)$ where $\mathbb{K}(k)$ is a rational function field and $\sigma(k) = k + 1$.
(2) The *q-rational case*: $\mathbb{F} = \mathbb{K}(z)$ where $\mathbb{K}(z)$ is a rational function field, $\mathbb{K} = \mathbb{K}'(q)$ is a rational function field ($\mathbb{K}'$ is a field) and $\sigma(z) = q\,z$.
(3) The *mixed case*: $(\mathbb{K}(k)(z_1, \dots, z_v), \sigma)$ where $\mathbb{K}(k)(z_1, \dots, z_v)$ is a rational function field, $\mathbb{K} = \mathbb{K}'(q_1, \dots, q_v)$ is a rational function field ($\mathbb{K}'$ is a field), $\sigma(k) = k + 1$, and $\sigma(z_i) = q_i\, z_i$ for $1 \le i \le v$.

We remark that these difference fields can be embedded into the ring of sequences $(\mathrm{Seq}(\mathbb{K}), S)$ as expected. For the rational case see Example 5.1, and for the other two cases we refer to [22, Ex. 5.3]. Further aspects can be found in [6].

On top of such a ground field, a tower of extensions is built recursively depending on the input that is passed to Sigma. Let $(\mathbb{A}, \sigma)$ be the already constructed difference ring with constant field $\mathbb{K}$. Then the tower can be extended by one of the following three types of extensions [8, 21]; compare Definition 4.9.

(1) **Σ-extension**: Given $\beta \in \mathbb{A}$, take the polynomial ring $\mathbb{A}[t]$ (t is transcendental over $\mathbb{A}$) and extend the automorphism σ from $\mathbb{A}$ to $\mathbb{A}[t]$ subject to the relation $\sigma(t) = t + \beta$. If $\mathrm{const}(\mathbb{A}[t], \sigma) = \mathrm{const}(\mathbb{A}, \sigma)$, the difference ring $(\mathbb{A}[t], \sigma)$ is called a *Σ-extension* of $(\mathbb{A}, \sigma)$.
(2) **Π-extension**: Given a unit $\alpha \in \mathbb{A}^*$, take the Laurent polynomial ring $\mathbb{A}[t, t^{-1}]$ (t is transcendental over $\mathbb{A}$) and extend the automorphism σ from $\mathbb{A}$ to $\mathbb{A}[t, t^{-1}]$ subject to the relation $\sigma(t) = \alpha\, t$ (and $\sigma(t^{-1}) = \frac{1}{\alpha}\, t^{-1}$). If $\mathrm{const}(\mathbb{A}[t, t^{-1}], \sigma) = \mathrm{const}(\mathbb{A}, \sigma)$, the difference ring $(\mathbb{A}[t, t^{-1}], \sigma)$ is called a *Π-extension* of $(\mathbb{A}, \sigma)$.
(3) **R-extension**: Given a primitive λth root of unity $\alpha \in \mathbb{K}$ with $\lambda \ge 2$, take the algebraic ring $\mathbb{A}[t]$ subject to the relation $t^{\lambda} = 1$ and extend the automorphism σ from $\mathbb{A}$ to $\mathbb{A}[t]$ subject to the relation $\sigma(t) = \alpha\, t$. If $\mathrm{const}(\mathbb{A}[t], \sigma) = \mathrm{const}(\mathbb{A}, \sigma)$, the difference ring $(\mathbb{A}[t], \sigma)$ is called an *R-extension* of $(\mathbb{A}, \sigma)$.

More generally, we call a difference ring $(\mathbb{E}, \sigma)$ an *$R\Pi\Sigma$-extension* of a difference ring $(\mathbb{A}, \sigma)$ if it is built by a tower

$$\mathbb{A} = \mathbb{E}_0 \leq \mathbb{E}_1 \leq \cdots \leq \mathbb{E}_e = \mathbb{E} \tag{65}$$

of R-, Π-, and Σ-extensions starting from the difference ring $(\mathbb{A}, \sigma)$. Note that by construction we have that $\mathrm{const}(\mathbb{E}, \sigma) = \mathrm{const}(\mathbb{A}, \sigma) = \mathbb{K}$. Finally, we restrict to the following case that is relevant for this article.

Definition 8.2 We call a difference ring $(\mathbb{E}, \sigma)$ a *simple $R\Pi\Sigma$-ring with constant field* $\mathbb{K}$ if it is an $R\Pi\Sigma$-extension of a difference ring $(\mathbb{A}, \sigma)$ built by the tower (65) with the following properties:

(1) $(\mathbb{A}, \sigma)$ is one of the three difference fields from Definition 8.1;
(2) for i with $1 \leq i \leq e$ the following holds: if $(\mathbb{E}_i, \sigma)$ is a Π-extension of $(\mathbb{E}_{i-1}, \sigma)$ with $\mathbb{E}_i = \mathbb{E}_{i-1}[t_i, t_i^{-1}]$, then $\sigma(t_i)/t_i \in \mathbb{A}^*$.

Note that within such a simple $R\Pi\Sigma$-ring the generators of

(a) R-extensions model algebraic products of the form α^k where α is a primitive root of unity;
(b) Π-extensions model (q–)hypergeometric/mixed hypergeometric products depending on the chosen base field $(\mathbb{A}, \sigma)$;
(c) Σ-extensions represent nested sums whose summands are built recursively by polynomial expressions in terms of objects that are introduced in (a), (b) and (c).

Given such a simple $R\Pi\Sigma$-ring with constant field $\mathbb{K}$, we can exploit the algorithmic properties summarized in Theorem 5.4 that are incorporated within the summation package `Sigma`. For a detailed description of parts (1) and (2a) of Theorem 5.4 we refer to [22, Section 7.2]; for part (2b) of Theorem 5.4 we refer to [22, Section 5].

In the following we sketch some further aspects. Namely, given an expression $X(k)(= X_k)$ in terms of nested sums over hypergeometric (resp. q-hypergeometric or mixed hypergeometric) products, one can always construct algorithmically an $R\Pi\Sigma$-ring $(\mathbb{E}, \sigma)$ together with an evaluation function $\mathrm{ev} : \mathbb{E} \times \mathbb{Z}_{\geq 0} \to \mathbb{K}$ with the following two properties (A) and (B).

(A) $(\mathbb{E}, \sigma)$ is constructed explicitly by the tower of extensions (65) with the generators t_i ($\mathbb{E}_i = \mathbb{E}_{i-1}[t_i]$ for R- or Σ-extensions and $\mathbb{E}_i = \mathbb{E}_{i-1}[t_i, t_i^{-1}]$ for a Π-extension) where for $1 \leq i \leq e$, there is an explicitly given product or a nested sum over products, say $F_i(k)$, and a $\lambda_i \in \mathbb{Z}_{\geq 0}$ such that $\mathrm{ev}(t_i, k) = F_i(k)$ holds for all $k \geq \lambda_i$. In particular, the resulting map $\tau : \mathbb{E} \to \mathrm{Seq}(\mathbb{K})$ with $\tau(f) \equiv (\mathrm{ev}(f, k))_{k \geq 0}$ yields a $\mathbb{K}$-embedding.

Example 8.3 Consider the $R\Pi\Sigma$-ring $(\mathbb{K}(k)[s], \sigma)$ from Example 4.8. There we obtained ev with $\mathrm{ev}(s, k) = H_k$ for all $k \geq \lambda$ with $\lambda = 0$.

(B) One can construct an element $x \in \mathbb{E}$ and a $\lambda \in \mathbb{Z}_{\geq 0}$ such that $X(i) = \mathrm{ev}(x, i)$ holds for all $i \geq \lambda$. In particular, this $x \in \mathbb{E}$ can be rephrased again as an expression in terms of products or sums defined over such products in the following way: replacing the generators t_i in f by the attached sums or products[18] one gets an expression $X'(k)$ in terms of nested sums over products such that $X(k) = \mathrm{ev}(x, k) = X'(k)$ holds for all $k \in \mathbb{Z}_{\geq 0}$ with $k \geq \lambda$.

In addition, the summation paradigms of refined parameterized telescoping [17–22] and recurrence solving can be carried out in such simple $R\Pi\Sigma$-rings. In a nutshell, we can solve the telescoping problem and enhanced versions of it in the $R\Pi\Sigma$-ring $(\mathbb{E}, \sigma)$ or equivalently in the product-sum sequence ring $(\mathbb{S}, S)$. This enables one to discover, e.g., the identities given in Sect. 7.

Furthermore, the difference ring algorithms combined with the algorithms given in [11] work also for difference rings where one starts with the free difference field $(\mathbb{G}, \sigma)$ introduced in Sect. 6.1 as base field, adjoins the generators given in Definition 8.1, and puts a tower of $R\Pi\Sigma$-extensions on top; compare Sect. 6.1.

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[18] In the q-case (resp. in the mixed case) we also have to replace z by q^k (resp. z_i by q_i^k for $1 \leq i \leq v$).

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Differential Equations and Dispersion Relations for Feynman Amplitudes

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Abstract The derivation of the Cutkosky's cutting rule by means of the Veltman's Largest Time Equation is described in detail, and the use of cut graphs, imaginary parts and dispersive representations within the Differential Equation approach to the evaluation of Feynman graph amplitudes is discussed.

1 Introduction

The explicit evaluation of the imaginary part of a Feynman graph amplitude can be significantly simpler than the evaluation of the whole amplitude; the imaginary part can then be used, by means of a dispersion relation, to reconstruct the whole amplitude.

This talk will discuss the possibility of using imaginary parts and dispersive representation within the differential equations approach to Feynman amplitudes; indeed, it turns out that in some cases (when the unitarity cuts are also maximal cuts) the imaginary part can provide with the solutions of the associated homogeneous equation, while quite in general writing a dispersive representation for the inhomogeneous terms may be of great help in obtaining the whole solution when using the Euler's variation of the constants approach.

Section 2 contains a thorough description of the derivation of the unitarity cutting rules by Dick Cutkosky [1] obtained through the Largest Time Equation of Tini Veltman [2], and some examples of its application. Section 3 discusses in details the 1-loop `Bubble` amplitude with its unitary and generalised (maximal) cuts, Sect. 4 the role of the imaginary parts within the Differential Equation approach.

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Section 5 deals with the `Sunrise` amplitude and its connections to the elliptic functions, Sect. 6 with the 3-loop `Banana` graph. Section 7, finally, describes the dispersive representations and their use when dealing with the inhomogeneous terms of the Differential Equations.

2 Veltman's Largest Time Equation

Cut graphs and cut propagators were introduced in 1960 by Dick Cutkosky in his paper *Singularities and discontinuities of Feynman amplitudes* [1], whose Abstract says "It is shown that the discontinuity across a branch cut starting from any Landau singularity is obtained by replacing Feynman propagators by delta functions for those lines which appear in the Landau diagram. The general formula is a simple generalization of the unitarity condition".

The word *cut* appears already in the abstract, but refers, in the analytic function terminology, to the discontinuity of the considered Feynman amplitude. If such an amplitude is given by a complex function $f(s)$ of some Mandelstam variable s, for s real and above a threshold s_0, i.e. for $s > s_0$ one has

$$2i\,\mathtt{Im}f(s) = f(s+i\varepsilon) - f(s-i\varepsilon)$$

where $2i\,\mathtt{Im}f(s)$ is the discontinuity of $f(s)$ across the *cut* $s_0 < s < +\infty$.

The propagators, to be replaced by delta functions (the mass-shell conditions for the propagating particles) for obtaining the imaginary part (also equal to the discontinuity of the graph), are usually called *cut propagators*; further, they cut the Feynman graph into the product of two subgraphs (the *unitarity cut*), and the whole result is referred to as the *Cutkosky cutting rule*.

The Cutkosky derivation relies on analytic functions theory; in his paper of 1963, *Unitarity and causality in a renormalizable field theory with unstable particles* [2] Tini Veltman recovered the Cutkosky rule by using only the space-time properties of the Feynman propagators. The Veltman's derivation will be shortly described in this Section, following closely the treatment of [3].

To start with, let us write the (scalar) Feynman propagator as

$$\Delta(x) = \int \frac{d^4p}{(2\pi)^4}\frac{-i}{p^2+m^2-i\varepsilon}\,\mathrm{e}^{ipx}\ ,$$

with $p^2 = \mathbf{p}\cdot\mathbf{x} - p_0x_0$. The above formula refers to $1+3=4$ dimensions, but it is of immediate extension to continuous dimensions d with 1 time and $(d-1)$ space dimensions.

From the definition, one immediately derives the following formulas

$$\Delta(x) = \Delta(-x) = \int \frac{d^4p}{(2\pi)^4}\frac{-i}{p^2+m^2-i\varepsilon}\,\mathrm{e}^{ipx}\ , \tag{1}$$

$$\Delta(x) = \theta(x_0)\Delta^+(x) + \theta(-x_0)\Delta^-(x)\ , \tag{2}$$

$$\Delta^+(x) = \int \frac{d^4p}{(2\pi)^4}(2\pi)\theta(+p_0)\ \delta(p^2+m^2)\mathrm{e}^{ipx}\ , \tag{3}$$

$$\Delta^-(x) = \int \frac{d^4p}{(2\pi)^4}(2\pi)\theta(-p_0)\ \delta(p^2+m^2)\mathrm{e}^{ipx}\ , \tag{4}$$

$$\Delta^+(-x) = \Delta^-(x)\ , \tag{5}$$

$$\Delta^*(x) = \Delta^*(-x) = \int \frac{d^4p}{(2\pi)^4}\frac{i}{p^2+m^2+i\varepsilon}\ \mathrm{e}^{ipx}\ , \tag{6}$$

$$\Delta^*(x) = \theta(x_0)\Delta^-(x) + \theta(-x_0)\Delta^+(x)\ . \tag{7}$$

$$(\ \Delta^+(x)\ )^* = \Delta^-(x)\ . \tag{8}$$

The functions $\Delta(x)$, $\Delta^{\pm}(x)$ *etc.* will be graphically represented with the following lines

x_1 $x_2 = \Delta(x_1 - x_2) = \Delta(x_2 - x_1)$ (9)

x_1  $x_2 = \Delta^*(x_1 - x_2) = \Delta^*(x_2 - x_1)\ ,$ (10)

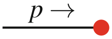
x_1  $x_2 = \Delta^-(x_1 - x_2) = \Delta^+(x_2 - x_1)\ ,$ (11)

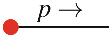
x_1  $x_2 = \Delta^+(x_1 - x_2) = \Delta^-(x_2 - x_1)\ .$ (12)

The first line, x_1 x_2 is not oriented, i.e. it corresponds to the propagator $\Delta(x_1 - x_2)$ from x_1 to x_2, or, which the same, the propagator $\Delta(x_2 - x_1)$ from x_2 to x_1, and the same applies to x_1  x_2..

The last two lines, on the contrary, are oriented; x_1  x_2 corresponds to $\Delta^-(x_1 - x_2)$ from x_1 to x_2, or $\Delta^+(x_2 - x_1)$ from x_2 to x_1, while x_1  x_2 corresponds to $\Delta^+(x_1 - x_2)$ from x_1 to x_2, or $\Delta^-(x_2 - x_1)$ from x_2 to x_1. As we will see, they correspond to the *cut propagators*.

In the momentum representation, one has

$p \rightarrow$  $= 2\pi\theta(p_0)\delta(p^2+m^2)\ ,$

$p \rightarrow$  $= 2\pi\theta(-p_0)\delta(p^2+m^2)\ ,$ (13)

showing that in a *cut propagator* (i.e. a line joining an uncircled to a circled vertex) according to Eqs. (3), (4) there is a *positive* energy flow towards the circled vertex, while in a line without circled vertices or with both vertices circled, according to Eqs. (2), (7) the energy can flow in both directions.

Graphically, Eq. (2) can be represented as

$$
\begin{aligned}
x_1 \;\rule[0.5ex]{3em}{0.4pt}\; x_2 \;=\; & \theta(x_{10}-x_{20}) \;\; x_1 \bullet\!\rule[0.5ex]{3em}{0.4pt}\; x_2 \\
& + \theta(x_{20}-x_{10}) \;\; x_1 \;\rule[0.5ex]{3em}{0.4pt}\!\bullet\, x_2 \;,
\end{aligned}
\tag{14}
$$

and Eq. (7) as

$$
\begin{aligned}
x_1 \bullet\!\rule[0.5ex]{3em}{0.4pt}\!\bullet\, x_2 \;=\; & \theta(x_{10}-x_{20}) \;\; x_1 \;\rule[0.5ex]{3em}{0.4pt}\!\bullet\, x_2 \\
& + \theta(x_{20}-x_{10}) \;\; x_1 \bullet\!\rule[0.5ex]{3em}{0.4pt}\; x_2 \;.
\end{aligned}
\tag{15}
$$

Given two points x, x_M, with $x_{M0} > x_0$, thanks to the above equations one finds, again in the graphic representation, the relations

$$
\begin{aligned}
\texttt{if}: \quad x_{M0} > x_0 \qquad & x \;\rule[0.5ex]{3em}{0.4pt}\; x_M = \; x \;\rule[0.5ex]{3em}{0.4pt}\!\bullet\, x_M \;, \\
& x \bullet\!\rule[0.5ex]{3em}{0.4pt}\; x_M = \; x \bullet\!\rule[0.5ex]{3em}{0.4pt}\!\bullet\, x_M \;;
\end{aligned}
\tag{16}
$$

the above relations tell us that, if $x_{M0} > x_0$, the presence of a (red) circle on x_M makes no difference, independently from the presence, or absence, of a circle on x, the other extreme of the line.

A Feynman graph in configuration space is given by N interaction vertex points $x_1, x_2, .., x_N$, suitably joined by propagator lines. The corresponding Feynman graph amplitude $F(x)$ (where x stands for all the N vertex points, considering for simplicity the scalar case only, and omitting coupling constants) is the product of

- a factor i for each interaction vertex,
- a (scalar) propagator $x_i \;\rule[0.5ex]{3em}{0.4pt}\; x_j \;\; = \Delta(x_i - x_j) = \Delta(x_j - x_i)$ for each line joining any two points x_i, x_j.

As a consequence of Eq. (9), in particular,

$$
F(-x) = F(x) \;. \tag{17}
$$

As a further simplification, all the propagators will be given a same mass m, but the discussion which will follow applies to the case of different masses as well. The above amplitude $F(x_i)$ must then be integrated on all the internal points (i.e. the points not connected to the external particle lines).

Given an N vertices graph, consider the set of all the 2^N related graphs, obtained by taking the original graph and putting a (red) circle on each of the N vertices, in all the possible ways, and for each of the 2^N new graph define a new amplitude, by following the graphical representations of Eqs. (9)–(12), as the product of the following factors:

- a factor i for each original vertex, $(-i)$ for each circled vertex;
- a factor x_i ——— x_j $= \Delta(x_i - x_j) = \Delta(x_j - x_i)$ for each line joining two uncircled vertices (x_i, x_j);
- x_i●——— x_j $= \Delta^+(x_i - x_j) = \Delta^-(x_j - x_i)$ for each line joining a circled x_i to an uncircled x_j; or, which is the same
- x_i ———● x_j $= \Delta^-(x_i - x_j) = \Delta^+(x_j - x_i)$ for each line joining an uncircled x_i to a circled x_j;
- x_i●———● x_j $= \Delta^*(x_i - x_j) = \Delta^*(x_j - x_i)$ for each line joining two circled vertices (x_i, x_j).

As it is easy to check, the *circling* operation is related to complex conjugation; given any graph with a subset of *circled* vertices, the corresponding graph where the vertices of that subset are without circles, and all the others vertices are with circles is its complex conjugate. In particular, if the amplitude of the original Feynman graph with N vertices is $F(x)$, the amplitude of the graph with N circles is $F^*(x)$, i.e.

$$F(x) + F^*(x) = 2\mathrm{Re}F(x) \; . \tag{18}$$

Let us recall that (in the S-matrix contest) one is usually interested in a quantity

$$A(x) = -iF(x) \; , \tag{19}$$

so that

$$\begin{aligned} F(x) &= iA(x) \; , \\ \mathrm{Re}F(x) + i\,\mathrm{Im}F(x) &= i\,\mathrm{Re}A(x) - \mathrm{Im}A(x) \; , \\ \mathrm{Re}F(x) &= -\mathrm{Im}T(x) \; ; \end{aligned} \tag{20}$$

for that reason, the real part of $F(x)$ is usually referred to as the *imaginary part*, or *discontinuity*, see Sect. 7, of the amplitude.

If if $\tilde{F}(p)$ is then the Fourier transform of $F(x)$

$$\tilde{F}(p) = \int dx \; F(x) \mathrm{e}^{-ipx}$$

one has, recalling in particular Eq. (17)

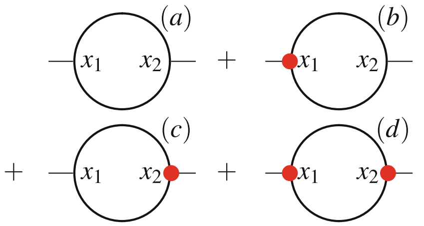
$$
\begin{aligned}
\left(\tilde{F}(p)\right)^* &= \int dx \left(F(x) \mathrm{e}^{-ipx} \right)^* \\
&= \int dx \big(F(x)\big)^* \, \mathrm{e}^{ipx} \\
&= \int dx \big(F(-x)\big)^* \, \mathrm{e}^{-ipx} \\
&= \int dx \; F^*(x) \, \mathrm{e}^{-ipx} \;,
\end{aligned}
$$

so that

$$
\begin{aligned}
\mathtt{Re}\tilde{F}(p) &= \int dx \; \mathtt{Re}F(x)\mathrm{e}^{-ipx} \;, \\
\mathtt{Im}\tilde{F}(p) &= \int dx \; \mathtt{Im}F(x)\mathrm{e}^{-ipx} \;,
\end{aligned}
\tag{21}
$$

i.e. the real part of the Fourier transform of the amplitude is the Fourier transform of the real part of the amplitude (and the same applies to the imaginary part).

The Veltman's *Largest Time Equation* states that the sum of all the 2^N *circled* amplitudes defined above, including the original amplitude $F(x_i)$, vanishes. The proof can best be followed in a first simple and explicit example, the one-loop bubble, for which the largest time equation can be graphically represented as



$$= 0 \,. \tag{22}$$

Now the proof: let $x_{0,M}$ be the largest of all the $x_{0,i}$ times, say $x_{0,2} > x_{0,1}$ in the above example. Take (in any order) the first of the 2^N *circled* graphs in which the vertex x_M is not *circled*, say graph (a) above, and look for its partner graph in which the vertex x_M is *circled*, but all the other vertices x_i have the same *circles*; in our example, it corresponds to graph (c). According to the rules defining the *circled* graphs and Eq. (14), because $x_{20} > x_{1,0}$,the amplitude of graph (a) is

$$\varDelta(x_2 - x_1)\; \varDelta(x_2 - x_1) = \varDelta^+(x_2 - x_1)\; \varDelta^+(x_2 - x_1)$$

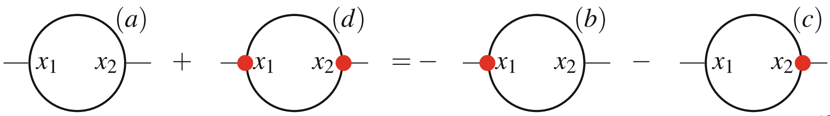
while the amplitude for the graph (c), remembering the factor -1 due to the circle in x_2, is

$$-\Delta^+(x_2 - x_1)\,\Delta^+(x_2 - x_1)\;.$$

The sum of the amplitudes corresponding to the two graphs (a) and (b) therefore vanishes.

Consider then the next graph without a circle on the vertex x_2, graph (b) in our example, pair it with its partner, which is graph (d): for the same reasons as for the first pair of graphs, the sum of the amplitudes corresponding to (b) and (d) also vanishes; and so until all the other *circled* graphs (if any) are paired and found to cancel each other, so that the sum of all the 2^{N-1} pairs formed by the 2^N *circled* graphs vanishes.

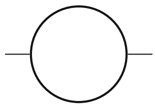
Equation (22) can then be rewritten as



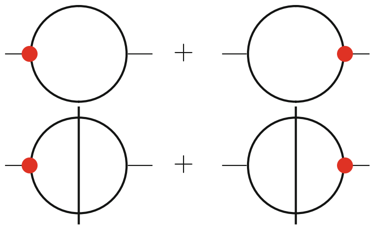
(23)

Recalling that the amplitude (d) is the complex conjugate of the amplitude (a),

From now on, having in mind Eqs. (19)–(21), let us define, in the momentum representation,

$iA(p) = p$  , (24)

where p is the momentum entering in the graph; the largest time equation then gives

$2\,\mathrm{Im}A(p) =$  (25)

where, in the second line, the two *cut propagator lines* are joined to give a *cut graph*.

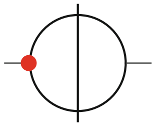
From Eq. (24) one has (in d continuous dimensions, and in the different masses case, with $M > m$)

$$A(p) = -i \int \frac{d^d k}{(2\pi)^d} \frac{1}{D_1 - i\varepsilon} \frac{1}{D_2 - i\varepsilon}\;, \tag{26}$$

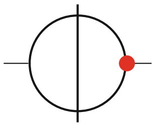
with

$$D_1 = k^2 + m^2 = -k_0^2 + \mathbf{k}^2 + m^2 \ ,$$
$$D_2 = (p-k)^2 + M^2 = -(p_0 - k_0)^2 + (\mathbf{p} - \mathbf{k})^2 + M^2 \ ,$$

where $\mathbf{k}$ stands for the $(d-1)$ space dimensions of the d-dimensional vector k, so that finally



$$= \int \frac{d^d k}{(2\pi)^{d-2}} \theta(-k_0)\delta(D_1)\theta(-(p_0-k_0))\delta(D_2) \ , \tag{27}$$



$$= \int \frac{d^d k}{(2\pi)^{d-2}} \theta(k_0)\delta(D_1)\theta(p_0-k_0)\delta(D_2) \ . \tag{28}$$

Quite in general, the δ-function constraints

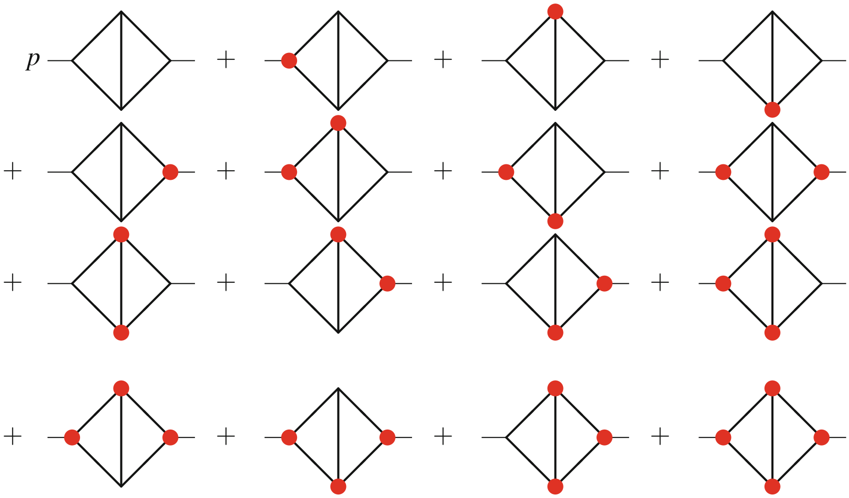
$$\delta(D_1) = \delta(k^2 + m^2) = -k_0^2 + \mathbf{k}^2 + m^2 \ ,$$
$$\delta(D_2) = \delta((p-k)^2 + M^2) = -(p_0 - k_0)^2 + (\mathbf{p} - \mathbf{k})^2 + M^2 \ ,$$

imply

$$|k_0| > m \ , \quad |p_0 - k_0| > M \ . \tag{29}$$

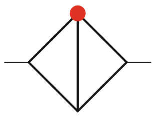
Let us consider, for simplicity, only the case of timelike p in its restframe, where it has components $p = (p_0, 0)$. In Eq. (27), due to the presence of the factors $\theta(-k_0), \theta(-(p_0 - k_0))$ the conditions (29) require, to be satisfied, $p_0 < -(M+m)$, in agreement with Eq. (13) (in a cut propagator, the energy flows towards the circle, and, due to energy conservation, the energy must leave the graph along the incoming external particle line). Similarly, Eq. (28) is different from zero only if $p_0 > (M+m)$ (or *above threshold*). In both cases, if $u = -p^2 = p_0^2$ is the Mandelstam variable associated to the vector p, one has that the condition $u > (M+m)^2$ must be satisfied for obtaining a non vanishing result.

As another example, consider the two loop (massive) *kite* graph, whose largest time equation can be depicted as

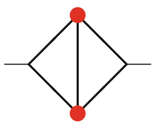


$= 0$

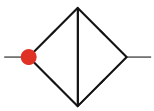
The *kite* has 4 vertices, so there are $2^4 = 16$ *circled* graphs; but many of them vanish. One has, for instance,

 $= 0\,;$

indeed, all the three cut lines meeting in the upper vertex according to Eq. (13) carry positive energy there, violating energy conservation at that vertex. Similarly,

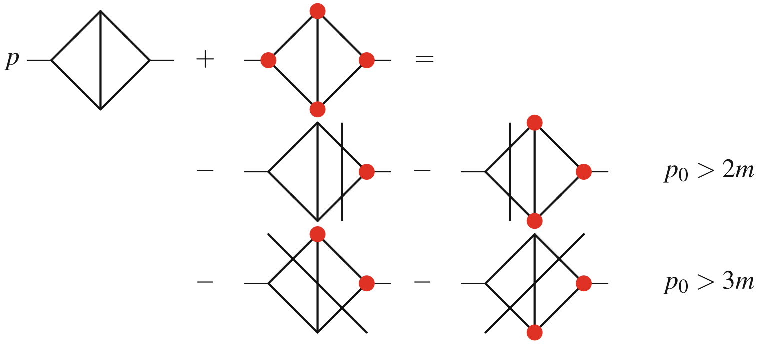
 $= 0\,,$

because there is an energy flow to the upper or lower vertices and among them, according to Eq. (7), but no way of leaving them. Further, for timelike $p = (p_0, 0)$ with $p_0 > 0$,

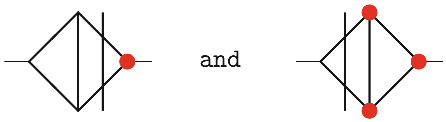
 $= 0\,,$

as the energy from the incoming particle and the two cut propagator lines flows to the left vertex and has no way of leaving it.

For timelike $p = (p_0, 0)$ with $p_0 > 0$, dropping the *circled* graphs which vanish, the largest time equation becomes

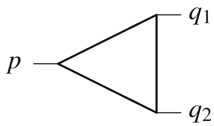


Let us comment that the amplitudes corresponding to

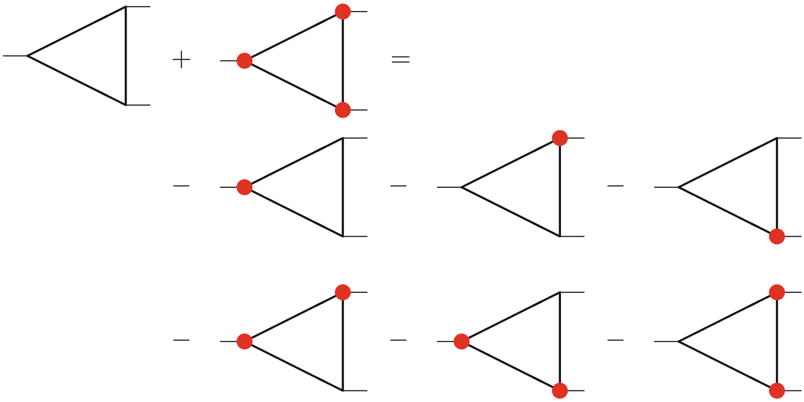


are the complex conjugate of each other, so that their sum is real (as it should be...), and are different from zero if $p_0 > 2m$ (two particle cut), while for $p_0 > 3m$ (three particle cut) also the last two graphs contribute.

As one more example, consider the 1-loop vertex



The largest time equation is immediately written

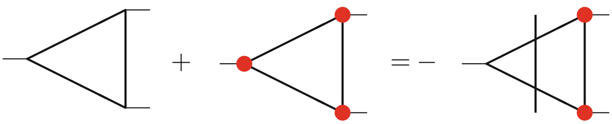


(30)

but the discussion of its meaning is less immediate than in the self-mass case.

The vertex amplitude is a function of the three Mandelstam variables $(-p^2)$, $(-q_1^2)$, $(-q_2)^2$, and any of the above *circled* graphs can contribute to the imaginary part depending, on equal footing, of the actual values of those variables. The complete discussion of the general dependence on the three variables is highly non trivial; a practical approach might be to start from the region in which all the three variables are in the Euclidean region, where all the *circled* graphs vanish, and then moving judiciously one of the variables at the time to the Minkosky region ...

Considering the case in which all the internal masses are equal to m, one can arrive for instance at the kinematical region in which the vector p is timelike and has components $p = (p_0, 0)$, with $p_0 > 2m$ and, say, $(-q_1^2) = (-q_2)^2 = m^2$; the largest time Eq. (30) then becomes



where the cut graph does not vanish if $p_0 > 2m$.

3 The 1-Loop Bubble

In this section we consider again, in some more details but in $d = 2$ dimensions, the amplitude $A(p)$ with timelike $p = (p_0, 0)$ already introduced in Eq. (26)

$$A(p) = -i \int \frac{dk_0 dk_z}{(2\pi)^2} \frac{1}{D_1 - i\varepsilon} \frac{1}{D_2 - i\varepsilon} , \tag{31}$$

$$D_1 = -k_0^2 + k_z^2 + m^2 ,$$

$$D_2 = -(p_0 - k_0)^2 + k_z^2 + M^2 .$$

The largest time equation reads

$$\begin{aligned}\mathtt{Im}A(p) &= \frac{1}{2}\int dk_0 dk_z\ \theta(-k_0)\delta(D_1)\theta(k_0-p_0)\delta(D_2)\\ &+ \frac{1}{2}\int dk_0 dk_z\ \theta(k_0)\delta(D_1)\theta(p_0-k_0)\delta(D_2)\ ,\end{aligned} \tag{32}$$

and an explicit (simple) calculation gives

$$\begin{aligned}\mathtt{Im}A(p) &= \frac{1}{2}\theta(+p_0-(M+m))\frac{1}{\sqrt{(p_0^2-(M+m)^2)(p_0^2-(M-m)^2)}}\\ &+ \frac{1}{2}\theta(-p_0-(M+m))\frac{1}{\sqrt{(p_0^2-(M+m)^2)(p_0^2-(M-m)^2)}}\ .\end{aligned} \tag{33}$$

It can be of interest to compare the previous result with the explicit calculation of the whole amplitude; recalling

$$\frac{1}{x-i\varepsilon} = \frac{x+i\varepsilon}{x^2+\varepsilon^2} = P\left(\frac{1}{x}\right) + i\pi\delta(x)$$

where $P(1/x)$ stands for the principal value, and by writing accordingly any propagator $1/(D-i\varepsilon)$ as

$$\frac{1}{D-i\varepsilon} = P\left(\frac{1}{D}\right) + i\pi\delta(D)\ , \tag{34}$$

Equation (31) becomes

$$\begin{aligned}A(p) = \int \frac{dk_0 dk_z}{(2\pi)^2}\Bigg[&\pi P\left(\frac{1}{D_1}\right)\delta(D_2) + \pi\delta(D_1)P\left(\frac{1}{D_2}\right)\\ &+ i\left(\pi^2\delta(D_1)\delta(D_2) - P\left(\frac{1}{D_1}\right)P\left(\frac{1}{D_2}\right)\right)\Bigg]\ .\end{aligned} \tag{35}$$

The direct calculation gives, for $p_0 = Z > (M+m)$

$$\begin{aligned}\mathtt{Re}A(p) &= \int \frac{dk_0 dk_z}{(2\pi)^2}\left[\pi P\left(\frac{1}{D_1}\right)\delta(D_2) + \pi\delta(D_1)P\left(\frac{1}{D_2}\right)\right]\\ &= -\frac{1}{2\pi\sqrt{(Z^2-(M-m)^2)(Z^2-(M+m)^2)}}\\ &\times \ln\frac{\sqrt{Z^2-(M-m)^2}+\sqrt{Z^2-(M+m)^2}}{\sqrt{Z^2-(M-m)^2}-\sqrt{Z^2-(M+m)^2}}\end{aligned} \tag{36}$$

and

$$\int \frac{dk_0 dk_z}{(2\pi)^2}\left[\pi^2\delta(D_1)\delta(D_2)\right] = \frac{1}{4\sqrt{(Z^2-(M-m)^2)(Z^2-(M+m)^2)}} \tag{37}$$

$$\int \frac{dk_0 dk_z}{(2\pi)^2}\left[P\left(\frac{1}{D_1}\right)P\left(\frac{1}{D_2}\right)\right] = -\frac{1}{4\sqrt{(Z^2-(M-m)^2)(Z^2-(M+m)^2)}} \tag{38}$$

so that

$$\begin{aligned}\mathtt{Im}A(p) &= \int \frac{dk_0 dk_z}{(2\pi)^2}\left[\pi^2\delta(D_1)\delta(D_2) - P\left(\frac{1}{D_1}\right)P\left(\frac{1}{D_2}\right)\right] \\ &= \frac{1}{2\sqrt{(Z^2-(M-m)^2)(Z^2-(M+m)^2)}}\,,\end{aligned} \tag{39}$$

in agreement (of course) with Eq. (33) for $p_0 = Z > (M+m)$.

It is to be noted that in the "naive" decomposition of $A(p)$ into its real and imaginary part, Eq. (35), the imaginary part receives two contributions, Eqs. (37) and (38), while the Cutkosky–Veltman cutting rule Eqs. (32), (33) for $p_0 > (M+m)$ gives a single contribution, corresponding, as Eq. (37), to the product of two δ-functions, but with different numerical factors and positivity conditions on the energies.

The two contributions to the imaginary part (37), (38) are always present, but their difference, see Eqs. (35), (39), vanishes when the condition $|p_0| > (M+m)$ is not satisfied. If, for instance, $0 < p_0 = U < (M-m)$, an explicit calculation gives that the two expressions take the same value,

$$\int \frac{dk_0 dk_z}{(2\pi)^2}\left[\pi^2\delta(D_1)\delta(D_2)\right] = \frac{1}{4\sqrt{((M-m)^2-U^2)((M+m)^2-U^2)}} \tag{40}$$

$$\int \frac{dk_0 dk_z}{(2\pi)^2}\left[P\left(\frac{1}{D_1}\right)P\left(\frac{1}{D_2}\right)\right] = \frac{1}{4\sqrt{((M-m)^2-U^2)((M+m)^2-U^2)}} \tag{41}$$

so that their difference, se Eqs. (35), (39), vanishes as expected.

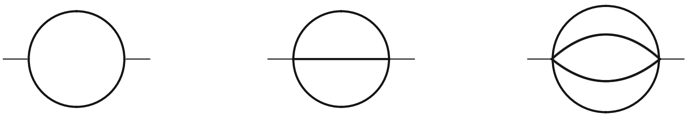
4 Imaginary Parts of the Amplitudes and Differential Equations

Take some Feynman amplitude $A(u)$ which satisfies a given differential equation in the variable u; the equation will have, in general, a homogeneous part, involving only $A(u)$, and an inhomogenous part, involving *simpler* amplitudes, supposedly known, corresponding to graphs in which some of the propagators appearing in $A(u)$ are missing.

As $ReA(u)$, $ImA(u)$ satisfy separately the real and imaginary parts of the equation, the equation for $ImA(u)$ it is expected to be simpler than the original equation. In the simplest cases, as for instance the 1-loop `Bubble`, the inhomogeneous terms are just real tadpoles, whose imaginary part vanishes, and the differential equation for the imaginary part of $A(u)$ is just the homogeneous part of the complete equation. More in general, however, also the inhomogeneous terms can develop an imaginary part, anyhow expected to be somewhat simpler than the full amplitude, so that the resulting equation is somewhat (or just marginally?) simpler than the original equation.

If all the inhomogeneous terms are tadpoles, (so that the differential equation for the imaginary part of the amplitude is exactly the homogeneous part of the equation), and one is able to evaluate directly the imaginary part of the graph (say by using the largest time equation), one can relay on that calculation for obtaining a first solution of the homogeneous equation, as a first step of the discussion and understanding of the complete equation.

The first obvious examples are the `Bubble`, `Sunrise` and `Banana` amplitudes



Let us start from the `Bubble` amplitude $\mathtt{Bub}(u)$, for different masses but considering only the $d = 2$ limit for simplicity; the homogeneous part of the equation for $\mathtt{Bub}(u)$ is

$$\frac{d}{du}\mathtt{Bub}(u) = -\frac{1}{2}\left(\frac{1}{u-(M+m)^2} + \frac{1}{u-(M-m)^2}\right)\mathtt{Bub}(u) \, , \tag{42}$$

whose solution, up to a multiplicative constant, irrelevant here, for $u > (M+m)^2$ is

$$\mathtt{Bub}(u) = \frac{1}{\sqrt{(u-(M+m)^2)(u-(M-m)^2)}} \, . \tag{43}$$

(Let us recall that, when considering only the real solutions of the previous equation, the multiplicative constants must be specified separately for each of the u intervals with end points $-\infty$, $(M-m)^2$, $(M+m)^2$ and ∞).

The result is obviously in agreement with the already seen imaginary part of $A(p)$, Eqs. (33), (39) obtained, according to the largest time equation, by considering the cut graphs with the *proper* signs of the energy solutions of the δ-function conditions. However, also Eqs. (37), (40), corresponding to the integrals of the same δ-functions, but without physical conditions on the signs of the energy solutions (and therefore not directly related to the Feynman amplitude) are proportional to the same square root Eq. (43) and are therefore solutions of the homogeneous equation (42).

To clarify this point, recall that the equation for the original Feynman amplitude was obtained by repeated use of the IBP's (*Integration by Parts Identities*) [4] for the integral of the product of two propagators in the loop variable $d^d k$ with integration contours from $-\infty$ to $+\infty$ specified around the propagator poles by the usual $m^2 \to m^2 - i\varepsilon$ Feynman prescription. An essential feature of those IBP's is the absence of *end point contributions*, as the integrands of the Feynman graphs can be considered as vanishing at infinity as a consequence of the properties of the continuous dimensional integration.

But end point contributions are absent also when the integration contour is a closed loop which does not cross a discontinuity cut of the integrand, (anyhow absent in the Feynman graph amplitudes), but containing some singularity (in our case the poles of the propagators), so that the integrals do not vanish trivially, symbolically something like

$$\oint_{C_1} dz\, \frac{df}{dz} = \oint_{C_2} dz\, \frac{df}{dz} = 0\,,$$

where C_1 is the contour from $-\infty$ to $+\infty$ and C_2 the contour around some pole(s). By writing a Feynman propagator as $1/(D - i\varepsilon)$, where D is a quadratic polynomial in the integration loop momentum, say $D = k^2 + m^2 = -(k_0^2 - K^2 - m^2)$ with two poles at $k_0 = \pm\sqrt{K^2 + m^2}$, in the Feynman amplitude the integration contour C_1 of k_0 runs along the real axis passing passing below and above the negative and positive poles. Replacing the Feynman propagator $1/(D - i\varepsilon)$ by, say, $\theta(k_0)\delta(D)$ amounts to keep the same factor $1/(D - i\varepsilon)$ in the intagrand, but to replace the previous *standard* integration path of k_0 by a (small) circle around the positive k_0 pole; similarly, replacing $1/(D - i\varepsilon)$ by $\delta(D) = (\theta(-k_0) + \theta(k_0))\ \delta(D)$ amounts to integrate on two (small) circles around both zeroes, *etc.* for the other propagators.

As the integrands do not change, and end point contributions are always absent, the structure of the IBP's for the integrals with the modified contours are the same as the IBP's for the original Feynman amplitude; therefore, also the differential equations for the modified countours are, at least *formally*, the same differential equations obtained for the original Feynman amplitude.

Why *formally*?

The IBP's can generate, among many other terms, a numerator consisting of polynomials in the scalar products of the various occurring vectors. Assume that there is a propagator $1/(D - i\varepsilon)$ in the integrand of the original Feynman amplitude, and that a factor D is generated by the IBP's in the numerator; as

$$D\, \frac{1}{D - i\varepsilon} = 1$$

in the resulting term the propagator $1/(D - i\varepsilon)$ is missing, so that the resulting term belongs to a (socalled) *subtopology* of the considered Feynman amplitude, ending up, in the equation for the amplitude, to an inhomogeneous term.

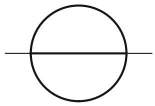
In the amplitudes in which the propagator is *cut*, i.e. in which $1/D - i\varepsilon$ is replaced by $\delta(D)$ (with or without θ-function specifications of the sign of the roots), the would-be inhomogeneous term, corresponding to $D/(D - i\varepsilon) = 1$ in the original amplitude, is missing, because

$$D\,\delta(D) = 0\,.$$

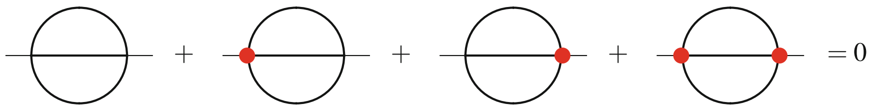
In the case of the Bubble, the double cut $\delta(D_1)\delta(D_2)$ implies that any inhomogeneous term corresponding to the absence of one of the propagators is absent; as the two propagators are both cut (so called *maximal cut*, or *maximally cut graph*), there are no inhomogeneous terms. The homogeneous equation for the imaginary part is so recovered.

As the equation is a first order equation, with just one solution, there is no surprise that all the cut amplitudes, being all solutions of a same homogeneous equation, are equal (more exactly, proportional).

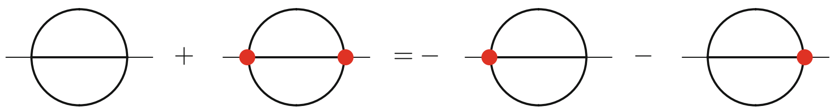
5 Sunrise

Now the Sunrise (scalar, equal masses) amplitude .

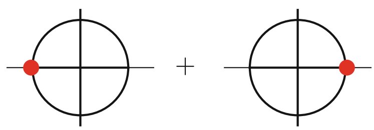
The largest time equation has the same structure as the Bubble, and gives

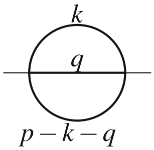


so that



or

$2\mathrm{ImSun}(u) =$ 

Introducing the momenta as p 

in the equal mass case the three propagators are

$$D_1 = k^2 + m^2, \qquad D_2 = q^2 + m^2, \qquad D_3 = (p-k-q)^2 + m^2$$

In $d = 2$ dimensions (for simplicity; and neglecting further the overall normalization), with $u = W^2 = (-p^2)$, the `Sunrise` amplitude is

$$\mathtt{Sun}(u) = -i \int \frac{d^2k\, d^2q}{(D_1 - i\varepsilon)(D_2 - i\varepsilon)(D_3 - i\varepsilon)} \, .$$

The homogeneous (second order) differential equation for $\mathtt{Sun}(u)$ is (in $d = 2$ dimensions)

$$\left\{ \frac{d^2}{du^2} + \left[\frac{1}{u} + \frac{1}{u - m^2} + \frac{1}{u - 9m^2} \right] \frac{d}{du} + \frac{1}{m^2} \left[-\frac{1}{3u} + \frac{1}{4(u - m^2)} + \frac{1}{12(u - 9m^2)} \right] \right\} \mathtt{Sun}(u) = 0$$

The triple cut of the largest time equation (which is also a maximal cut) is nothing but the *physical three particle phase space* at energy $W > 3m,\ u = W^2 > 9m^2$, know long since as the Dalitz–Fabri plot for the 3π's K-meson decay [5, 6].

Calling $I_0(u)$ that phase space, for $u = W^2$, $W > 3m$ one has, again up to a normalization factor,

$$\mathtt{ImSun}(u) = I_0(u) = \int_{4m^2}^{(W-m)^2} \frac{db}{\sqrt{R_4(u,b)}} \, , \tag{44}$$

where $R_4(u, b)$ is the fourth order polynomial in b

$$R_4(u,b) = b(b - 4m^2)((W-m)^2 - b)((W+m)^2 - b).$$

One can check [7, 8] that $I_0(u)$ is indeed a solution, by using a kind of suitable integration by parts identities involving $R_4(u, b)$, in which the vanishing of $R_4(u, b)$ at the end-points of the integration interval plays an essential role. Therefore, also all the integrals in b of the same integrand between any other two zeroes of $R_4(u, b)$ (or any other contour including those points) are solutions of the equation.

Standard considerations for contour integrals along a closed path show then that only two of them are independent, say the previous $I_0(u)$ and, for instance

$$J_0(u) = \int_0^{4m^2} \frac{db}{\sqrt{-R_4(u,b)}} \; .$$

Once the integral representation of the two independent solutions of the homogeneous equation is obtained, one can switch to *special function* mathematics, which gives

$$I_0(u) = \frac{2}{\sqrt{(W+3m)(W-m)^3}} \, K\left(\frac{(W-3m)(W+m)^3}{(W+3m)(W-m)^3}\right) \; ,$$
$$J_0(u) = \frac{2}{\sqrt{(W+3m)(W-m)^3}} \, K\left(1 - \frac{(W-3m)(W+m)^3}{(W+3m)(W-m)^3}\right) \; , \tag{45}$$

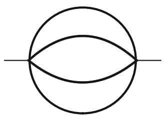
where $K(x)$ is a complete elliptic integral.

Knowing the homogeneous solutions, one can then use the Euler's formulas for obtaining the solution of the complete inhomogeneous equation, as well as the next terms in the $(d-2)$ expansion etc., as suitable repeated integrations of rational fractions times the homogeneous solutions in $d = 2$ dimensions seen above, $I_0(u)$ and $J_0(u)$. As $I_0(u)$ and $J_0(u)$ are complete elliptic integrals, it is natural to call, somewhat loosely, (generalized) Elliptic Polylogarithms all the (new) integrals appearing when following the Euler's method, by analogy with the (generalized) Polylogarithms appearing when the solutions of the differential equations can be expressed as repeated integrals of rational functions only.

More rigorous, unambiguous definitions of Elliptic Polylogarithms exist, linking them to the general theory and formalism of elliptic functions. In the impossibility of providing a comprenssive list of the many contributions to this field, let us just recall, among the first, the paper by David Broadhurst [9] and then jump to almost all the contributors to this Conference, in particular Johannes Blümlein [10], Pierre Vanhove [11] and Stefan Weinzierl [12], and their references to previous works.

6 The `Banana` Amplitude

A few words on the (equal mass) `Banana` amplitude.



`The Banana graph`

The homogeneous equation for the `Banana` scalar amplitude with equal masses is a third order equation, at first sight of impossible solution. But, as an obvious extension of the `Sunrise` case, we find that the imaginary part of the amplitude is the maximally cut graph, which therefore satisfies the homogeneous equation. On the other hand, that imaginary part is also the 4-body equal mass physical phase space, which can be easily evaluated as the *merging* of two 2-particles phase spaces.

By following that approach, Primo and Tancredi [13] obtained, in a relatively simple way, a double integral representation for the phase space, whose integrand is the (inverse) square root of a sixth order polynomial in the two integration variables. By suitably changing the integration regions they succeeded also in obtaining three linearly independent integrals, corresponding to the three independent solutions of the third order equation, which were found to be the products of two complete elliptic integrals of appropriate arguments.

Even in this case, a bottom up approach, relying on physical and mathematically simple considerations (such as the phase space of four equal mass particles), provided a first step in the solution of an otherwise daunting mathematical problem.

7 Dispersion Relations and Differential Equations

Let us consider again the scalar self-mass amplitude of Eq. (31) in the simple $d = 2$ case, depending on a single external vector p with components $p = (p_0, p_z)$ through the Mandelstam variable $u = p_0^2 - p_z^2$, written, with a minor change of notation, as

$$B(u) = -i \int \frac{dk_0 dk_z}{(2\pi)^2} \frac{1}{D_1 - i\varepsilon} \frac{1}{D_2 - i\varepsilon} \,, \tag{46}$$

where D_1, D_2 are the same as in Eq. (31).

If p is spacelike, $p = (0, V)$, $u = -V^2 < 0$, an explicit calculation gives

$$\begin{aligned} B(-V^2) = & \frac{1}{2\pi\sqrt{((M+m)^2+V^2)((M-m)^2+V^2)}} \\ & \times \ln \frac{\sqrt{(M+m)^2+V^2} + \sqrt{(M-m)^2+V^2}}{\sqrt{(M+m)^2+V^2} - \sqrt{(M-m)^2+V^2}} \,. \end{aligned} \tag{47}$$

The above quantity is surely real; as $p_0 = 0$, we can perform a Wick rotation on the time component $k_0 = -ik_4$. $dk_0 = idk_4$, after which the denominators of the propagators become positive definite, all the $i\varepsilon$ can be ignored and the integrand is real and regular in the whole integration region. The Feynman graph integral (46) defines for p spacelike and $u = -V^2$ a real function of u, $B(-V^2) = B(u)$ which can however be analytically continued to any value (positive or even complex) of u; if we call the continuation $\mathscr{B}(u)$, we have

$$\texttt{if} : u < 0 \qquad\qquad \mathscr{B}(u) = B(u) \,. \tag{48}$$

But the Feynman integral (46) is well defined for any real value of the components of p, including of course the case of p timelike, say $p = (W, 0)$, with $u = W^2 > 0$. In this case the inverse propagators can vanish, the $m^2 - i\varepsilon$ prescription matters, and according to Eq. (34) an imaginary part is anyhow present in the integrand and, as in the case of Eqs. (36), (39), the final result can be complex if $u > u_0$, where u_0 is a threshold depending on the masses. So that in general for $W^2 > u_0$ one can write

$$B(W^2) = \mathtt{Re}B(W^2) \ + \ i\theta(W^2 - u_0)\mathtt{Im}B(W^2) \, . \tag{49}$$

By comparison of Eqs. (36), (39), (47) and (48) one finds, for any real value of u

$$\mathscr{B}(u + i\varepsilon) = \mathtt{Re}B(u) \ + \ i\theta(u - u_0)\mathtt{Im}B(u) \, , \tag{50}$$

$$\mathscr{B}(u - i\varepsilon) = \mathtt{Re}B(u) \ - \ i\theta(u - u_0)\mathtt{Im}B(u) \, , \tag{51}$$

where, let us repeat once more, $\mathtt{Re}B(u)$, $\mathtt{Im}B(u)$ are defined by the original Feynman graph (which is a function of the real parameter u through the *real* components of the vector p), so that the physical amplitude is $\mathscr{B}(u + i\varepsilon)$.

From Eqs. (50), (51) one sees that the function $\mathscr{B}(u)$ has a cut along the positive real axis starting at u_0, with discontinuity equal to $2i\,\mathtt{Im}B(u)$, the imaginary part of the graph given by the unitarity cutting rules discussed in the previous sections and therefore entirely fixed by the Feynman graph amplitude, As a consequence, the function $\mathscr{B}(u)$ satisfies the dispersion relation

$$\mathscr{B}(u) = \frac{1}{\pi} \int_{u_0}^{\infty} \frac{dv}{v - u} \mathtt{ImB}(v) \, , \tag{52}$$

valid for any value of u, where u_0 is a threshold and the imaginary part $\mathtt{ImA}(v)$, discussed in the previous sections, is the *discontinuity* in u of the amplitude. Let us recall, again, that the values provided by the Feynman graph correspond, see Eq. (50), to $\mathscr{B}(u + i\varepsilon)$ for u real (and $+i\varepsilon$ irrelevant if $u < u_0$).

It is immediate to derive from Eq. (52) a *subtracted* dispersion relation, such as

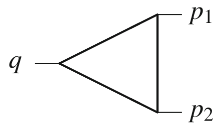
$$\mathscr{B}(u) = \mathscr{B}(0) + u\frac{1}{\pi} \int_{u_0}^{\infty} \frac{dv}{v(v - u)} \mathtt{ImB}(v)$$

which can be useful to fix boundary conditions or convergence problems.

A first (obvious) use of the dispersion relations is to evaluate $\mathtt{ImB}(v)$, and then try to obtain the complete amplitude by evaluating the dispersive integral; but that relays on the actual evaluation of the imaginary part itself, and within a differential equation approach the equation for the imaginary part is not particularly simpler or easier to solve than the complete equation when inhomogeneous terms are also present.

A second approach looks more promising: write the inhomogeneous terms in dispersive form. To illustrate this possibility with an example, let us look at the vertex amplitude, already introduced in Sect. 2,

$$\texttt{Vrt}(d;s) =$$



$$= \int \frac{i d^d k}{(k^2+m^2-i\varepsilon)((k-p_1)^2+m^2-i\varepsilon)((k-p_1-p_2)^2+m^2-i\varepsilon)} \tag{53}$$

where $d^d k$ refers to the d-dimensional integration and normalization factors, in the kinematical configuration $q = p_1 + p_2$, $p_1^2 = p_2^2 = 0$ and $-q^2 = s$ (q^2 is positive when q is spacelike). The complete differential equation for $\texttt{Vrt}(d;s)$ reads

$$\begin{aligned}\frac{d}{ds}\texttt{Vrt}(d;s) = -\frac{1}{s}\texttt{Vrt}(d;s) &+ \frac{(d-2)}{8m^4}\left(\frac{1}{s-4m^2} - \frac{1}{s}\right)\texttt{Tad}(d;m) \\ &+ \frac{(d-3)}{4\,m^2}\left(\frac{1}{s-4m^2} - \frac{1}{s}\right)B(d;s)\ ,\end{aligned}$$

where $B(d;s)$ is the analog of Eq. (46) in d-dimensions, while $\texttt{Tad}(d;m)$ is the tadpole of mass m

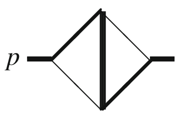
$$\texttt{Tad}(d;m) = -i\int \frac{d^d k}{k^2+m^2},$$

independent of s. By writing $B(d;s)$ in dispersive form, see Eq. (52), the equation for $\texttt{Vrt}(d;s)$ becomes

$$\begin{aligned}\frac{d}{ds}\texttt{Vrt}(d;s) = -\frac{1}{s}\texttt{Vrt}(d;s) &+ \frac{(d-2)}{8m^4}\left(\frac{1}{s-4m^2} - \frac{1}{s}\right)\texttt{Tad}(d;m) \\ + \frac{(d-3)}{4\,m^2}\frac{1}{\pi}\int_{u_0}^{\infty} dv\ &\texttt{ImB}(d,v)\left(\frac{1}{s-4m^2} - \frac{1}{s}\right)\frac{(-1)}{s-v}\ .\end{aligned} \tag{54}$$

As a first step, the equation in s can be solved by fully ignoring the integration in v and the actual value of $\texttt{ImB}(d,v)$, treating the new factor depending on s, $1/(s-v)$ on the same footing as the factors $1/s$ and $1/(s-4m^2)$ already appearing in the equation, i.e. considering the quantity v as a kind of new constant or parameter. Only after the accomplishment of the first step one has to consider the actual value of $\texttt{ImB}(d,v)$, and worry about the integration in v.

Another, less trivial example, is given by the family of the scalar integrals present in the QED 2-loop self-mass *kite*, already studied by Sabry [14]



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where the thick line is the electron line, and the thin lines are the massless photon propagators of the two loops (the imaginary part of the equal mass kite graph was already discussed in Sect. 2).

In the d-continuous dimensional regularization [16], the problem involves a total of 8 Master Integrals, among them the scalar amplitude with all the 5 propagators at the first power, which will be called $f_8(d; u)$, and the scalar (equal mass) sunrise, to be called here $f_6(d; u)$. In QED one is (obviously) interested in the $d \to 4$ limit; as in that limit $f_6(d; u)$ develops an u.v. double pole, it can be convenient (even if also somewhat confusing...) to rescale all the amplitudes by suitable powers of $(d-4)$, so that the rescaled set of equations has a finite limit at $d = 4$. (As a further *simplification*, which might however increase the potential confusion, it is also useful to use the Tarasov dimensional shift [15] from $d = 4$ to $d = 2$). In terms of the rescaled amplitudes, the equation for $f_8(d; u)$ reads

$$\begin{aligned} \frac{d}{du} f_8(d; u) = (d-4)\left(\frac{1}{u-m^2} - \frac{1}{2u}\right) f_8(d; u) \\ + \frac{(d-4)^3}{24}\left(\frac{1}{m^2} - \frac{8}{u-m^2}\right) f_6(d; u) \\ + \ldots \end{aligned} \tag{55}$$

where the dots stand for a few inhomogeneous terms which turn out to be expressible with ordinary Polylogarithms (of no interest here).

The homogeneous equation for $f_8(d; u)$ is simple, the non trivial part is within the inhomogeneous term $f_6(d; u)$, which is the *elliptic* `Sunrise`.

When expanding Eq. (55) in powers of $(d-4)$, the first non trivial order, corresponding to $(d-4)^3$, is

$$\begin{aligned} \frac{d}{du} f_8^{(3)} u) = \left(\frac{1}{m^2} - \frac{8}{u-m^2}\right) f_6^{(0)}(u) \\ + \frac{1}{u-m^2}\left(\frac{\pi^2}{96} - \frac{1}{16} G(0, m^2, u)\right) + \frac{1}{8u} G(m^2, m^2, u) \end{aligned} \tag{56}$$

where $G(0, m^2, u)$, $G(m^2, m^2, u)$ are ordinary Polylogarithms, while $f_6^{(0)}(u)$ is the (scalar) amplitude of the sunrise in $d = 2$ dimensions. At this point, recalling Eq. (44), one can write $f_6^{(0)}(u)$ through the dispersion relation

$$f_6^{(0)}(u) = \int_{9m^2}^{\infty} \frac{dv}{v-u} I_0(v).$$

When the above relation is inserted into Eq. (56), the integration of the differential equation becomes trivial and gives

$$f_8^{(3)}u) = \frac{1}{8}G(0, m^2, m^2, u) - \frac{1}{16}G(m^2, 0, m^2, u) - \frac{\pi^2}{96}G(m^2, u)$$
$$- \frac{1}{24}\int_{9m^2}^{\infty} dv\ I_0(v)\left(\frac{1}{m^2} - \frac{8}{v - m^2}\right)G(v, u)\ ,$$

where the dispersive *kernel* $I_0(v)$ of the sunrise dispersive representation is completely factorised, a feature which remains valid at higher orders in $(d-4)$, with $I_0(v)$ replaced by the imaginary part of the sunrise at the corresponding order.

8 Conclusions

We have recalled the derivation by Tini Veltman [2] of the *Largest Time Equation* for a Feynman graph amplitude, and its equivalence to the *Unitarity Cutting Rules* of Dick Cutkosky [1], accompanying the discussion with a number of examples.

The cut graph amplitudes (both the unitarity and the generalised cuts) are simpler to evaluate than the original amplitudes, but they still contain significant information on their structure, which can be used in the solution of their differential equations.

In the best cases, they are closely related to simple and well known physical quantities, such as the many particle phase space, which can then provide with a valuable hint in solving the associated homogeneous equation, the first step in studying the differential equations for the concerned amplitudes through the Euler's variation of the constants approach.

The dispersion relation representation, based on the previous evaluation of the relevant imaginary part of the amplitude, can further be used as a kind of universal tool for "merging" the amplitudes of the *subtopology*, corresponding to the inhomogenous terms of the differential equation for the whole amplitude, into the complete solution of the equation. When following this approach, the contribution of each *subtopology* is written as

$$\int dv\ K(v)\frac{1}{v-u} = -\int dv\ K(v)\frac{1}{u-v}\ ,$$

where u is the variable of the differential equation, v, $K(v)$ are the dispersive variable and the imaginary part of the *subtopology*. The dispersive factor $1/(u-v)$ fits naturally in the by now well established frame of the Generalised Polylogarithms in the variable u, introducing only one more parameter (or *letter*) v. The equation in u can be solved without worrying about the actual value of $K(v)$, and the problem of the integration in v can be tackled once the equation in u is solved. The procedure does not require the explicit knowledge of the dispersive kernel, and can be used even for kernels whose analytic structure is still to be investigated.

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Feynman Integrals, Toric Geometry and Mirror Symmetry

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Abstract This expository text is about using toric geometry and mirror symmetry for evaluating Feynman integrals. We show that the maximal cut of a Feynman integral is a GKZ hypergeometric series. We explain how this allows to determine the minimal differential operator acting on the Feynman integrals. We illustrate the method on sunset integrals in two dimensions at various loop orders. The graph polynomials of the multi-loop sunset Feynman graphs lead to reflexive polytopes containing the origin and the associated variety are ambient spaces for Calabi-Yau hypersurfaces. Therefore the sunset family is a natural home for mirror symmetry techniques. We review the evaluation of the two-loop sunset integral as an elliptic dilogarithm and as a trilogarithm. The equivalence between these two expressions is a consequence of (1) the local mirror symmetry for the non-compact Calabi-Yau three-fold obtained as the anti-canonical hypersurface of the del Pezzo surface of degree 6 defined by the sunset graph polynomial and (2) that the sunset Feynman integral is expressed in terms of the local Gromov-Witten prepotential of this del Pezzo surface.

1 Introduction

Scattering amplitudes are fundamental quantities used to understand fundamental interactions and the elementary constituents in Nature. It is well known that scattering amplitudes are used in particle physics to compare the theoretical predictions to experimental measurements in particle colliders (see [1] for instance). More recently the use of modern developments in scattering amplitudes have been extended to gravitational physics like unitarity methods to gravitational wave physics [2–6].

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The l-loop scattering amplitude $A^D_{n,l}(\underline{s}, \underline{m}^2)$ between n fields in D dimensions is a function of the kinematics invariants $\underline{s} = \{s_{ij} = (p_i + p_j)^2, 1 \leq i, j \leq n\}$ where p_i are the incoming momenta of the external particle, and the internal masses $\underline{m}^2 = (m_1, \ldots, m_r)$.

We focus on the questions : what kind of function is a Feynman integral? What is the best analytic representation?

The answer to these questions depend very strongly on which properties one wants to display. An analytic representation suitable for an high precision numerical evaluation may not be the one that displays the mathematical nature of the integral.

For instance the two-loop sunset integral has received many different, but equivalent, analytical expressions: hypergeometric and Lauricella functions [7, 8], Bessel integral representation [9–11], Elliptic integrals [12, 13], Elliptic polylogarithms [14–20] and trilogarithms [20].

The approach that we will follow here will be guided by the geometry of the graph polynomial using the parametric representation of the Feynman integral. In Sect. 2 we review the description of the Feynman integral I_Γ for a graph Γ in parametric space. We focus on the properties of the second Symanzik polynomial as a preparation for the toric approach used in Sect. 3. In Sect. 2.2 we show that the maximal cut π_Γ of a Feynman integral has a parametric representation similar to the one of the Feynman integral I_Γ where the only difference is the cycle of integration. The toric geometry approach is described in Sect. 3. In Sect. 3.2 we explain that the maximal cut integral is an hypergeometric series from the Gel'fand-Kapranov-Zelevinski (GKZ) construction. In Sect. 3.4.2, we show on examples how to derive the minimal differential operator annihilating the maximal cut integral. In Sect. 4 we review the evaluation of the two-loop sunset integral in two space-time dimensions. In Sect. 4.1 we give its expression as an elliptic dilogarithm

$$I_\ominus(p^2, \xi_1^2, \xi_2^2, \xi_3^2) \propto \varpi \sum_{i=1}^{6} c_i \sum_{n\geq 1} (\mathrm{Li}_2(q^n z_i) - (\mathrm{Li}_2(-q^n z_i)) \tag{1}$$

where ϖ is a period of the elliptic curve defined by the graph polynomial, q the nome function of the external momentum p^2 and internal masses ξ_i^2 for $i = 1, 2, 3$. In Sect. 4.2 we show that the sunset integral evaluates as sum of trilogarithm functions in (163)

$$\begin{aligned} I_\ominus(p^2, \xi_1^2, \xi_2^2, \xi_3^2) &\propto \varpi \; (3(\log Q)^3 \\ &+ \sum_{(n_1,n_2,n_3)\geq 0} \left(d_{n_1,n_2,n_3} + \delta_{n_1,n_2,n_3} \log(-p^2)\right) \mathrm{Li}_3\left(\prod_{i=1}^{3} \xi_i^{2n_i} Q^{n_i}\right). \end{aligned} \tag{2}$$

In Sect. 4.3 we show that the equivalence between theses two expression is the result of a local mirror map, $q \leftrightarrow Q$ in (165), for the non-compact Calabi-Yau three-fold obtained as the anti-canonical bundle over the del Pezzo 6 surface defined by the sunset graph polynomial. Remarkably the sunset Feynman integral is expressed in terms of the genus zero local Gromov-Witten prepotential [20]. Therefore this provides a natural application for Batyrev's mirror symmetry techniques [21]. One remarkable fact is that the computation can be done using the existing technology of mirror symmetry developed in other physical [22–24] or mathematics [25] contexts.

2 Feynman Integrals

A connected Feynman graph Γ is determined by the number n of propagators (internal edges), the number l of loops, and the number v of vertices. The Euler characteristic of the graph relates these three numbers as $v = n - l + 1$, therefore only the number of loops l and the number n of propagators are needed.

In a momentum representation an l-loop with n propagators Feynman graph reads

$$I_\Gamma(\underline{s}, \underline{\xi}^2, \underline{\nu}, D) := \frac{(\mu^2)^\omega}{\pi^{\frac{lD}{2}}} \frac{\prod_{i=1}^n \Gamma(\nu_i)}{\Gamma(\omega)} \int_{(\mathbb{R}^{1,D-1})^l} \frac{\prod_{i=1}^l d^D\ell_i}{\prod_{i=1}^n (q_i^2 - m_i^2 + i\varepsilon)^{\nu_i}}, \tag{3}$$

where D is the space-time dimension, and we set $\omega := \sum_{i=1}^n \nu_i - lD/2$ and q_i is the momentum flowing in between the vertices i and $i+1$. With μ^2 a scale of dimension mass squared. From now we set $m_i^2 = \xi_i^2\mu^2$ and $p_i \to p_i\mu$, with these new variables the μ^2 dependence disappear. The internal masses are positive $\xi_i^2 \geq 0$ with $1 \leq i \leq n$. Finally $+i\varepsilon$ with $\varepsilon > 0$ is the Feynman prescription for the propagators for a space-time metric of signature $(+ - \cdots -)$. The arguments of the Feynman integral are $\underline{\xi}^2 := \{\xi_1^2, \ldots, \xi_n^2\}$ and $\underline{\nu} := \{\nu_1, \ldots, \nu_n\}$ and $\underline{s} := \{s_{ij} = (p_i + p_j)^2\}$ with p_i with $i = 1, \ldots, v_e$ with $0 \leq v_e \leq v$ the external momenta subject to the momentum conservation condition $p_1 + \cdots + p_{v_e} = 0$. There are n internal masses ξ_i^2 with $1 \leq i \leq n$, is v_e is the number of external momenta we have v_e external masses p_i^2 with $1 \leq i \leq v_e$ (some of the mass could vanish but we do a generic counting here), and $\frac{v_e(v_e-3)}{2}$ independent kinematics invariants $s_{ij} = (p_i + p_j)^2$. The total number of kinematic parameters is

$$N_\Gamma(n,l) = n + \frac{v_e(v_e-1)}{2} \leq N_\Gamma(n,l)^{max} = n + \frac{(n-l+1)(n-l)}{2}. \tag{4}$$

We set

$$I_\Gamma(\underline{s}, \underline{m}, D) := I_\Gamma(\underline{s}, \underline{m}, 1, \ldots, 1, D), \tag{5}$$

and for ν_i positive integers we have

$$I_\Gamma(\underline{s}, \underline{m}, \underline{\nu}, D) = \prod_{i=1}^n \left(\frac{\partial}{\partial(\xi_i^2)}\right)^{\nu_i} I_\Gamma(\underline{s}, \underline{m}, D). \tag{6}$$

2.1 The Parametric Representation

Introducing the variables x_i with $1 \leq i \leq n$ such that

$$\sum_{i=1}^{n} x_i(q_i^2 - \xi_i^2) = (\ell_1^\mu, \ldots, \ell_l^\mu) \cdot \Omega \cdot (\ell_1^\mu, \ldots, \ell_l^\mu)^T + (\ell_1^\mu, \ldots, \ell_l^\mu) \cdot (Q_1^\mu, \ldots, Q_l^\mu) - J, \tag{7}$$

and performing standard Gaussian integrals on the x_i (see [26] for instance) one obtains the equivalent parametric representation that we will use in these notes

$$I_\Gamma(\underline{s}, \underline{\xi}, \underline{\nu}, D) = \int_{\Delta_n} \Omega_\Gamma, \tag{8}$$

the integrand is the $n-1$-form

$$\Omega_\Gamma = \prod_{i=1}^{n} x_i^{\nu_i - 1} \, \frac{\mathscr{U}^{\omega - \frac{D}{2}}}{\mathscr{F}^\omega} \, \Omega_0, \tag{9}$$

where Ω_0 is the differential $n-1$-form on the real projective space $\mathbb{P}^{n-1}$

$$\Omega_0 := \sum_{j=1}^{n} (-1)^{j-1} \, x_j \, dx_1 \wedge \cdots \wedge \widehat{dx_j} \wedge \cdots \wedge dx_n \,, \tag{10}$$

where $\widehat{dx_j}$ means that dx_j is omitting in this sum. The domain of integration Δ_n is defined as

$$\Delta_n := \{[x_1, \cdots, x_n] \in \mathbb{P}^{n-1} | x_i \in \mathbb{R}, x_i \geq 0\}. \tag{11}$$

The second Symanzik polynomial $\mathscr{F} = \mathscr{U}\left((Q_1^\mu, \ldots, Q_l^\mu) \cdot \Omega^{-1} \cdot (Q_1^\mu, \ldots, Q_l^\mu)^T - J\right)$, takes the form

$$\mathscr{F}(\underline{s}, \underline{\xi}^2, x_1, \ldots, x_n) = \mathscr{U}(x_1, \ldots, x_n) \left(\sum_{i=1}^{n} \xi_i^2 x_i \right) - \sum_{1 \leq i \leq j \leq n} s_{ij} \mathscr{G}_{ij}(x_1, \ldots, x_n) \tag{12}$$

where the first Symanzik polynomial $\mathscr{U}(x_1, \ldots, x_n) = \det \Omega$ and $\mathscr{G}_{ij}(x_1, \ldots, x_n)$ are polynomial in the x_i variables only.

- The first Symanzik polynomial $\mathscr{U}(x_1, \ldots, x_n)$ is an homogeneous polynomial of degree l in the Feynman parameters x_i and it is at most linear in each of the x_i variables. It does not depend on the physical parameters. This polynomial is also known as the Kirchhoff polynomial of graph Γ. Which is as well the determinant of the Laplacian of the graph see [27, Eq. (35)] for a definition.
- The polynomial $\mathscr{U}(x_1, \ldots, x_n)$ can be seen as the determinant of the period matrix Ω of the punctured Feynman graph [26], i.e. the graph with amputated external

legs. Or equivalently it can be obtained by considering the degeneration limit of a genus l Riemann surfaces with n punctures. This connection plays an important in understanding the quantum field theory Feynman integrals as the $\alpha' \to 0$ limit of the corresponding string theory integrals [28, 29].

- The graph polynomial $\mathscr{F}$ is homogeneous of degree $l+1$ in the variables $(x_1, \ldots, x_n)$. This polynomial depends on the internal masses ξ_i^2 and the kinematic invariants $s_{ij} = (p_i \cdot p_j)/\mu^2$. The polynomials $\mathscr{G}_{ij}$ are at most linear in all the variables x_i since this is given by the spanning 2-trees [27]. Therefore if all internal masses are vanishing then $\mathscr{F}$ is linear in the Feynman parameters x_i.
- The $\mathscr{U}$ and $\mathscr{F}$ are independent of the dimension of space-time. The space-time dimension enters only in the powers of $\mathscr{U}$ and $\mathscr{F}$ in the parametric representation for the Feynman graphs. Therefore one can see the Feynman integral as a meromorphic function of $(\underline{\nu}, D)$ in $\mathbb{C}^{1+n}$ as discussed in [30].
- All the physical parameters, the internal masses ξ_i^2 and the kinematic variables $s_{ij} = (p_i \cdot p_j)/\mu^2$ (that includes the external masses) enter linearly. This will be important for the toric approach described in Sect. 3.

2.2 Maximal Cut

We show that the maximal cut of a Feynman graph has a nice parametric representation. Let us consider the maximal cut

$$\pi_\Gamma(\underline{s}, \underline{\xi}^2, D) := \frac{1}{\Gamma(\omega)(2i\pi)^n \pi^{\frac{lD}{2}}} \int_{(\mathbb{R}^{1,D-1})^L} \prod_{i=1}^{l} d^D \ell_i \prod_{i=1}^{n} \delta(q_i^2 - m_i^2 + i\varepsilon), \quad (13)$$

of the Feynman integral $I_\Gamma(\underline{s}, \underline{\xi}^2, D)$ which is obtained from the Feynman integral in (3) by replacing all propagators by a delta-function

$$\frac{1}{d^2} = \frac{1}{2i\pi}\delta(d^2). \quad (14)$$

Using the representation of the δ-function

$$\delta(x) = \int_{-\infty}^{+\infty} dw e^{iwx}, \quad (15)$$

we obtain that the integral is

$$\pi_\Gamma(\underline{s}, \underline{m}, D) := \frac{1}{\Gamma(\omega)(2i\pi)^n \pi^{\frac{lD}{2}}} \int_{\mathbb{R}^{(1,D-1)L}} e^{-i\sum_{i=1}^n x_i(\ell_i^2 + m_i^2 - i\varepsilon)} \prod_{i=1}^{l} d^D \ell_i \prod_{i=1}^{n} dx_i\,. \quad (16)$$

At this stage the integral is similar to the one leading to the parametric representation with the replacement $x_r \to i x_r$ with $x_r \in \mathbb{R}$. Setting $\tilde{x}_r = i x_r$ and performing the Gaussian integrals over the loop momenta, we get

$$\pi_n(\underline{s}, \underline{\xi}^2, D) := \frac{1}{(2i\pi)^n} \int_{i\mathbb{R}^n} \frac{\widetilde{\mathscr{U}}^{\omega - \frac{D}{2}}}{\widetilde{\mathscr{F}}^{\omega}} \prod_{i=1}^{n} \delta\left(1 - \sum_{i=1}^{n} \tilde{x}_i\right) d\tilde{x}_i \,. \tag{17}$$

using the projective nature of the integrand we have $\frac{\widetilde{\mathscr{U}}^{\omega-D/2}}{\widetilde{\mathscr{F}}^{\omega}} = i^{-n} \frac{\mathscr{U}^{\omega-D/2}}{\mathscr{F}^{\omega}}$ and the integral can be rewritten as the torus integral

$$\pi_\Gamma(\underline{s}, \underline{\xi}^2, D) := \frac{1}{(2i\pi)^n} \int_{|x_1|=\cdots=|x_{n-1}|=1} \frac{\mathscr{U}^{\omega-D/2}}{\mathscr{F}^{\omega}} \prod_{i=1}^{n-1} dx_i \,. \tag{18}$$

This integral shares the same integrand with the Feynman integral I_Γ in (8) but the cycle of integration differs since we are integrating over a n-torus. We show in Sect. 3.2 that this maximal cut arises naturally from the toric formalism.

2.3 The Differential Equations

In general a Feynman integral $I_\Gamma(\underline{s}, \underline{\xi}^2, \underline{\nu}, D)$ satisfies an inhomogeneous system of differential equations

$$\mathscr{L}_\Gamma I_\Gamma = \mathscr{S}_\Gamma, \tag{19}$$

where the inhomogeneous term $\mathscr{S}_\Gamma$ essentially arises from boundary terms corresponding to reduced graph topologies where internal edges have been contracted. Knowing the maximal cut integral allows to determine differential operators $\mathscr{L}_\Gamma$

$$\mathscr{L}_\Gamma \pi_\Gamma(\underline{s}, \underline{\xi}^2, D) = 0, \tag{20}$$

This fact has been exploited in [31–34] to obtain the minimal order differential operator. The important remark in this construction is to use that the only difference between the Feynman integral I_Γ and the maximal cut π_Γ is the choice of cycle of integration. Since the Picard–Fuchs operator $\mathscr{L}_\Gamma$ acts as

$$\mathscr{L}_\Gamma \pi_\Gamma(\underline{s}, \underline{\xi}^2, D) = \int_{\gamma_n} \mathscr{L}_\Gamma \Omega_F = \int_{\gamma_n} d(\beta_\Gamma) = 0 \tag{21}$$

this integral vanishes because the cycle $\gamma_n = \{|x_1| = \cdots = |x_n| = 1\}$ has no boundaries $\partial\gamma_n = \emptyset$. In the case of the Feynman integral I_Γ this is not longer true as

$$\mathscr{L}_\Gamma I_\Gamma(\underline{s}, \underline{\xi}^2, D) = \int_{\Delta_n} d(\beta_\Gamma) = \int_{\partial\Delta_n} \beta_\Gamma = \mathscr{S}_\Gamma \neq 0 \,. \tag{22}$$

The boundary contributions arises from the configuration with some of the Schwinger coordinate $x_i = 0$ vanishing which corresponds to the so-called reduced topologies that are known to arises when applying the integration-by-part algorithm (see [35–37] for instance).

We illustrate this logic on some elementary examples of differential equations for multi-valued integrals relevant for the one- and two-loop massive sunset integrals discussed in this text.

2.3.1 The Logarithmic Integral

We consider the integral

$$I_1(t) = \int_a^b \frac{dx}{x(x-t)}\,, \tag{23}$$

and its cut integral

$$\pi(t) = \int_\gamma \frac{dx}{x(x-t)}\,, \tag{24}$$

where γ is a cycle around the point $x = t$. Clearly we have

$$\frac{d}{dx}\left(\frac{1}{t-x}\right) = \frac{1}{x(x-t)} + t\frac{d}{dt}\left(\frac{1}{x(x-t)}\right)\,, \tag{25}$$

therefore the integral $\pi(t)$ satisfies the differential equation

$$t\frac{d}{dt}\pi(t) + \pi(t) = \int_\gamma \frac{d}{dx}\left(\frac{1}{t-x}\right) = 0\,, \tag{26}$$

and the integral $I_1(t)$ satisfies

$$t\frac{d}{dt}I_1(t) + I_1(t) = \int_a^b \frac{d}{dx}\left(\frac{1}{t-x}\right) = \frac{1}{b(b-t)} - \frac{1}{a(a-t)}\,. \tag{27}$$

Changing variables from t to p^2 or an internal mass will give the familiar differential equation for the one-loop bubble that will be commented further in Sect. 3.4.

2.3.2 Elliptic Curve

The second example is the differential equation for the period of an elliptic curve $\mathscr{E} : y^2z = x(x-z)(x-tz)$ which is the geometry of the two-loop sunset integral. Consider the differential of the first kind on the elliptic curve

$$\omega = \frac{dx}{\sqrt{x(x-1)(x-t)}}\,, \tag{28}$$

this form can be seen as a residue evaluated on the elliptic curve $\omega = \mathrm{Res}_{\mathscr{E}}\,\Omega$ of the form on the projective space $\mathbb{P}^2$

$$\Omega = \frac{\Omega_0}{y^2z - x(x-z)(x-tz)}\,. \tag{29}$$

where $\Omega_0 = zdx \wedge dy + ydz \wedge dx + xdy \wedge dz$ is the natural top form on the projective space $[x : y : z]$. Systematic ways of deriving Picard–Fuchs operators for elliptic curve is given by Griffith's algorithm [38]. Consider the second derivative with respect to the parameter t

$$\frac{d^2}{dt^2}\Omega = 2\frac{x^2(x-z)^2z^2}{(y^2z - x(x-z)(x-tz))^2}\Omega_0 \tag{30}$$

the numerator belongs to the Jacobian ideal[1] of the polynomial $p(x, y, z) := y^2z - x(x-z)(x-tz)$, $J_1 = \langle \partial_x p(x, y, z) = -3x^2 + 2(t+1)xz - tz^2 2, \partial_y p(x, y, z) = 2yz, \partial_z p(x, y, z) = (t+1)x^2 + y^2 - 2txz\rangle$, since

$$x^2(x-z)^2z^2 = m^1_x \partial_x p(x, y, z) + m^1_y \partial_y p(x, y, z) + m^1_z \partial_z p(x, y, z)\,. \tag{31}$$

This implies that

$$\begin{aligned}\frac{d^2}{dt^2}\Omega &= \frac{\partial_x m^1_x + \partial_y m^1_y + \partial_z m^1_z}{(y^2z - x(x-z)(x-tz))^2}\Omega_0 \\ &\quad + d\left(\frac{(ym^1_z - zm^1_y)dx + (zm^1_x - xm^1_z)dy + (xm^1_y - ym^1_x)dz}{(y^2z - x(x-z)(x-tz))^2}\right)\end{aligned} \tag{32}$$

therefore

[1] An ideal I of a ring R, is the subset $I \subset R$, such that 1) $0 \in I$, 2) for all $a, b \in I$ then $a + b \in I$, 3) for $a \in I$ and $b \in R$, $a \cdot b \in R$. For $P(x_1, \ldots, x_n)$ an homogeneous polynomial in $R = \mathbb{C}[x_1, \ldots, x_n]$ the Jacobian ideal of P is the ideal generated by the first partial derivative $\{\partial_{x_i} P(x_1, \ldots, x_n)\}$ [39]. Given a multivariate polynomial $P(x_1, \ldots, x_n)$ its Jacobian ideal is easily evaluated using `Singular` command `jacob(P)`. The hypersuface $P(x_1, \cdots, x_n) = 0$ for an homogeneous polynomial, like the Symanzik polynomials, is of codimension 1 in the projective space $\mathbb{P}^{n-1}$. The singularities of the hypersurface are determined by the irreducible factors of the polynomial. This determines the cohomology of the complement of the graph hypersurface and the number of independent master integrals as shown in [40].

$$\frac{d^2}{dt^2}\Omega + p_1(t)\frac{d}{dt}\Omega = \frac{-p_1(t)x(x-z)z + \partial_x m_x^1 + \partial_y m_y^1 + \partial_z m_z^1}{(y^2z - x(x-z)(x-tz))^2}\Omega_0$$
$$+ d\left(\frac{(ym_z^1 - zm_y^1)dx + (zm_x^1 - xm_z^1)dy + (xm_y^1 - ym_x^1)dz}{(y^2z - x(x-z)(x-tz))^2}\right). \tag{33}$$

One easily derives that $\partial_x m_x^1 + \partial_y m_y^1 + \partial_z m_z^1$ is in the Jacobian ideal generated by J_1 and $x(x-z)z$ with the result that

$$\partial_x m_x^1 + \partial_y m_y^1 + \partial_z m_z^1 = m_x^2\partial_x p(x,y,z) + m_y^2\partial_y p(x,y,z) + m_z^2\partial_z p(x,y,z)$$
$$+ \frac{2t-1}{t(t-1)}x(x-z)z, \tag{34}$$

therefore $p_1(t) = \frac{2t-1}{t(t-1)}$ and the Picard–Fuchs operator reads

$$\frac{d^2}{dt^2}\Omega + \frac{2t-1}{t(t-1)}\frac{d}{dt}\Omega - \frac{\partial_x m_x^2 + \partial_y m_y^2 + \partial_z m_z^2}{(y^2z - x(x-z)(x-tz))^2}\Omega_0 =$$
$$d\left(\frac{(ym_z^1 - zm_y^1)dx + (zm_x^1 - xm_z^1)dy + (xm_y^1 - ym_x^1)dz}{(y^2z - x(x-z)(x-tz))^2}\right)$$
$$+ d\left(\frac{(ym_z^2 - zm_y^2)dx + (zm_x^2 - xm_z^2)dy + (xm_y^2 - ym_x^2)dz}{y^2z - x(x-z)(x-tz)}\right). \tag{35}$$

since $\partial_x m_x^2 + \partial_y m_y^2 + \partial_z m_z^2 = -\frac{1}{4t(t-1)}$ we have that

$$\left(4t(t-1)\frac{d^2}{dt^2} - 4(2t-1)\frac{d}{dt} + 1\right)\omega = -2\partial_x\left(\frac{y}{(x-t)^2}\right). \tag{36}$$

For α and β a (sympletic) basis of $H_1(\mathscr{E},\mathbb{Z})$ the period integrals $\varpi_1(t) := \int_\alpha \omega$ and $\varpi_2(t) := \int_\beta \omega$ both satisfy the differential equation

$$\left(4t(t-1)\frac{d^2}{dt^2} - 4(1-2t)\frac{d}{dt} + 1\right)\varpi_i(t) = 0\,. \tag{37}$$

Again this differential operator acting on an integral with a different domain of integration can lead to an homogeneous terms as this is case for the two-loop sunset Feynman integral.

The all procedure is easily implemented in `Singular` [41] with the following set of commands

```
In [1]: // Griffith-Dwork method for
deriving the Picard-Fuchs operator for the elliptic curve
 y^2z=x(x-z)(x-tz)

In [2]: ring A=(0,t),(x,y,z),dp;

In [3]: poly f=y^2*z-x*(x-z)*(x-t*z);

In [4]: ideal I1=jacob(f); I1

Out[4]: I1 [1]=-3*x2+(2t+2)*xz+(-t)*z2
         I1 [2] =2*yz
         I1 [3] =(t+1)*x2+y2+(-2t)*xz

In [5]: matrix M1=lift(I1,x^2*(x-z)^2*z^2); M1

Out[5]: M1 [1,1]=2/(3t+3)*xz3
         M1[1,2]=-1/(2t+2)*x2yz+1/(6t+6)*yz3
         M1[3,1]=1/(t+1)*x2z2-1/(3t+3)*z4

In [6]: // checking the decomposition
x^2*(x-z)^2*z^2-M1[1,1]*I[1]-M1[1,2]*I[2]-M1[1,3]*I[3]

Out[6]: 0

In [7]:  poly dC1=diff(M [1,1],x)  +diff(M [2,1],y)
+diff(M [3,1],z);
dC1

Out[7]:  dC1=3/(t+1)*x2z-1/(t+1)*z3

In [8]:  ideal I2=jacob(f),x*(x-z)*z;

In [9]:  matrix M2=lift(I2,dC1); M2

Out[9]: M2 [1,1]=1/(2t2+2t)*z
         M2 [2,1]=1/(4t2-4t)*y
         M2[3,1]=-1/(2t2-2t)*z
         M2[4,1]=(2t-1)/(t2-t)

In [10]: // checking the decomposition
dC1-M2[1,1]*I[1]-M2 [2,1]*I[2]-M2[1,3]*I[3]
-M2[4,1]*x*(x-z)*z

Out[10]: 0

In [11]:  poly
dC2=diff(M2[1,1],x)+diff(M2[2,1],y)
+diff(M2 [3,1],z);
dC2

Out[11]: -1/(4t2-4t)
```

3 Toric Geometry and Feynman Graphs

We will show how the toric approach provides a nice way to obtain this maximal cut integral. The maximal cut integral $\pi_\Gamma(\underline{s}, \underline{\xi}^2, D)$ is the particular case of generalised Euler integrals

$$\int_\sigma \prod_{i=1}^{r} P_i(x_1, \ldots, x_n)^{\alpha_i} \prod_{i=1}^{n} x_i^{\beta_i} dx_i \tag{38}$$

studied by Gel'fand, Kapranov and Zelevinski (GKZ) in [42, 43]. There $P_i(x_1, \ldots, x_n)$ are Laurent polynomials, α_i and β_i are complex numbers and σ is a cycle. The cycle entering the maximal cut integral in (18) is the product of circles $\sigma = \{|x_1| = |x_2| = \cdots = |x_n| = 1\}$. But other cycles arise when considering different cuts of Feynman graphs. The GKZ approach provides a totally combinatorial approach to differential equation satisfied by these integrals.

As well in the case when $P(\underline{x}, \underline{z}) = \sum_i z_{i_1,\ldots,i_r} \prod_{i=1}^n x_i^{\alpha_i}$ is the Laurent polynomial defining a Calabi-Yau hypersurface $\{P(\underline{x}, \underline{z}) = 0\}$, Batyrev showed that there is one canonical period integral [44, 45]

$$\Pi(\underline{z}) := \frac{1}{(2i\pi)^n} \int_{|x_1|=\cdots=|x_n|=1} \frac{1}{P(\underline{x}, \underline{z})} \prod_{i=1}^{n} \frac{dx_i}{x_i}\,. \tag{39}$$

This corresponds to the maximal cut integral (18) In the case where $\omega = D/2 = 1$ which is satisfied by the $(n-1)$-loop sunset integral $D = 2$ dimensions. The graph hypersurface of the $(n-1)$-loop sunset (see (47)) is always a Calabi-Yau $(n-1)$-fold. See for more comments about this at the end of Sect. 4.3.1. We refer to the reviews [46, 47] for some introduction to toric geometry for physics.

3.1 Toric Polynomials and Feynman Graphs

The second Symanzik polynomial $\mathscr{F}(\underline{s}, \underline{\xi}^2, x_1, \ldots, x_n)$ defined in (12) is a specialisation of the homogeneous (toric) polynomial[2] of degree $l+1$ at most quadratic in each variables in the projective variables $(x_1, \ldots, x_n) \in \mathbb{P}^{n-1}$

---

[2]Consider an homogeneous polynomial of degree d

$$P(\underline{z}, \underline{x}) = \sum_{\substack{0 \le r_i \le n \\ r_1+\cdots+r_n=d}} z_{i_1,\ldots,i_n} \prod_{i=1}^{n} x_i^{r_i}$$

this is called a *toric polynomial* if it is invariant under the following actions

$$z_i \to \prod_{j=1}^{n} t_i^{\alpha_{ij}} z_i; \qquad x_i \to \prod_{j=1}^{n} t_i^{\beta_{ij}} x_i$$

$$\mathscr{F}_l^{toric}(\underline{z}, x_1, \ldots, x_n) = \mathscr{U}_l^{tor}(x_1, \ldots, x_n) \left(\sum_{i=1}^n \xi_i^2 x_i \right) - \mathscr{V}_l^{tor}(x_1, \ldots, x_n), \quad (40)$$

where for $l \leq n$

$$\mathscr{U}_l^{tor}(x_1, \ldots, x_n) := \sum_{\substack{0 \leq r_i \leq 1 \\ r_1+\cdots+r_n=l}} u_{i_1,\ldots,i_n} \prod_{i=1}^n x_i^{r_i}, \quad (41)$$

where the coefficients $u_{i_1,\ldots,i_n} \in \{0, 1\}$. The expression in (40) is the most generic form compatible with the properties of the Symanzik polynomials listed in Sect. 2.1.

There are $\frac{n!}{(n-l)!l!}$ independent coefficient in the polynomial $\mathscr{U}_l^{tor}(x_1, \ldots, x_n)$. Of course this is a huge over counting, as this does not take into account the symmetries of the graphs and the constraints on the non-vanishing of some coefficients. This will be enough for the toric description we are using here. In order to keep most of the combinatorial power of the toric approach we will only do the specialisation of the toric coefficients with the physical slice corresponding of Feynman graph polynomial at the end on solutions. This will avoid having to think at constrained system of differential equations which is a difficult problem discussed recently in [40].

The kinematics part has the toric polynomial

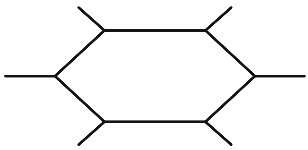
$$\mathscr{V}_l^{tor}(x_1, \ldots, x_n) := \sum_{\substack{0 \leq r_i \leq 1 \\ r_1+\cdots+r_n=l+1}} z_{i_1,\ldots,i_n} \prod_{i=1}^n x_i^{r_i}, \quad (42)$$

where the coefficients $z_{i_1,\cdots,i_n} \in \mathbb{C}$. The number of independent toric variables $z_{\underline{i}}$ in $\mathscr{V}^{tor}(x_1, \ldots, x_n)$ is $\frac{n!}{(n-l-1)!(l+1)!}$.

3.1.1 Some Important Special Cases

There are few important special cases.

- At one-loop order $l = 1$ and the number of independent toric variables in $\mathscr{V}^{tor}(x_1, \ldots, x_n)$ is exactly the number of independent kinematics for an n-gon one-loop amplitude



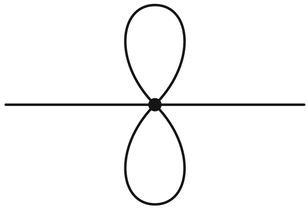
In this case the most general toric one-loop polynomial is

---

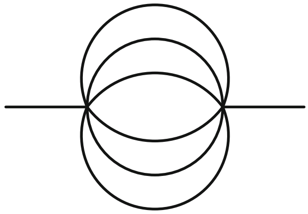
for $(t_1, \ldots, t_n) \in \mathbb{C}^n$ and α_{ij} and β_{ij} integers. The second Symanzik polynomial have a natural torus action acting on the mass parameters and the kinematic variables as we will see on some examples below. We refer to the book [39] for more details.

$$\mathscr{F}_1^{tor}(x_1,\cdots,x_n) = \left(\sum_{i=1}^n x_i\right)\left(\sum_{i=1}^n \xi_i^2 x_i\right) - \mathscr{V}_1^{tor}(x_1,\cdots,x_n). \tag{43}$$

- For $l = n$ there is only one vertex the graph is n-bouquet which is a product of n one-loop graphs. These graphs contribute to the reduced topologies entering the determination of the inhomogeneous term $\mathscr{S}_\Gamma$ of the Picard–Fuchs equation (19). They don't contribute to the maximal cut π_Γ for $l > 1$.



- The case $l = n - 1$ corresponds to the $(n-1)$-loop two-point sunset graphs



In that case the kinematic polynomial is just

$$\mathscr{V}_{n-1}^{tor}(x_1,\ldots,x_n) = z_{1,\ldots,1} x_1 \cdots x_n, \tag{44}$$

and the toric polynomial

$$\mathscr{F}_{n-1}^{tor}(x_1,\ldots,x_n) = x_1\cdots x_n \left(\sum_{i=1}^n \frac{u_{1,\ldots,0,\ldots,1}}{x_i}\right)\left(\sum_{i=1}^n \xi_i^2 x_i\right) - z_{1,\ldots,1} x_1\cdots x_n, \tag{45}$$

where the index 0 in $u_{1,\ldots,0,\ldots,1}$ is at position i. Actually by redefining the parameter $z_{1,\ldots,1}$ the generic toric polynomial associated to the sunset graph are

$$\mathscr{F}_{\ominus}^{tor}(x_1,\ldots,x_n) = x_1\cdots x_n \left(\sum_{\substack{1\leq i,j\leq n\\ i\neq j}} z_{ij}\frac{x_i}{x_j} - z_0\right), \tag{46}$$

where $z_{ij} \in \mathbb{C}$ and $z_0 \in \mathbb{C}\backslash\{0\}$. This polynomial has $1 - n + n^2$ parameters where a sunset graph as $n + 1$ physical parameters given by n masses and one kinematics invariant

$$\mathscr{F}^{l}_{\ominus}(p^2, \underline{\xi}^2, \underline{x}) = x_1 \cdots x_{l+1} \left(\sum_{i=1}^{l+1} \frac{1}{x_i}\right) \left(\sum_{i=1}^{l+1} \xi_i^2 x_i\right) - p^2 x_1 \cdots x_{l+1}\,. \tag{47}$$

So there are too many parameters from $n \geq 3$ but this generalisation will be useful for the GKZ description used in the next sections.

3.2 *The GKZ Approach : A Review*

In the section we briefly review the GKZ construction based on [42, 43] see as well [48]. We consider the Laurent polynomial of $n-1$ variables $P(z_1, \ldots, z_r) = \mathscr{F}^{tor}\underline{z}, x_1, \ldots, x_n/(x_1 \cdots x_n)$ from the toric polynomial of Sect. 3.1. The coefficients of monomials are z_i (by homogeneity we set $x_n = 1$)

$$P(z_1, \ldots, z_r) = \sum_{\mathbf{a}=(a_1,\ldots,a_{n-1})\in\mathbf{A}} z_{\boldsymbol{a}} \prod_{i=1}^{n-1} x_i^{a_i}, \tag{48}$$

with $\mathbf{a} = (a_1, \ldots, a_{n-1})$ is an element of $\mathbf{A} = (\mathbf{a}_1, \ldots, \mathbf{a}_r)$ a finite subset of $\mathbb{Z}^{n-1}$. The number of elements in A is r the number of monomials in $P(z_1, \ldots, z_r)$.

We consider the natural fundamental period integral [49]

$$\Pi(\underline{z}) := \frac{1}{(2i\pi)^{n-1}} \int_{|x_1|=\cdots=|x_{n-1}|=1} P(z_1, \ldots, z_r)^m \prod_{i=1}^{n-1} \frac{dx_i}{x_i}, \tag{49}$$

which is the same as maximal cut π_Γ in (18) for $D = 2\omega = -m$. The derivative with respect to $z_{\mathbf{a}}$ reads

$$\frac{\partial}{\partial z_{\boldsymbol{a}}} \Pi(\underline{z}) = \frac{1}{(2i\pi)^{n-1}} \int_{|x_1|=\cdots=|x_{n-1}|=1} m P(z_1, \ldots, z_r)^{m-1} \prod_{i=1}^{n-1} x_i^{a_i} \frac{dx_i}{x_i}, \tag{50}$$

therefore for every vector $\boldsymbol{\ell} = (\ell_1, \ldots, \ell_r) \in \mathbb{Z}^{n-1}$ such that

$$\ell_1 + \cdots + \ell_r = 0, \qquad \ell_1 \mathbf{a}_1 + \cdots + \ell_r \mathbf{a}_r = \boldsymbol{\ell} \cdot \mathbf{A} = 0, \tag{51}$$

then holds the differential equation

$$\left(\prod_{l_i>0} \partial_{z_i}^{l_i} - \prod_{l_i<0} \partial_{z_i}^{-l_i}\right) \Pi(\underline{z}) = 0. \tag{52}$$

Introducing the so-called $\mathscr{A}$-hypergeometric functions[3] $\Phi_{\mathbb{L},\gamma}(z_1,\dots,z_r)$ of r complex variables $(z_1,\dots,z_r)\in\mathbb{C}^r$

$$\Phi_{\mathbb{L},\boldsymbol{\gamma}}(z_1,\dots,z_r)=\sum_{(\ell_1,\dots,\ell_r)\in\mathbb{L}}\prod_{j=1}^{r}\frac{z_j^{\gamma_j+\ell_j}}{\Gamma(\gamma_j+\ell_j+1)},\tag{53}$$

depending on the complex parameters $\boldsymbol{\gamma}:=(\gamma_1,\dots,\gamma_r)\in\mathbb{C}^r$ and the lattice

$$\mathbb{L}:=\{(\ell_1,\dots,\ell_r)\in\mathbb{Z}|\sum_{i=1}^{r}\ell_i\mathbf{a}_i=0,\ell_1+\cdots+\ell_r=0\},\tag{54}$$

with r elements $\{\mathbf{a}_1,\dots,\mathbf{a}_r\}\in\mathbb{Z}^n$. These functions are solutions of the so-called $\mathscr{A}$-hypergeometric system of differential equations given by a vector $\mathbf{c}\in\mathbb{C}^n$ and :

- For every $\boldsymbol{\ell}=(\ell_1,\dots,\ell_r)\in\mathbb{L}$ there is one differential operator

$$\Box_{\boldsymbol{\ell}}:=\prod_{\ell_i>0}\partial_{z_i}^{\ell_i}-\prod_{\ell_i<0}\partial_{z_i}^{-\ell_i},\tag{55}$$

  such that $\Box_{\boldsymbol{\ell}}\Phi_{\mathbb{L},\gamma}(z_1,\dots,z_r)=0$
- n differential operators $\mathbf{E}:=(E_1,\dots,E_{n-1})$

$$\mathbf{E}:=\mathbf{a}_1z_1\frac{\partial}{\partial z_1}+\cdots+\mathbf{a}_rz_r\frac{\partial}{\partial z_r},\tag{56}$$

  such that for $\mathbf{c}=(c_1,\dots,c_{n-1})$ we have

$$(\mathbf{E}-\mathbf{c})\Phi_{\mathbb{L},\gamma}(z_1,\dots,z_r)=0.\tag{57}$$

  Notice that $E_1=\sum_{i=1}^{n}z_i\frac{\partial}{\partial z_i}$ is the Euler operator and c_1 is the degree of homogeneity of the hypergeometric function.
  These operators satisfy the commutation relations

$$\begin{aligned}\mathbf{z^uE}-\mathbf{Ez^u}&=-(\mathbf{A}\cdot\mathbf{u})\,\mathbf{z^u},\\ \partial_z^{\mathbf{u}}\mathbf{E}-\mathbf{E}\partial_z^{\mathbf{u}}&=(\mathbf{A}\cdot\mathbf{u})\,\partial_z^{\mathbf{u}},\end{aligned}\tag{58}$$

  with $\mathbf{z^u}:=\prod_{i=1}^{r}z_r^{u_r}$ and $\partial_z^{\mathbf{u}}:=\prod_{i=1}^{r}\partial_{z_r}^{u_r}$.

Using the GKZ construction one can easily derive a system of differential operator annihilating the maximal of any Feynman integral after identification of the toric variables with the physical parameters. The system of differential operators obtained from the GKZ system can be massaged into a set of Picard–Fuchs differential operators in a spirit similar to the one used in mirror symmetry [22, 39, 51].

[3]The convergence of these series is discussed in [50, §3–2] and [48, §5.2].

Since it is rather complicated to restrict differential operators but it is easier to restrict functions, it is therefore preferable to determine the $\mathscr{A}$-hypergeometric representation of the maximal cut integral and derive the minimal differential operator annihilating this integral. For well chosen vector $\boldsymbol{\ell} \in \mathbb{L}$ the differential operator factorises with a factor being given by the minimal (Picard–Fuchs) differential operator acting on the Feynman integral.

An important remark is that the maximal cut integral

$$\pi_\Gamma = \int_{|x_1|=\cdots=|x_{n-1}|=1} \frac{1}{\mathscr{F}_\Gamma} \prod_{i=1}^{n-1} dx_i, \tag{59}$$

is a particular case of fundamental period $\Pi(\underline{z})$ in (49) with $m = -1$ and therefore is given by a $\mathscr{A}$-hypergeometric function once we have identified the toric variables z_i with the physical parameters.

In the next section we illustrate this approach on some simple but fundamental examples.

3.3 Hypergeometric Functions and GKZ System

The relation between hypergeometric functions and the GKZ differential system can be simply understood as follows (see [48, 52, 53]).

3.3.1 The Gauß Hypergeometric Series

Consider the case of $\mathbb{L} = (1, 1, -1, 1)\mathbb{Z} \subset \mathbb{Z}^4$ and the vector $\gamma = (0, c-1, -a, -b) \in \mathbb{C}^4$ and c a positive integer. The GKZ hypergeometric function is

$$\Phi_{\mathbb{L},\gamma}(u_1,\ldots,u_4) = \sum_{n\in\mathbb{Z}} \frac{u_1^n u_2^{1-c+n} u_3^{-a-n} u_4^{-b-n}}{\Gamma(1+n)\Gamma(c+n)\Gamma(1-n-a)\Gamma(1-n-b)}, \tag{60}$$

which can be rewritten as

$$\Phi_{\mathbb{L},\gamma}(u_1,\ldots,u_4) = \frac{u_2^{c-1} u_3^{-a} u_4^{-b}}{\Gamma(c)\Gamma(1-a)\Gamma(1-b)}\, {}_2F_1\left(\begin{matrix} a,\ b \\ c \end{matrix}\,\middle|\, \frac{u_1u_2}{u_3u_4}\right). \tag{61}$$

The GKZ system is

$$\left(\frac{\partial^2}{\partial u_1 \partial u_2} - \frac{\partial^2}{\partial u_3 \partial u_4}\right) \Phi_{\mathbb{L},\gamma}(u_1,\ldots,u_4) = 0,$$
$$\left(u_1\frac{\partial}{\partial u_1} - u_2\frac{\partial}{\partial u_2} + 1 - c\right) \Phi_{\mathbb{L},\gamma}(u_1,\ldots,u_4) = 0,$$

$$\left(u_1\frac{\partial}{\partial u_1}+u_3\frac{\partial}{\partial u_3}+a\right)\Phi_{\mathbb{L},\gamma}(u_1,\ldots,u_4)=0,$$
$$\left(u_1\frac{\partial}{\partial u_1}+u_4\frac{\partial}{\partial u_4}+b\right)\Phi_{\mathbb{L},\gamma}(u_1,\ldots,u_4)=0\,. \tag{62}$$

By differentiating we find

$$\left(u_2\frac{\partial^2}{\partial u_1\partial u_2}-u_1\frac{\partial^2}{\partial u_1^2}+c\frac{\partial}{\partial u_1}\right)\Phi_{\mathbb{L},\gamma}(u_1,\ldots,u_4)=0,$$
$$\left(u_3u_4\frac{\partial^2}{\partial u_3\partial u_4}-\left(u_1\frac{\partial}{\partial u_1}+a\right)\left(u_1\frac{\partial}{\partial u_1}+b\right)\right)\Phi_{\mathbb{L},\gamma}(u_1,\ldots,u_4)=0\,. \tag{63}$$

combining these equations one finds

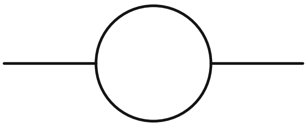
$$\left(u_1^2\frac{\partial}{\partial u_1}+(1+a+b)u_1\frac{\partial}{\partial u_1}+ab\right)\Phi_{\mathbb{L},\gamma}(u_1,\ldots,u_4)$$
$$=\frac{u_3u_4}{u_2}\left(u_1\frac{\partial^2}{\partial u_1^2}+c\frac{\partial}{\partial u_1}\right)\Phi_{\mathbb{L},\gamma}(u_1,\ldots,u_4). \tag{64}$$

Setting $F(z)=\Gamma(c)\Gamma(1-a)\Gamma(1-b)\Phi_{\mathbb{L},\gamma}(z,1,1,1)$ gives that $F(z)={}_2F_1\left({a\,b \atop c}\middle|z\right)$ satisfies the Gauß hypergeometric differential equation

$$z(z-1)\frac{d^2F(z)}{dz^2}+((a+b+1)z+c)\frac{dF(z)}{dz}+abF(z)=0\,. \tag{65}$$

3.4 *The Massive One-Loop Graph*

In this section we show how to apply the GKZ formalism on the one-loop bubble integral



3.4.1 Maximal Cut

The one-loop sunset (or bubble) graph as the graph polynomial

$$\mathscr{F}_\circ(x_1,x_2,t,\xi_1^2,\xi_2^2)=p^2x_1x_2-(\xi_1^2x_1+\xi_2^2x_2)(x_1+x_2)\,. \tag{66}$$

The most general toric degree two polynomial in $\mathbb{P}^2$ with at most degree two monomial is given by

$$\mathscr{F}_\circ^{tor}(x_1, x_2, z_1, z_2, z_3) = z_1 x_1^2 + z_2 x_2^2 + z_3 x_1 x_2 \,. \tag{67}$$

This toric polynomial has three parameters which is exactly the number of independent physical parameters. The identification of the variables is given by

$$z_1 = -\xi_1^2, \qquad z_2 = -\xi_2^2, \qquad z_3 = p^2 - (\xi_1^2 + \xi_2^2)\,, \tag{68}$$

We consider the equivalent toric Laurent polynomial

$$P(x_1, x_2) = \frac{\mathscr{F}_\circ^{tor}}{x_1 x_2} = \sum_{i=1}^{3} z_i x_1^{a_i^1} x_2^{a_i^2}\,, \tag{69}$$

so that p^2 in (66) corresponds to the constant term (or the origin the Newton polytope) and setting $\mathbf{a}_i = (1, a_i^1, a_i^2)$ we have

$$\mathbf{A}_\circ = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & 0 & 0 \end{pmatrix} . \tag{70}$$

The lattice is defined by

$$\mathbb{L}_\circ := \{\boldsymbol{\ell} := (\ell_1, \ell_2, \ell_3) \in \mathbb{Z}^3 | \ell_1 \mathbf{a}_1 + \ell_2 \mathbf{a}_2 + \ell_3 \mathbf{a}_3 = \boldsymbol{\ell} \cdot \mathbf{A}_\circ = 0\}\,. \tag{71}$$

This means that the elements of $\mathbb{L}_\circ$ are in the kernel of $\mathbf{A}_\circ$. This lattice in $\mathbb{Z}^3$ has rank one

$$\mathbb{L}_\circ = (1, 1, -2)\mathbb{Z}\,. \tag{72}$$

Notice that all the elements automatically satisfy the condition $\ell_1 + \ell_2 + \ell_3 = 0$.

Because the rank is one the GKZ system of differential equations is given by

$$\begin{aligned} e_1 &:= \frac{\partial^2}{\partial z_1 \partial z_2} - \frac{\partial^2}{(\partial z_3)^2}, \\ d_1 &:= \sum_{r=1}^{3} z_r \frac{\partial}{\partial z_r}, \\ d_2 &:= z_1 \frac{\partial}{\partial z_1} - z_2 \frac{\partial}{\partial z_2}, \end{aligned} \tag{73}$$

By construction for $\alpha \in \mathbb{C}$

$$e_1(\mathscr{F}_\circ^{tor})^\alpha = 0,$$
$$d_1(\mathscr{F}_\circ^{tor})^\alpha = \alpha\,(\mathscr{F}_\circ^{tor})^\alpha, \tag{74}$$

and

$$d_2(\mathscr{F}_\circ^{tor})^\alpha = \frac{1}{2}\,\left(\partial_{x_1}(x_1(\mathscr{F}_\circ^{tor})^\alpha) - \partial_{x_2}(x_2(\mathscr{F}_\circ^{tor})^\alpha)\right)\,, \tag{75}$$

therefore the action of the derivative d_2 vanishes on the integral but not the integrand

$$d_2\int_\gamma (\mathscr{F}_\circ^{tor})^\alpha = 0 \qquad \text{for} \qquad \partial\gamma = \emptyset\,. \tag{76}$$

The GKZ hypergeometric series is defined as for $\gamma_i \notin \mathbb{Z}$

$$\Phi^\circ_{\mathbb{L},\boldsymbol{\gamma}} = \sum_{\boldsymbol{\ell}\in\mathbb{L}_\circ}\prod_{i=1}^{3}\frac{z_i^{l_i+\gamma_i}}{\Gamma(l_i+\gamma_i+1)}, \tag{77}$$

in this sum we have $\boldsymbol{\ell} = n(1,1,-2)$ with $n\in\mathbb{Z}$, and the condition $\sum_{i=1}^3 \gamma_i \mathbf{a}_i = (0,0,-1)$ which can be solved using $\boldsymbol{\gamma} = (\gamma_1,\gamma_2,\gamma_3) = \gamma(1,1,-2)+(0,0,-1)$, leading to

$$\Phi^\circ_{\mathbb{L},\boldsymbol{\gamma}} = \frac{1}{z_3}\sum_{n\in\mathbb{Z}}\frac{u_1^n}{\Gamma(n+\gamma+1)^2\Gamma(-2n+\gamma)}, \tag{78}$$

where we have introduced the new toric coordinate

$$u_1 := \frac{z_1 z_2}{z_3^2} = \frac{\xi_1^2\xi_2^2}{\left(p^2-(\xi_1^2+\xi_2^2)\right)^2}\,. \tag{79}$$

This is the natural coordinate dictated by the invariance of the period integral under the transformation $(x_1,x_2)\to(\lambda x_1,\lambda x_2)$ and $(z_1,z_2,z_3)\to(z_1/\lambda, z_2/\lambda, z_3/\lambda)$.

This GKZ hypergeometric function is a combination of ${}_3F_2$ hypergeometric functions

$$\Phi^\circ_{\mathbb{L},\boldsymbol{\gamma}} = \frac{1}{z_3^{1-2\gamma}}\left(\frac{u_1^{\gamma-1}}{\Gamma(\gamma)\Gamma(\gamma+2)}\,{}_3F_2\left(\begin{matrix}1,\ 1-\gamma,\ 1-\gamma\\ 1+\frac{\gamma}{2},\ \frac{3}{2}+\frac{\gamma}{2}\end{matrix}\middle|\frac{1}{4u_1}\right)\right.$$
$$\left.+\frac{u_1^\gamma}{\Gamma(\gamma+1)^2}\,{}_3F_2\left(\begin{matrix}1,\ \frac{1}{2}-\frac{\gamma}{2},\ \frac{1}{2}-\frac{\gamma}{2}\\ 1+\gamma,\ 1+\gamma\end{matrix}\middle|4u_1\right)\right)\,. \tag{80}$$

For $\gamma = 0$ the series is trivially zero as the system is resonant and needs to be regularised [50, 54] . The regularisation is to use the functional equation for the Γ-function $\Gamma(z)\Gamma(1-z) = \pi/\sin(\pi z)$ to replace the pole term by

$$\lim_{\varepsilon\to 0}\frac{\Gamma(\varepsilon)}{\Gamma(-2n+\varepsilon)}=\Gamma(1+2n),\qquad n\in\mathbb{Z}\backslash\{0\},\tag{81}$$

and write the associated regulated period as

$$\pi_\circ=\lim_{\varepsilon\to 0}\frac{1}{z_3}\sum_{n\in\mathbb{N}}\frac{u_1^n\Gamma(\varepsilon)}{\Gamma(n+1)^2\Gamma(-2n+\varepsilon)}\,,\tag{82}$$

which is easily shown to be

$$\begin{aligned}\pi_\circ(z_1,z_2,z_3)&=\frac{1}{z_3}{}_2F_1\left(\begin{matrix}\frac{1}{2}\ 1\\ 1\end{matrix}\middle|4u_1\right)=\frac{1}{\sqrt{z_3^2-4z_1z_2}}\,,\\ &=\frac{1}{\sqrt{(p^2-(\xi_1+\xi_2)^2)(p^2-(\xi_1-\xi_2)^2)}}\,.\end{aligned}\tag{83}$$

This expression of course matches the expression for the maximal cut (18) integral $\pi_\circ(p^2,\xi_1^2,\xi_2^2,2)$ in two dimensions

$$\pi_\circ(p^2,\xi_1^2,\xi_2^2,2)=\frac{1}{(2i\pi)^2}\int_{|x_1|=|x_2|=1}\frac{dx_1dx_2}{\mathscr{F}_\circ(x_1,x_2)}\,.\tag{84}$$

3.4.2 The Differential Operator

From the expression of the maximal cut $\pi_\circ$ in (83) as an hypergeometric series, which satisfies a second order differential equation (65), we can extract a differential operator with respect to p^2 or the masses ξ_i^2 annihilating the maximal cut. This differential equation is not the minimal one as it can be factorised leaving minimal order differential operators are annihilating the maximal cut are such that $L^\circ_{PF,(1)}\pi_\circ(p^2,\xi_1^2,\xi_2^2)=0$ and $L^\circ_{PF,(2)}\pi_\circ(p^2,\xi_1^2,\xi_2^2)=0$ with

$$L^\circ_{PF,(1)}=p^2\frac{d}{dp^2}+\frac{p^2(p^2-\xi_1^2-\xi_2^2)}{(p^2-(\xi_1+\xi_2)^2)(p^2-(\xi_1-\xi_2)^2)}\,,\tag{85}$$

and

$$L^\circ_{PF,(2)}=\xi_1^2\frac{d}{d\xi_1^2}-\frac{\xi_1^2(p^2-\xi_1^2+\xi_2^2)}{(p^2-(\xi_1+\xi_2)^2)(p^2-(\xi_1-\xi_2)^2)}\,,\tag{86}$$

with of course a similar operator with the exchange of ξ_1 and ξ_2. These operators do not annihilate the integrand but lead to total derivatives

$$L^\circ_{PF,(1)}\frac{1}{\mathscr{F}_\circ(\underline{x},p^2,\underline{\xi}^2)}=\partial_{x_1}\left(\frac{p^2(2\xi_2^2-(p^2-(\xi_1^2+\xi_2^2))x_1)}{(p^2-(\xi_1+\xi_2)^2)(p^2-(\xi_1-\xi_2)^2)\mathscr{F}_2(x_1,1,p^2,\underline{\xi}^2)}\right),\tag{87}$$

and

$$L^{\circ}_{PF,(2)}\,\frac{1}{\mathscr{F}_{\circ}(\underline{x},p^2,\underline{\xi}^2)}=\partial_{x_1}\left(\frac{((p^2-\xi_2^2)^2-\xi_1^2(p^2+\xi_2^2))x_1-\xi_2^2(p^2+\xi_1^2-\xi_2^2)}{(p^2-(\xi_1+\xi_2)^2)(p^2-(\xi_1-\xi_2)^2)\,\mathscr{F}_2(x_1,1,p^2,\underline{\xi}^2)}\right). \tag{88}$$

These operators can be obtained from the operator $td/dt+1$ derived in Sect. 2.3.1 and the change of variables $t=\frac{\sqrt{\left(p^2-\xi_1^2-\xi_2^2\right)^2-4\xi_1^2\xi_2^2}}{\xi_1^2}$. For the boundary term one needs to pay attention that the shift induces a dependence on the physical parameters in the domain of integration.

3.4.3 The Massive One-Loop Sunset Feynman Integral

Having determined the differential operators acting on the maximal cut it is now easy to obtain the action of these operators on the one-loop integral. The action of the Picard–Fuchs operators on the Feynman integral $I_{\circ}(p^2,\xi_1^2,\xi_2^2,2)$ are given by

$$L^{\circ}_{PF,(1)}\,I_{\circ}(p^2,\xi_1^2,\xi_2^2,2)=-\frac{2}{(p^2-(\xi_1+\xi_2)^2)(p^2-(\xi_1-\xi_2)^2)}\,, \tag{89}$$

and

$$L^{\circ}_{PF,(2)}\,I_{\circ}(p^2,\xi_1^2,\xi_2^2,2)=\frac{\xi_1^2-\xi_2^2-p^2}{(p^2-(\xi_1+\xi_2)^2)(p^2-(\xi_1-\xi_2)^2)}\,. \tag{90}$$

It is then easy to obtain that in $D=2$ dimensions the one-loop massive bubble evaluates to

$$\begin{aligned}I_{\circ}(p^2,\xi_1^2,\xi_2^2)=&\frac{1}{\sqrt{(p^2-(\xi_1+\xi_2)^2)(p^2-(\xi_1-\xi_2)^2)}}\\&\times\log\left(\frac{p^2-(\xi_1^2+\xi_2^2)-\sqrt{(p^2-(\xi_1+\xi_2)^2)(p^2-(\xi_1-\xi_2)^2)}}{p^2-(\xi_1^2+\xi_2^2)+\sqrt{(p^2-(\xi_1+\xi_2)^2)(p^2-(\xi_1-\xi_2)^2)}}\right).\end{aligned} \tag{91}$$

3.5 *The Two-Loop Sunset*

The sunset graph polynomial is the most general cubic in $\mathbb{P}^2$ with maximal order two degree for each variables

$$\mathscr{F}_{\ominus}(x_1,x_2,x_3,t,\underline{\xi}^2)=x_1x_2x_3\left(p^2-(\xi_1^2x_1+\xi_2^2x_2+\xi_3^2x_3)\left(\frac{1}{x_1}+\frac{1}{x_2}+\frac{1}{x_3}\right)\right), \tag{92}$$

which corresponds to the toric polynomial

$$\mathscr{F}_{\ominus}^{tor} = x_1x_2x_3\left(\frac{x_3z_1}{x_1} + \frac{x_2z_2}{x_1} + \frac{x_3z_3}{x_2} + \frac{x_1z_4}{x_3} + \frac{x_2z_5}{x_3} + \frac{x_1z_6}{x_2} + z_7\right). \tag{93}$$

To the contrary to the one-loop case there are more toric parameters z_i than physical variables. The identification of the physical variables is

$$-\xi_1^2 = z_4 = z_6, \quad -\xi_2^2 = z_2 = z_5, \quad -\xi_3^2 = z_1 = z_3, \quad p^2 - (\xi_1^2 + \xi_2^2 + \xi_3^2) = z_7, \tag{94}$$

As before writing the toric polynomial as

$$P_{\ominus} = \sum_{i=1}^{7} z_i x_1^{a_i^1} x_2^{a_i^2} x_3^{a_i^3}, \tag{95}$$

and setting $\mathbf{a}_i = (1, a_i^1, a_i^2, a_i^3)$ we have

$$\mathbf{A}_{\ominus} = \begin{pmatrix}\mathbf{a}_1\\ \vdots\\ \mathbf{a}_7\end{pmatrix} = \begin{pmatrix}1 & -1 & 0 & 1\\ 1 & -1 & 1 & 0\\ 1 & 0 & -1 & 1\\ 1 & 1 & 0 & -1\\ 1 & 0 & 1 & -1\\ 1 & 1 & -1 & 0\\ 1 & 0 & 0 & 0\end{pmatrix}, \tag{96}$$

The lattice is now defined by

$$\mathbb{L}_{\ominus} := \{\boldsymbol{\ell} := (\ell_1, \dots, \ell_7) \in \mathbb{Z}^7 | \ell_1\mathbf{a}_1 + \cdots + \ell_7\mathbf{a}_7 = \boldsymbol{\ell}\cdot\mathbf{A}_{\ominus} = 0\}. \tag{97}$$

This lattice in $\mathbb{Z}^7$ has rank four $\mathbb{L}_{\ominus} = \oplus_{i=1}^4 L_i\mathbb{Z}$ with the basis

$$\begin{pmatrix}L_1\\ \vdots\\ L_4\end{pmatrix} = \begin{pmatrix}1 & 0 & 0 & 0 & 1 & 1 & -3\\ 0 & 1 & 0 & 0 & 0 & 1 & -2\\ 0 & 0 & 1 & 0 & 1 & 0 & -2\\ 0 & 0 & 0 & 1 & -1 & -1 & 1\end{pmatrix}, \tag{98}$$

From this we derive the sunset GKZ system

$$\begin{aligned} e_1 &:= \frac{\partial^3}{\partial z_1 \partial z_5 \partial z_6} - \frac{\partial^3}{(\partial z_7)^3},\\ e_2 &:= \frac{\partial^2}{\partial z_2 \partial z_6} - \frac{\partial^2}{(\partial z_7)^2}, \end{aligned}$$

$$
\begin{aligned}
e_3 &:= \frac{\partial^2}{\partial z_3 \partial z_5} - \frac{\partial^2}{(\partial z_7)^2},\\
e_4 &:= \frac{\partial^2}{\partial z_4 \partial z_7} - \frac{\partial^2}{\partial z_5 \partial z_6}
\end{aligned}
\tag{99}
$$

by construction $e_i(\mathscr{F}^{tor}_{\ominus})^{\alpha} = 0$ with $\alpha \in \mathbb{C}$ for $1 \leq i \leq 4$. We have as well this second set of operators from the operators

$$
\begin{aligned}
d_1 &:= \sum_{r=1}^{7} z_r \frac{\partial}{\partial z_r},\\
d_2 &:= z_1 \frac{\partial}{\partial z_1} + z_2 \frac{\partial}{\partial z_2} - z_4 \frac{\partial}{\partial z_4} - z_6 \frac{\partial}{\partial z_6},\\
d_3 &:= z_2 \frac{\partial}{\partial z_2} - z_3 \frac{\partial}{\partial z_3} + z_5 \frac{\partial}{\partial z_5} - z_6 \frac{\partial}{\partial z_6},\\
d_4 &:= z_1 \frac{\partial}{\partial z_1} + z_3 \frac{\partial}{\partial z_3} - z_4 \frac{\partial}{\partial z_4} - z_5 \frac{\partial}{\partial z_5}
\end{aligned}
\tag{100}
$$

The interpretation of these operators is the following

- The Euler operator $d_1 \mathscr{F}^{\alpha}_{tor} = \alpha \, \mathscr{F}^{\alpha}_{tor}$ for $\alpha \in \mathbb{C}$.
- To derive the action of these operators on the maximal cut period integral

$$
\pi^{tor}_{\ominus}(z_1, \ldots, z_7) = \frac{1}{(2i\pi)^3} \int_{\gamma} \frac{1}{\mathscr{F}^{tor}_{\ominus}} \prod_{i=1}^{3} dx_i \,, \tag{101}
$$

  we remark that if $\mathscr{F}^{tor}_{\ominus} = x_1 x_2 x_3 \, P_{\ominus}$ we have

$$
\begin{aligned}
d\left(\frac{1}{P_{\ominus}} \frac{dx_1}{x_1}\right) &= \frac{-z_1 x_1/x_2 + z_3 x_2 + z_4 x_2/x_1 - z_6/x_2}{P_{\ominus}^2} \frac{dx_1}{x_1} \wedge \frac{dx_2}{x_2},\\
d\left(\frac{1}{P_{\ominus}} \frac{dx_1}{x_1}\right) &= -\frac{z_1 x_1/x_2 + z_2 x_1 - z_4 x_2/x_1 - z_5/x_1}{P_{\ominus}^2} \frac{dx_1}{x_1} \wedge \frac{dx_2}{x_2},
\end{aligned}
\tag{102}
$$

  therefore since the cycle γ has no boundary

$$
\begin{aligned}
d_2 \pi^{tor}_{\ominus} &= \int_{\gamma} d\left(\frac{1}{P_{\ominus}} \frac{dx_1}{x_1}\right) = 0,\\
d_3 \pi^{tor}_{\ominus} &= -\int_{\gamma} d\left(\frac{1}{P_{\ominus}} \frac{dx_2}{x_2}\right) = 0,\\
d_4 \pi^{tor}_{\ominus} &= \int_{\gamma} d\left(\frac{1}{P_{\ominus}} \left(\frac{dx_1}{x_1} + \frac{dx_2}{x_2}\right)\right) = 0 \,.
\end{aligned}
\tag{103}
$$

- The natural toric coordinates are

$$u_1 := \frac{z_1 z_5 z_6}{z_7^3}, \qquad u_2 := \frac{z_2 z_6}{z_7^2}, \qquad u_3 := \frac{z_3 z_5}{z_7^2}, \qquad u_4 := \frac{z_4 z_7}{z_5 z_6}, \tag{104}$$

which reads in terms of the physical parameters

$$\begin{aligned} u_2 &= \frac{\xi_1^2 \xi_2^2}{\left(p^2 - (\xi_1^2 + \xi_2^2 + \xi_3^2)\right)^2}, \quad u_3 = \frac{\xi_2^2 \xi_3^2}{\left(p^2 - (\xi_1^2 + \xi_2^2 + \xi_3^2)\right)^2}, \\ u_4 &= \frac{p^2 - (\xi_1^2 + \xi_2^2 + \xi_3^2)}{\xi_2^2}, \quad u_1 = u_2 u_3 u_4. \end{aligned} \tag{105}$$

They are the natural variables associated with the toric symmetries of the period integral

$$\begin{aligned} (x_1, x_2) &\to (\lambda x_1, x_2), \quad (z_1, z_2, z_3, z_4, z_5, z_6, z_7) \to (z_1/\lambda, z_2/\lambda, z_3, z_4\lambda, z_5\lambda, z_6, z_7), \\ (x_1, x_2) &\to (x_1, \lambda x_2), \quad (z_1, z_2, z_3, z_4, z_5, z_6, z_7) \to (z_1\lambda, z_2, z_3/\lambda, z_4/\lambda, z_5, z_6\lambda, z_7), \\ (x_1, x_2) &\to (\lambda x_1, \lambda x_2), \quad (z_1, z_2, z_3, z_4, z_5, z_6, z_7) \to (z_1, z_2/\lambda, z_3/\lambda, z_4, z_5\lambda, z_6\lambda, z_7). \end{aligned} \tag{106}$$

The sunset GKZ hypergeometric series is defined as for $\gamma_i \notin \mathbb{Z}$ with $1 \leq i \leq 7$

$$\Phi^{\ominus}_{\mathbb{L},\boldsymbol{\gamma}}(z_1, \ldots, z_7) = \sum_{\boldsymbol{\ell} \in \mathbb{L}} \prod_{i=1}^{7} \frac{z_i^{l_i + \gamma_i}}{\Gamma(l_i + \gamma_i + 1)}, \tag{107}$$

in this sum we have $\boldsymbol{\ell} = \sum_{i=1}^4 n_i L_i$ with $n_i \in \mathbb{Z}$, and the condition $\sum_{i=1}^7 \gamma_i \mathbf{a}_i = (-1, 0, 0, 0)$ which can be solved using $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_7) = \sum_{i=1}^4 \gamma_i \mathscr{L}_i + (0, \ldots, 0, -1)$. Using the leading to toric variables the solution reads

$$\begin{aligned} \Phi^{\ominus}_{\mathbb{L},\boldsymbol{\gamma}}(z_1, \ldots, z_7) &= \frac{1}{z_7} \sum_{(n_1, \ldots, n_4) \in \mathbb{Z}} \frac{u_1^{n_1+\gamma_1} u_2^{n_2+\gamma_2} u_3^{n_3+\gamma_3} u_4^{n_4+\gamma_4}}{\prod_{i=1}^4 \Gamma(n_i + \gamma_i + 1)} \times \\ &\times \frac{1}{\Gamma(n_1 + n_2 - n_4 + \gamma_1 + \gamma_2 - \gamma_4 + 1)\Gamma(n_1 + n_3 - n_4 + \gamma_1 + \gamma_3 - \gamma_4 + 1)} \\ &\times \frac{1}{\Gamma(-3n_1 - 2n_2 - 2n_3 + n_4 - 3\gamma_1 - 2\gamma_2 - 2\gamma_3 + \gamma_4)}. \end{aligned} \tag{108}$$

With $\boldsymbol{\gamma} = (0, 0, 0, 0, 0, 0, 0)$ the series is trivially zero as being resonant. The resolution is to the regularise the term has a zero by using for $\ell_7 < 0$

$$\lim_{\varepsilon \to 0} \frac{\Gamma(\varepsilon)}{\Gamma(\ell_7 + \varepsilon)} = (-1)^{\ell_7} \Gamma(1 - \ell_7), \tag{109}$$

and write the associated regulated period as

$$\pi_{\ominus}^{(2)}(p^2,\underline{\xi}^2) = \lim_{\varepsilon\to 0}\sum_{(n_1,n_2,n_3,n_4)\in\mathbb{N}} \frac{(\xi_1^2)^{n_1+n_2}(\xi_2^2)^{n_1+n_2+n_3-n_4}(\xi_3^2)^{n_1+n_3}}{\prod_{i=1}^4 \Gamma(1+n_i)}$$
$$\times\frac{(p^2-(\xi_1^2+\xi_2^2+\xi_3^2))^{-3n_1-2n_2-2n_3+n_4-1}(-1)^{-3n_1-2n_2-2n_3+n_4}\Gamma(\varepsilon)}{\Gamma(1+n_1+n_2-n_4)\Gamma(1+n_1+n_3-n_4)\Gamma(-3n_1-2n_2-2n_3+n_4+\varepsilon)}\,. \tag{110}$$

One can expand this expression as a series near $t=\infty$ to get that

$$\pi_{\ominus}^{(2)}(p^2,\xi_1^2,\xi_2^2,\xi_3^2) = \sum_{n\geq 0}(p^2)^{-n-1}\sum_{n_1+n_2+n_3=n}\left(\frac{n!}{n_1!n_2!n_3!}\right)^2 \xi_1^{2n_1}\xi_2^{2n_2}\xi_3^{2n_3}\,, \tag{111}$$

which is the series expansion of the maximal cut integral

$$\pi_{\ominus}^{(2)}(p^2,\underline{\xi}^2) = \frac{1}{(2i\pi)^3}\int_\gamma \frac{1}{\mathscr{F}_\ominus}\prod_{i=1}^3 dx_i\,, \tag{112}$$

where $\gamma=\{|x_1|=|x_2|=|x_3|=1\}$. The construction generalises easily to the case of the higher loop sunset integral in an easy way [55].

3.5.1 The Differential Operators

Now that we have the expression for the maximal cut it is easy to derive the minimal order differential operator annihilating this period. There are various methods to derive the Picard–Fuchs operator from the maximal cut. One method is to use the series expansion of the period around $s=1/t=0$. Another method is to reduce the GKZ system of differential operator in similar fashion as shown for the hypergeometric function in Sect. 3.3.1. This method leads to a fourth order differential operator which factorises a minimal second order operator. We notice that this approach is similar to the integration-by-part based approach

The minimal order differential operator is of second order

$$\mathscr{L}_{PF}^{\ominus} = \left(p^2\frac{d}{dp^2}\right)^2 + q_1(p^2,\underline{\xi}^2)\left(p^2\frac{d}{dp^2}\right) + q_0(p^2,\underline{\xi}^2)\,, \tag{113}$$

with the coefficients given in [20, 56]. The action of this differential operator on the maximal cut is given by

$$\mathscr{L}_{PF}^{\ominus}\pi_{\ominus}^{(2)} = \frac{1}{(2i\pi)^3}\int_\gamma \mathscr{L}_{PF}^{\ominus}\frac{1}{\mathscr{F}_\ominus}\prod_{i=1}^3 dx_i = \frac{1}{(2i\pi)^3}\int_\gamma\left(\sum_{i=1}^3\partial_i\beta_i\right)\prod_{i=1}^3 dx_i = 0\,. \tag{114}$$

The action of this operator on the Feynman integral is given by then we find that that full differential operator acting on the two-loop sunset integral is given by

$$\mathscr{L}_{PF}^{\ominus} I_{\ominus}(p^2, \underline{\xi}^2) = \int_{\substack{x_1 \geq 0 \\ x_2 \geq 0}} \left(\sum_{i=1}^{3} \partial_i \beta_i \right) \delta(x_3 = 1) \prod_{i=1}^{3} dx_i = \mathscr{S}_{\ominus} \,, \tag{115}$$

where the inhomogeneous term reads

$$\mathscr{S}_{\ominus} = \mathscr{Y}_{\ominus}(p^2, \underline{\xi}^2) + c_1(p^2, \underline{\xi}^2) \log\left(\frac{m_1^2}{m_3^2}\right) + c_2(p^2, \underline{\xi}^2) \log\left(\frac{m_2^2}{m_3^2}\right) , \tag{116}$$

with the Yukawa coupling[4]

$$\mathscr{Y}_{\ominus}(p^2, \underline{\xi}^2) = \frac{6(p^2)^2 - 4p^2(\xi_1^2 + \xi_2^2 + \xi_3^2) - 2\prod_{i=1}^{4} \mu_i}{(p^2)^2 \prod_{=1}^{4}(p^2 - \mu_i^2)} , \tag{117}$$

where $(\mu_1, \ldots, \mu_4) = ((-\xi_1 + \xi_2 + \xi_3)^2), (\xi_1 - \xi_2 + \xi_3)^2), (\xi_1 + \xi_2 - \xi_3)^2), (\xi_1 + \xi_2 + \xi_3)^2))$. A geometric interpretation is the integral [20]

$$\mathscr{Y}_{\ominus}(p^2, \underline{\xi}^2) = \int_{\mathscr{E}_{\ominus}} \Omega_{\ominus} \wedge p^2 \frac{d}{p^2} \Omega_{\ominus} \,, \tag{118}$$

where $\Omega_{\ominus}$ is the sunset residue differential form

$$\Omega_{\ominus} = \mathrm{Res}_{\mathscr{E}_{\ominus}=0} \frac{x_1 dx_2 \wedge dx_3 + x_3 dx_1 \wedge dx_2 + x_2 dx_3 \wedge dx_1}{\mathscr{F}_{\ominus}} , \tag{119}$$

on the sunset elliptic curve

$$\mathscr{E}_{\ominus} := \{p^2 x_1 x_2 x_3 - (\xi_1^2 x_1 + \xi_2^2 x_2 + \xi_3^2 x_3)(x_1 x_2 + x_1 x_3 + x_2 x_3) | (x_1, x_2, x_3) \in \mathbb{P}^2\} \,. \tag{120}$$

The Yukawa coupling satisfies the differential equation

$$p^2 \frac{d}{p^2} \mathscr{Y}_{\ominus}(t) = (2 - q_1(p^2, \underline{\xi}^2)) \mathscr{Y}_{\ominus}(p^2, \underline{\xi}^2) \,. \tag{121}$$

The coefficients c_1 and c_2 in (116) are the integral of the residue one form between the marked points on $Q_1 = [0, -\xi_3^2, \xi_2^2]$, $Q_2 = [-\xi_3^2, 0, \xi_1^2]$ and $Q_3 = [-\xi_2^2, \xi_1^2, 0]$ on the elliptic curve [20]

---

[4]This quantity is the usual Yukawa coupling of particle physics and string theory compactification. The Yukawa coupling is determined geometrically by the integral of the wedge product of differential forms over particular cycles [57]. The Yukawa couplings which depend non-trivially on the internal geometry appear naturally in the differential equations satisfied by the periods of the underlying geometry as explained for instance in these reviews [46, 58].

$$c_1(p^2, \underline{\xi}^2) := p^2 \frac{d}{p^2} \int_{Q_1}^{Q_3} \Omega_\ominus, \qquad c_2(p^2, \underline{\xi}^2) := p^2 \frac{d}{p^2} \int_{Q_2}^{Q_3} \Omega_\ominus\,. \tag{122}$$

3.6 The Generic Case

In this section we show how to determine the differential equation for the l-loop sunset integral from the knowledge of the maximal cut. The maximal cut of the l-loop sunset integral is given by

$$\pi_\ominus^{(l)}(p^2, \underline{\xi}^2) = \sum_{n\geq 0} t^{-n-1}\, A_\ominus(l, n, \xi_1^2, \dots, \xi_{l+1}^2)\,, \tag{123}$$

with

$$A_\ominus(l, n, \xi_1^2, \cdots, \xi_{l+1}^2) := \sum_{r_1+\cdots+r_{l+1}=n} \left(\frac{n!}{r_1!\cdots r_{l+1}!}\right)^2 \prod_{i=1}^{l+1} \xi_i^{2r_i}\,. \tag{124}$$

3.6.1 The All Equal Mass Case

For the all equal mass case one can easily determine the differential equation to all order [26] using the Bessel integral representation of [9]. We present here a different derivation.

For the all equal masses the coefficient of the maximal cut satisfies a nice recursion [59]

$$\sum_{k\geq 0} \left(n^{l+2} \sum_{1\leq i\leq k} \sum_{\substack{a_i+b_i=l+2\\ 1<a_{i+1}+1<a_i\leq l+1}} \prod_{i=1}^{k} (-a_i b_i) \left(\frac{n-i}{n-i+1}\right)^{a_i-1} \right) A_\ominus(l, n-k, \underline{1}) = 0, \tag{125}$$

where $a_i \in \mathbb{N}$. Standard method gives that the associated differential operator acting on $t\pi_\ominus^l(t, 1, \dots, 1) = \sum_{n\geq 0} (p^2)^{-n} A(l+1, n, 1, \dots, 1)$ reads

$$\begin{aligned}\mathscr{L}_{PF,\ominus}^{(l),1mass} &= \sum_{k\geq 0} (p^2)^k \sum_{1\leq i\leq k} \sum_{\substack{a_i+b_i=l+2, a_{k+1}=0\\ 1<a_{i+1}+1<a_i\leq l+1}} \left(k - p^2 \frac{d}{p^2}\right)^{l+2-a_1} \\ &\qquad \times \prod_{i=1}^{k} (-a_i b_i) \left(k - i - p^2 \frac{d}{dp^2}\right)^{a_i - a_{i+1}}\,.\end{aligned} \tag{126}$$

This operator has been derived in [26, §9] using different method.

They are differential operators of order l, the loop order, in d/dp^2 and the coefficients are polynomials of degree $l+1$

$$\mathscr{L}_{PF}^{(l),1mass} = (-p^2)^{\lceil l/2\rceil -1} \prod_{i=1}^{\lfloor l/2\rfloor+1} (p^2-\mu_i^2)\left(\frac{d}{dp^2}\right)^l + \cdots \tag{127}$$

where $\mu_i^2 := (\pm 1 \pm 1 \cdots \pm 1)^2$ is the set of the different thresholds. The operator $\mathscr{L}_{PF}^{(2),1mass}$ is the Picard–Fuchs operator of the family of elliptic curves for $\Gamma_1(6)$ for the all equal mass sunset [60], the operator $\mathscr{L}_{PF}^{(3),1mass}$ of the family of $K3$ surfaces [61]. Having determined the Picard–Fuchs operator it is not difficult to derive its action on the Feynman integral with the result that [26]

$$\mathscr{L}_{PF}^{(l),1mass}(I_\ominus(p^2,1,\ldots,1)) = -(l+1)!\,. \tag{128}$$

3.6.2 The General Mass Case

For unequal masses the recursion relation does not close only on the coefficients (124) and no simple closed formula is known for the differential operator on the maximal cut. The minimal differential operator annihilating the $\pi_\ominus^{(l)}(t,\underline{\xi}^2)$ can be obtained using the GKZ hypergeometric function discussed in the previous section.

For the l-loop sunset integral the GKZ lattice has rank l^2, $\mathbb{L} = \sum_{i=1}^{l^2} n_i\, L_i$. For instance for the three-loop sunset the regulated hypergeometric series representation of the maximal cut reads

$$\begin{aligned}\pi_\ominus^{(3)}(p^2,\underline{\xi}^2) = -\lim_{\varepsilon\to 0} \sum_{(n_1,\ldots,n_9)\in\mathbb{N}^9} & \frac{(\xi_1^2)^{n_1+n_2+n_3}(\xi_2^2)^{n_1+n_3+n_4+n_6-n_7-n_8+n_9}}{\prod_{i=1}^9 \Gamma(1+n_i)}\\ &\times \frac{(\xi_3^2)^{n_2+n_5+n_8}(\xi_4^2)^{n_1+n_4+n_6}}{\Gamma(n_1+n_4+n_6-n_7-n_8+1)\Gamma(n_2+n_5-n_6+n_8-n_9+1)}\\ &\times \frac{1}{\Gamma(n_1+n_3-n_5+n_6-n_7-n_8+n_9+1)}\\ &\times \frac{(-p^2+\xi_1^2+\xi_2^2+\xi_3^2+\xi_4^2)^{-3n_1-2n_2-2n_3-2n_4-n_5-2n_6+n_7-n_9-1}\Gamma(\varepsilon)}{\Gamma(-3n_1-2n_2-2n_3-2n_4-n_5-2n_6+n_7-n_9+\varepsilon)}.\end{aligned} \tag{129}$$

The minimal order differential operator annihilating the maximal cut $p^2\pi_\ominus^{(3)}(p^2,\underline{\xi}^2)$ with generic mass configurations, $\xi_1 \neq \xi_2 \neq \xi_3 \neq \xi_4$ and all the masses non vanishing, is an operator of order 6, with polynomial coefficients $c_k(t)$ of degree up to 29

$$L_{PF,\ominus}^3 = \sum_{k=0}^{6} c_k(t)\left(t\frac{d}{t}\right)^k. \tag{130}$$

For instance the differential operator for the mass configuration $\xi_i = i$ with $1 \le i \le 4$ is given by

$$\begin{aligned} c_6 &= (t-100)(t-36)(t-64)(t-4)^2(t-16)^2 \\ &\times \big(345t^{12} - 10275t^{11} + 243243t^{10} + 700860t^9 - 289019444t^8 + 9517886160t^7 \\ &- 169244843904t^6 + 2163112875520t^5 - 24375264125952t^4 \\ &+ 198627459010560t^3 - 896517312217088t^2 \\ &+ 1570362910310400t - 1192050032640000\big), \end{aligned} \tag{131}$$

and

$$\begin{aligned} c_5 &= (t-4)(t-16)\big(7245t^{17} - 1461150t^{16} + 108842709t^{15} - 4073021820t^{14} \\ &+ 79037467036t^{13} + 706049613520t^{12} - 122977114948800t^{11} \\ &+ 4897976525794560t^{10} - 118057966435402752t^9 \\ &+ 2042520337021317120t^8 - 28129034886941589504t^7 \\ &+ 321784682881513881600t^6 - 2877522528057659228160t^5 \\ &+ 17978948962533528043520t^4 - 69950845277551433089024t^3 \\ &+ 151178557780128065126400t^2 - 182250696371318292480000t \\ &+ 96676211287130112000000\big), \end{aligned} \tag{132}$$

and

$$\begin{aligned} c_4 &= 2\big(23460t^{19} - 4086975t^{18} + 273974766t^{17} - 9833465295t^{16} \\ &+ 173874227860t^{15} + 3780156754180t^{14} \\ &- 419091386081744t^{13} + 16647873781420800t^{12} \\ &- 425729411677916160t^{11} + 8098824799795968000t^{10} \\ &- 125136842089603031040t^9 + 1631034274362173030400t^8 \\ &+ 173643904146421013544 96t^7 + 140612615518097533829120t^6 \\ &- 807868060015143792148480t^5 + 3100095209313936311582720t^4 \\ &- 7563751451192001262780416t^3 + 11448586013594218187980800t^2 \\ &- 9812428506034109153280000t + 3374878648568905728000000\big), \end{aligned} \tag{133}$$

and

$$\begin{aligned} c_3 &= 12\big(8970t^{19} - 1147050t^{18} + 56442264t^{17} - 1477273050t^{16} - 447578647t^{15} \\ &+ 2416587481200t^{14} - 130189239609348t^{13} + 4001396495500560t^{12} \\ &- 86975712270293184t^{11} + 1511724058206439680t^{10} \end{aligned}$$

$$
\begin{aligned}
&- 22690173944998831104t^9 + 28997467949760092160 0t^8 \\
&- 29007626181964981370 88t^7 + 20882244400635484241920t^6 \\
&- 10109032702326061085 4912t^5 + 30876042892573654646 7840t^4 \\
&- 55905723724426733263 2576t^3 + 53317728311810960916 4800t^2 \\
&- 13303477731242016768 0000t - 14061994369037107200 0000\big), \qquad (134)
\end{aligned}
$$

and

$$
\begin{aligned}
c_2 = 24\big(&3105t^{19} - 260100t^{18} + 8740695t^{17} - 121279200t^{16} - 8982728081t^{15} \\
&+ 771645247175t^{14} - 29786960482306t^{13} + 741851366254700t^{12} \\
&- 14140682364004072t^{11} + 237224880534337760t^{10} \\
&- 3605462277123620992t^9 + 44725169880349560320t^8 \\
&- 405767142088142927872t^7 + 2549108215435181793280t^6 \\
&- 11307241496864563101696t^5 + 40972781273200446013440t^4 \\
&- 141797614014479525216256t^3 + 363118631232748702924800t^2 \\
&- 415180490608717332480000t + 210929915535556608000000\big), \qquad (135)
\end{aligned}
$$

and

$$
\begin{aligned}
c_1 = 24\,\big(&345t^{19} - 15000t^{18} + 345675t^{17} + 7323600t^{16} - 3165461083t^{15} \\
&+ 184943420750t^{14} - 5084383561348t^{13} + 91042473303800t^{12} \\
&- 1344824163401536t^{11} + 17444484465759680t^{10} \\
&- 146155444722244096t^9 - 426434786380119040t^8 \\
&+ 31798683088486989824t^7 - 488483076656283893760t^6 \\
&+ 5136134162164414021632t^5 - 40834519838668015534080t^4 \\
&+ 222597043391679285952512t^3 - 685074395310881085849600t^2 \\
&+ 830360981217434664960000t - 421859831071113216000000\big), \qquad (136)
\end{aligned}
$$

and

$$
\begin{aligned}
c_0 = 1728\,\big(&21908444t^{15} - 1482071825t^{14} + 40507170144t^{13} - 668436089250t^{12} \\
&+ 8209054542408t^{11} - 65000176183240t^{10} - 503218239747392t^9 \\
&+ 31962708303867520t^8 - 619576476284137472t^7 + 7554395788685281280t^6 \\
&- 73455221906789646336t^5 + 571135922816871792640t^4 \\
&- 3095113137012548304896t^3 + 9514922157095570636800t^2 \\
&- 11532791405797703680000t + 5859164320432128000000\big)\,. \qquad (137)
\end{aligned}
$$

A systematic study of the differential operators for the l loop sunset integral will appear in [55].

4 Analytic Evaluations for Sunset Integral

In this section we give different analytic expressions for the two-loop sunset integral. In one form the two-loop sunset integral is given by an elliptic dilogarithm as review in Sect. 4.1 or as a ordinary trilogarithm as review in Sect. 4.1. In Sect. 4.3 we explain that the equivalence between the two expressions is a manifestation of the mirror symmetry proven in [20].

4.1 The Sunset Integral as an Elliptic Dilogarithm

The geometry of the graph hypersurface is a family of elliptic curves

$$\mathcal{E}_{\ominus} := \{p^2 x_1 x_2 x_3 - (\xi_1^2 x_1 + \xi_2^2 x_2 + \xi_3^2 x_3)(x_1 x_2 + x_1 x_3 + x_2 x_3) | (x_1, x_2, x_3) \in \mathbb{P}^2\}\,. \tag{138}$$

One can use the information from the geometry of the graph polynomial and use a parameterisation of the physical variables making the geometry of the elliptic curve explicit.

The elliptic curve $\mathcal{E}_{\ominus}$ can be represented as $\mathbb{C}^\times/q^{\mathbb{Z}}$ where $q = \exp(2i\pi\tau)$ and τ is the period ratio of the elliptic curve. There a six special points on the elliptic curve $\mathcal{E}_{\ominus}$ the three points that intersect the domain of integration

$$P_1 := [0, 0, 1], \qquad P_2 := [0, 0, 1], \qquad P_3 := [0, 0, 1], \tag{139}$$

and three other points outside the domain of integration

$$Q_1 := [0, -\xi_3^2, \xi_2^2], \qquad Q_2 := [-\xi_3^2, 0, \xi_1^2], \qquad Q_3 := [-\xi_1^2, \xi_2^2, 0]. \tag{140}$$

If one denotes by $x(P_i)$ the image of the point P_i in $\mathbb{C}^\times/q^{\mathbb{Z}}$ and $x(Q_i)$ the image of the point Q_i we have $x(P_i) = -x(Q_i)$ with $i = 1, 2, 3$

$$\left(\frac{\theta_1(x(P_i)/x(P_j))}{\theta_c(x(P_i)/x(P_j))}\right)^2 = \frac{\xi_k}{\sqrt{t}\xi_i\xi_j}\,, \tag{141}$$

with (i, j, k) a permutation of $(1, 2, 3)$ and c a permutation of $(2, 3, 4)$.[5] It was shown in [20] that the sunset Feynman integral is given by

---

[5]The Jacobi theta functions are defined by $\theta_2(q) := 2q^{\frac{1}{8}} \prod_{n\geq 1}(1-q^n)(1+q^n)^2$, $\theta_3(q) := \prod_{n\geq 1}(1-q^n)(1+q^{n-\frac{1}{2}})^2$ and $\theta_4(q) := \prod_{n\geq 1}(1-q^n)(1-q^{n-\frac{1}{2}})^2$.

$$I_{\ominus}(p^2,\underline{\xi}^2) \equiv \frac{i\varpi_r}{\pi}\left(\hat{E}_2\left(\frac{x(P_1)}{x(P_2)}\right)+\hat{E}_2\left(\frac{x(P_2)}{x(P_3)}\right)+\hat{E}_2\left(\frac{x(P_3)}{x(P_1)}\right)\right) \quad \text{mod periods}, \tag{142}$$

where $\hat{E}_2(x)$ is the elliptic dilogarithm

$$\hat{E}_2(x) = \sum_{n\geq 0}\left(\mathrm{Li}_2\left(q^n x\right) - \mathrm{Li}_2\left(-q^n x\right)\right) - \sum_{n\geq 1}\left(\mathrm{Li}_2\left(q^n/x\right) - \mathrm{Li}_2\left(-q^n/x\right)\right). \tag{143}$$

The J-invariant of the sunset elliptic curve is

$$J_{\ominus} = 256\frac{(3-u_{\ominus}^2)^3}{4-u_{\ominus}^2}, \tag{144}$$

where the Hauptmodul is

$$u_{\ominus} = \frac{(p^2-\xi_1^2-\xi_2^2-\xi_3^2)^2-4(\xi_1^2\xi_2^2+\xi_1^2\xi_3^2+\xi_2^2\xi_3^2)}{\sqrt{16t\xi_1^2\xi_2^2\xi_3^2}}, \tag{145}$$

given in term of Jacobi theta functions

$$u_{\ominus}^{3,4} = \frac{\theta_3^4+\theta_4^4}{\theta_3^2\theta_4^2}, \quad u_{\ominus}^{2,3} = -\frac{\theta_3^4+\theta_2^4}{\theta_3^2\theta_2^2}, \quad u_{\ominus}^{2,4} = i\frac{\theta_2^4-\theta_4^4}{\theta_2^2\theta_4^2}, \tag{146}$$

and the period is given for each pair $(a,b) = (3,4), (2,3), (2,4)$ by

$$\varpi_r = \frac{t^{\frac{1}{4}}\pi\theta_a\theta_b}{(\xi_1^2\xi_2^2\xi_3^2)^{\frac{1}{4}}}, \tag{147}$$

is the elliptic curve period which is real on the line $t < (\xi_1+\xi_2+\xi_3)^2$.

By using the dilogarithm functional equations one can bring the expression (142) in a form similar to the one used in [62]

$$\sum_{i=1}^{3}\sum_{n\in\mathbb{Z}}\mathrm{Li}_2(q^n x_i). \tag{148}$$

This representation needs to be properly regularised as discussed in [62] whereas the representation in (143) is a converging sum. An equivalent representation used multiple elliptic polylogarithms [14–19] this representation has the advantage of generalising to other graphs [63–68].

For the all equal masses case, $1=\xi_1=\xi_2=\xi_3$, the family of elliptic curves

$$\mathscr{E}_{\ominus} := \{p^2x_1x_2x_3-(x_1+x_2+x_3)(x_1x_2+x_1x_3+x_2x_3)=0|(x_1,x_2,x_3)\in\mathbb{P}^2\}, \tag{149}$$

defines a pencil of elliptic curves in $\mathbb{P}^2$ corresponding to a modular family of elliptic curves $f : \mathcal{E}_\ominus \to X_1(6) = \{\tau \in \mathbb{C}|\Im\mathrm{m}(\tau) > 0\}/\Gamma_1(6)$ (see [60]). When all the masses are equal the map is easier since the elliptic curve is a modular curve for $\Gamma_1(6)$ and the coordinates of the points are mapped to sixth root of unity $x(P_r) = e^{\frac{2i\pi r}{6}}$ and $x(Q_r) = -e^{\frac{2i\pi r}{6}}$ with $r = 1, 2, 3$.

The integral is expressed as the following combination of elliptic dilogarithms

$$I_\ominus(p^2, 1, 1, 1) = \varpi_r(t)(i\pi - \log q) - 6\frac{\varpi_r(p^2)}{\pi} E_\ominus(q)\,, \tag{150}$$

where the Hauptmodul

$$p^2 = 9 + 72\frac{\eta(q^2)}{\eta(q^3)}\left(\frac{\eta(q^6)}{\eta(q)}\right)^5\,, \tag{151}$$

and the real period for $p^2 < \xi_1^2 + \xi_2^2 + \xi_3^2$

$$\varpi_r(p^2) = \frac{\pi}{\sqrt{3}}\,\frac{\eta(q)^6\eta(q^6)}{\eta(q^2)^3\eta(q^3)^2}\,. \tag{152}$$

In this case the elliptic dilogarithm is given by

$$\begin{aligned} E_\ominus(q) &= -\frac{1}{2i}\sum_{n\geq 0}\left(\mathrm{Li}_2\left(q^n\zeta_6^5\right) + \mathrm{Li}_2\left(q^n\zeta_6^4\right) - \mathrm{Li}_2\left(q^n\zeta_6^2\right) - \mathrm{Li}_2\left(q^n\zeta_6\right)\right)\\ &\quad + \frac{1}{4i}\left(\mathrm{Li}_2\left(\zeta_6^5\right) + \mathrm{Li}_2\left(\zeta_6^4\right) - \mathrm{Li}_2\left(\zeta_6^2\right) - \mathrm{Li}_2\left(\zeta_6\right)\right)\,. \end{aligned} \tag{153}$$

which we can write as a q-expansion

$$E_\ominus(q) = \frac{1}{2}\sum_{k\in\mathbb{Z}\backslash\{0\}}\frac{(-1)^{k-1}}{k^2}\,\frac{\sin(\frac{n\pi}{3}) + \sin(\frac{2n\pi}{3})}{1 - q^k}\,. \tag{154}$$

4.2 The Sunset Integral as a Trilogarithm

In this section we evaluate the sunset two-loop integral in a different way, leading to an expression in terms of trilogarithms. We leave the interpretation of the two equivalence with the previous evaluation to Sect. 4.3 where we explain that these results are a manifestation of local mirror symmetry.

We introduce the quantity the logarithmic Mahler measure $R_0(p^2, \underline{\xi}^2)$

$$R_0(p^2, \underline{xi}^2) = -i\pi + \int_{|x|=|y|=1} \log(p^2 - (\xi_1^2 x + \xi_2^2 y + \xi_3^2)(x^{-1} + y^{-1} + 1)) \frac{d \log x d \log y}{(2\pi i)^2}, \tag{155}$$

which evaluates to

$$R_0 = \log(-p^2) - \sum_{n\geq 1} \frac{(p^2)^{-n}}{n} A_{\ominus}(2, n, \xi_1^2, \xi_2^2, \xi_3^2), \tag{156}$$

where $A_{\ominus}(2, n, \xi_1^2, \xi_2^2, \xi_3^2)$ is defined in (124). Differentiating with respect to p^2 leads to maximal cut

$$\frac{d}{dp^2} R_0(p^2, \xi_1^2, \xi_2^2, \xi_3^2) = \pi_{\ominus}^{(2)}(p^2, \xi_1^2, \xi_2^2, \xi_3^2), \tag{157}$$

where $\pi_{\ominus}^{(2)}(p^2, \xi_1^2, \xi_2^2, \xi_3^2)$ is defined in (123). It was shown in [20] that the sunset integral has the expansion

$$I_{\ominus}(p^2, \underline{\xi}^2) = -2i\pi\, \pi_{\ominus}^{(2)}(t, \underline{\xi}^2) \left(3R_0^3 + \sum_{\substack{\ell_1+\ell_2+\ell_3=\ell>0 \\ (\ell_1,\ell_2,\ell_3)\in\mathbb{N}^3\backslash(0,0,0)}} \ell(1-\ell R_0) N_{\ell_1,\ell_2,\ell_3} \prod_{i=1}^{3} \xi_i^{2\ell_i} e^{\ell_i R_0} \right), \tag{158}$$

where the invariant numbers N_{ℓ_1,ℓ_2,ℓ_3} can be computed from the Yukawa coupling (118) using [20, proposition 7.6]

$$6 - \sum_{\substack{\ell_1+\ell_2+\ell_3=\ell>0 \\ (\ell_1,\ell_2,\ell_3)\in\mathbb{N}^3\backslash(0,0,0)}} \ell^3 N_{\ell_1,\ell_2,\ell_3} R_0^\ell \prod_{i=1}^{3} \xi_i^{2\ell_i} = \frac{(6(p^2)^2 - 4p^2(\xi_1^2+\xi_2^2+\xi_3^2) + 2\mu_1\cdots\mu_4)}{p^2 \prod_{i=1}^4 (p^2-\mu_i^2)\, (\pi_{\ominus}^{(2)}(p^2, \underline{\xi}^2))^3}. \tag{159}$$

These quantities can be expressed in terms of the virtual integer numbers of rational curves of degree $\ell = \ell_1 + \ell_2 + \ell_3$ by the covering formula

$$N_{\ell_1,\ell_2,\ell_3} = \sum_{d|\ell_1,\ell_2,\ell_3} \frac{1}{d^3} n_{\frac{\ell_1}{d},\frac{\ell_2}{d},\frac{\ell_3}{d}}. \tag{160}$$

A first few Gromov-Witten numbers are given by (these invariants are symmetric in their indices so list only one representative)

(ℓ_1,ℓ_2,ℓ_3)	(100)	$\overset{k>0}{(k00)}$	(110)	(210)	(111)	(310)	(220)	(211)	(221)
N_{ℓ_1,ℓ_2,ℓ_3}	2	$2/k^3$	-2	0	6	0	$-1/4$	-4	10
n_{ℓ_1,ℓ_2,ℓ_3}	2	0	-2	0	6	0	0	-4	10

(161)

(ℓ_1, ℓ_2, ℓ_3)	(410)	(320)	(311)	(510)	(420)	(411)	(330)	(321)	(222)
N_{ℓ_1,ℓ_2,ℓ_3}	0	0	0	0	0	0	$-2/27$	-1	$-189/4$
n_{ℓ_1,ℓ_2,ℓ_3}	0	0	0	0	0	0	0	-1	-48

(162)

Introducing the variables $Q_i = \xi_i^2 e^{R_0}$ we can rewrite the sunset integral as

$$
\begin{aligned}
-\frac{I_\ominus(p^2, \underline{\xi}^2)}{2i\pi\pi_\ominus^{(2)}(p^2, \underline{\xi}^2)} &= 3R_0^3 + \sum_{\substack{\ell_1+\ell_2+\ell_3=\ell>0\\(\ell_1,\ell_2,\ell_3)\in\mathbb{N}^3\setminus(0,0,0)}} \ell(1-\ell R_0)N_{\ell_1,\ell_2,\ell_3}\prod_{i=1}^3 \xi_i^{2\ell_i}e^{\ell_i R_0}\\
&= 3R_0^3 + \sum_{(n_1,n_2,n_3)\geq(0,0,0)} (d_{n_1,n_2,n_3} + \delta_{n_1,n_2,n_3}\log(-p^2))\,\mathrm{Li}_3(Q_1^{n_1}Q_2^{n_2}Q_3^{n_3}), \quad (163)
\end{aligned}
$$

where $\mathrm{Li}_3 = \sum_{n\geq1} x^n/n^3$ is the trilogarithm and the first coefficients are given by

(ℓ_1, ℓ_2, ℓ_3)	(100)	(110)	(200)	(111)	(210)	(300)	(400)	(220)	(310)	(211)
d_{ℓ_1,ℓ_2,ℓ_3}	2	0	$9/4$	-6	-6	$58/27$	$79/48$	0	$-8/3$	40
$\delta_{\ell_1,\ell_2,\ell_3}$	-2	2	8	-54	0	$-16/27$	$-3/8$	3	0	64

(164)

In Sect. 4.3 we will explain that these numbers are local Gromov-Witten numbers N_{ℓ_1,ℓ_2,ℓ_3} and the sunset Feynman integral is the Legendre transformation of the local prepotential as shown [20].

Using the relation between the complex structure of $2i\pi\tau = \log q$ of the elliptic curve and R_0 (see [20, proposition 7.6] and Sect. 4.3)

$$
\log q = 2\sum_{i=1}^3 \log(Q_i^2) - \sum_{\substack{\ell_1+\ell_2+\ell_3=\ell>0\\(\ell_1,\ell_2,\ell_3)\in\mathbb{N}^3\setminus(0,0,0)}} \ell^2 N_{\ell_1,\ell_2,\ell_3}\prod_{i=1}^3 Q_i^{\ell_i}, \quad (165)
$$

one can check the equivalence between the expressions (142) and (158).

4.2.1 The All Equal Masses Case

In this section we compute the local invariants for the all equal masses case $\xi_1 = \xi_2 = \xi_3 = 1$ the sunset integral reads

$$
I_\ominus(p^2, 1, 1, 1) = \pi_\ominus^{(2)}(p^2, 1, 1, 1)\left(3R_0^3 + \sum_{\substack{\ell_1+\ell_2+\ell_3=\ell>0\\(\ell_1,\ell_2,\ell_3)\in\mathbb{N}^3\setminus(0,0,0)}} \ell(1-\ell\log Q)N_{\ell_1,\ell_2,\ell_3}\, Q_0^\ell\right). \quad (166)
$$

with $Q_0 = \exp(R_0)$ where

$$R_0 = -\log(-p^2) + \sum_{\ell>0} \frac{(p^2)^{-\ell}}{\ell} \sum_{p_1+p_2+p_3=\ell} \left(\frac{\ell!}{p_1!p_2!p_3!}\right)^2 , \tag{167}$$

and using the expression for p^2 in (151) we have that

$$R_0(q) = i\pi + \log q - \sum_{n\geq 1} (-1)^{n-1} \left(\frac{-3}{n}\right) n\, \mathrm{Li}_1\left(q^n\right) , \tag{168}$$

where $\left(\frac{-3}{n}\right) = 0, 1, -1$ for $n \equiv 0, 1, 2 \mod 3$. The maximal cut in (111) reads

$$p^2 \pi_{\ominus}^{(2)}(p^2, 1, 1, 1) = \frac{\eta(q^2)^6 \eta(q^3)}{\eta(q)^3 \eta(q^6)^2} . \tag{169}$$

We recall the p^2 is the hauptmodul in (151). The Gromov-Witten invariant N_ℓ can be computed using [20, proposition 7.6]

$$6 - \sum_{\ell\geq 1} \ell^3 N_\ell Q^\ell = \frac{6}{p^2(p^2-1)(p^2-9)\,(\pi_{\ominus}^{(2)}(q))^3} . \tag{170}$$

Introducing the virtual numbers n_ℓ of degree ℓ

$$N_\ell = \sum_{d|\ell} \frac{1}{d^3} n_{\frac{\ell}{d}} , \tag{171}$$

we have

$$\begin{aligned} n_k/6 = {} & 1, -1, 1, -2, 5, -14, 42, -136, 465, -1655, 6083, -22988, \\ & 88907, -350637, 1406365, -5724384, 23603157, -98440995, \\ & 414771045, -1763651230, 7561361577, -32661478080, \\ & 142046490441, -621629198960, 2736004885450, \\ & -12105740577346, 53824690388016, \ldots \end{aligned} \tag{172}$$

The relation between Q and q

$$Q = -q \prod_{n\geq 1} (1-q^n)^{n\delta(n)}; \qquad \delta(n) := (-1)^{n-1} \left(\frac{-3}{n}\right) , \tag{173}$$

which we will interpret as a mirror map in Sect. 4.3, in the expansion in (166) gives the dilogarithm expression in (150).

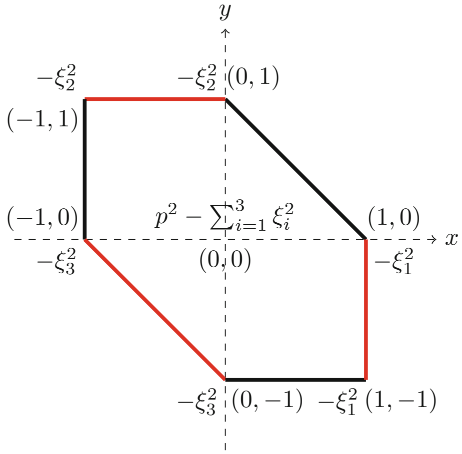


Fig. 1 The Newton polyhedron associated with the sunset second Symanzik polynomial. The coordinates (a, b) of the vertices we the powers of $x^a y^b$ and we give the value of the coefficient in $\phi_\ominus(p^2, \underline{\xi}^2, x, y, 1)$

4.3 *Mirror Symmetry and Sunset Integral*

In this section we review the result of [20] where it was shown that the sunset two-loop integral is the Legendre transform of the local Gromov-Witten prepotential and that the equivalence between the elliptic dilogarithm expression and the trilogarithm expansion of the previous section is a manifestation of local mirror symmetry. The techniques used in this section are standard in the study of mirror symmetry in string theory. We refer to the physicists oriented reviews [46, 47] for some presentation of the mathematical notions used in this section.

4.3.1 The Sunset Graph Polynomial and del Pezzo Surface

To the sunset Laurent polynomial

$$P_\ominus(p^2, \underline{\xi}^2, x_1, x_2, x_3) = p^2 - (x_1\xi_1^2 + x_2\xi_2^2 + x_3\xi_3^2)\left(\frac{1}{x_1} + \frac{1}{x_2} + \frac{1}{x_3}\right), \quad (174)$$

we associate the Newton polyhedron in Fig. 1. The vertices of the polyhedron are the powers of the monomial in x_1 and x_2 with $x_3 = 1$.

This corresponds to a maximal toric blow-up of three points in $\mathbb{P}^2$ leading to a del Pezzo surface of degree 6 $\mathscr{B}_3$.[6] The hexagon in Fig. 1 resulted from the blow-up (in red on the figure) of a triangle at the points $P_1 = [1 : 0 : 0]$, $P_2 = [0 : 1 : 0]$ and

[6] A del Pezzo surface is a two-dimensional Fano variety. A Fano variety is a complete variety whose anti-canonical bundle is ample. The anti-canonical bundle of a non-singular algebraic variety of dimension n is the line bundle defined as the nth exterior power of the inverse of the cotangent bundle. An ample line bundle is a bundle with enough global sections to set up an embedding of its base variety or manifold into projective space.

$P_3 = [0:0:1]$ by the mass parameters see [60, §6] and [20, §4]. The del Pezzo 6 surfaces are rigid.[7]

Notice that the external momentum p^2 appears only in the centre of the Newton polytope making this variable special.

One can construct a non-compact Calabi-Yau three-fold $\mathscr{M}_{\ominus}$ defined as the anti-canonical hypersurface over the del Pezzo surface $\mathscr{B}_3$. This non-compact three-fold is obtained as follows [20, §5]. Consider the Laurent polynomial

$$F_{\ominus} = a + bu^2v^{-1} + cu^{-1}v + u^{-1}v^{-1}\phi_{\ominus}(p^2, \underline{\xi}^2, x_1, x_2, x_3), \qquad (175)$$

with $a, b, c \in \mathbb{C}^*$. Its Newton polytope Δ is the convex hull of $\{(0, 0, 2, -1), (0, 0, -1, 1), \Delta_{\ominus} \times (-1, -1)\}$ where $\Delta_{\ominus}$ is the Newton polytope given by the hexagon in Fig. 1. The newton polytope Δ is reflexive because its polar polytope $\Delta^\circ := \{y \in \mathbb{R}^4 | \langle y, x\rangle \geq -1, \forall x \in \Delta\} = \text{convex hull}\{(0, 0, 1, 0), (0, 0, 0, 1), 6\Delta^\circ_{\ominus} \times (-2, -3)\}$ is integral. Notice that for the sunset polytope is self-dual $\Delta_{\ominus} = \Delta^\circ_{\ominus}$. A triangulation of Δ gives a complete toric fan[8] on Δ°, which then provides Fano variety $\mathbb{P}_\Delta$ of dimension four [70]. For general a, b, c and the generic physical parameters $p^2, \underline{\xi_1^2, \xi_2^2, \xi_3^2}$ in the sunset graph polynomial, the singular compactification $\mathscr{M}_{\ominus} := \overline{\{F = 0\}}$ is a smooth Calabi-Yau three-fold. This non-compact Calabi-Yau three-fold can be seen as a limit of compact Calabi-Yau three-fold following the approach of [23] to local mirror symmetry. One can consider a semi-stably degenerating a family of elliptically-fibered Calabi-Yau three-folds $\mathscr{M}_z$ to a singular compactification $\mathscr{M}_{\ominus}$ for $z = 0$ and to compare the asymptotic Hodge theory[9] of this B-model to that of the mirror (elliptically fibered) A-model Calabi-Yau $\mathscr{M}^\circ_{\ominus}$. Both $\mathscr{M}_{\ominus}$ and $\mathscr{M}^\circ_{\ominus}$ are elliptically fibered over the del Pezzo of degree 6 $\mathscr{B}_3$. Under the mirror map we have the isomorphism of A- and B-model $\mathbb{Z}$-variation of Hodge structure [20]

$$H^3(\mathscr{M}_{z_0}) \cong H^{even}(\mathscr{M}^\circ_{q_0})\,. \qquad (176)$$

This situation is not unique to the two-loop sunset. The sunset graph have a reflexive polytopes containing the origin. The origin of the polytope is associated with the coefficient $p^2 - \sum_{i=1}^n \xi_i^2$, and plays a very special role. The ambient space of the sunset polytope defines a Calabi-Yau hypersurfaces (the anti-canonical divisor defines a Gorenstein toric Fano variety). Therefore they are a natural home for Batyrev's mirror symmetry techniques [21].

[7]The graph polynomial (47) for higher loop sunset graphs defines Fano variety, which is as well a Calabi-Yau manifold.

[8]The fan of a toric variety is defined in the standard reference [69] and the review oriented to a physicists audience in [47].

[9]Feynman integrals are period integrals of mixed Hodge structures [26, 71]. At a singular point some cycles of integration vanish, the so-called vanishing cycles, and the limiting behaviour of the period integral is captured by the asymptotic behaviour of the cohomological Hodge theory. The asymptotic Hodge theory inherit some filtration and weight structure of the original Hodge theory.

4.3.2 Local Mirror Symmetry

Putting this into practise means recasting the computation in Sect. 4.2 and the mirror symmetry description in [20, §7] in the language of [24], matching the computation of the Gromov-Witten prepotential in [24, §6.6].

The first step is to remark that the holomorphic (3, 0) period of Calabi-Yau threefold $\mathscr{M}_\ominus$ reduces to the third period R_0 once integrated on a vanishing cycle [72, Appendix A], [73, §4] and [20, §5.7]

$$\int_{\text{vanishing cycle}} \mathrm{Res}_{F_\ominus=0}\left(\frac{1}{F_\ominus}\frac{du\wedge dv\wedge\wedge dx_1\wedge dx_2}{uvx_1x_2}\right)\propto R_0(p^2,\underline{\xi}^2), \tag{177}$$

where $F_\ominus$ is given in (175) and $R_0(p^2,\underline{\xi}^2)$ is given in (155). This second period is related to the analytic period near $p^2=\infty$ by $\pi_\ominus^{(2)}(p^2,\underline{\xi}^2)=\frac{d}{dp^2}R_0(p^2,\underline{\xi}^2)$.[10]

The Gromov-Witten invariant evaluated in (161) Sect. 4.2 are actually the BPS numbers for the del Pezzo 6 case evaluated in [24, §6.6] since

$$\sum_{\substack{\ell_1+\ell_2+\ell_3=\ell>0\\(\ell_1,\ell_2,\ell_3)\in\mathbb{N}^3\backslash(0,0,0)}} N_{\ell_1,\ell_2,\ell_3}R_0^{\ell}\prod_{i=1}^{3}\xi_i^{2\ell_i}=\sum_{(\tilde\ell_1,\tilde\ell_2,\tilde\ell_3)\in\mathbb{N}^3\backslash(0,0,0)} n_{\tilde\ell_1,\tilde\ell_2,\tilde\ell_3}\mathrm{Li}_3\left(\prod_{i=1}^{3}\xi_i^{2\tilde\ell_i}e^{\tilde\ell_i R_0}\right), \tag{178}$$

where we used the covering relation (160). With the following identifications[11] $Q_1=1$, $Q_2=\xi_1^2e^{R_0}$, $Q_3=\xi_2^2e^{R_0}$ and $Q_4=\xi_3^2e^{R_0}$, the expression in (178) reproduces the local genus 0 prepotential $F_0=F_0^{class}+\sum_{\boldsymbol{\beta}\in H^2(\mathscr{M},\mathbb{Z})}n_g^{\boldsymbol{\beta}}\mathrm{Li}_3(\prod_{r=1}^4 Q_r^{\beta_r})$ computed in [24, eq.(6.51)] with $F_0^{class}=\prod_{i=1}^3(R_0+\log(\xi_i^2))$ in our case.

From the complex structure of the elliptic curve we define the dual period $\pi_1(p^2,\underline{\xi}^2)=2i\pi\tau\pi_\ominus^{(2)}(p^2,\underline{\xi}^2)$ one the other homology cycle. Which gives the dual third period R_1, such that $\pi_1^{(2)}(p^2,\underline{\xi}^2)=\frac{d}{dp^2}R_1(p^2,\underline{\xi}^2)$. This dual period R_1 is therefore identified with the derivative of local prepotential F_0

$$\begin{aligned}2i\pi R_1&=\frac{\partial}{\partial R_0}F_0 \\ &=\sum_{1\le i<j\le 3}(R_0+\log(\xi_i^2))(R_0+\log(\xi_j^2))-\sum_{\substack{\ell_1+\ell_2+\ell_3=\ell>0\\(\ell_1,\ell_2,\ell_3)\in\mathbb{N}^3\backslash\{0,0,0\}}}\ell N_{\ell_1,\ell_2,\ell_3}\prod_{i=1}^{3}\xi_i^{2\ell_i}e^{\ell_i R_0},\end{aligned} \tag{179}$$

[10] It has been already noticed in [74] the special role played by the Mahler measure and mirror symmetry.

[11] We would like to thank Albrecht Klemm for discussions and communication that helped clarifying the link between the work in [20] and the analysis in [24].

as shown in [20, theorem 6.1] and [20, Corollary 6.3]. With these identifications it is not difficult to see that the sunset Feynman integral is actually given by the Legendre transform of R_1

$$I_{\ominus}(p^2, \underline{\xi}^2) = -2i\pi\pi^{(2)}_{\ominus}(p^2, \underline{\xi}^2)\left(\frac{\partial R_1}{\partial R_0}R_0 - R_1\right). \tag{180}$$

This shows the relation between the sunset Feynman integral computes the local Gromov-Witten prepotential. The local mirror symmetry map $Q \leftrightarrow q$ given in the relations (165) and (173) maps the B-model expression, where the sunset Feynman integral is a elliptic dilogarithm function of the complex structure $\log(q)/(2i\pi)$ of the elliptic curve and the A-model expansion in terms of the Kähler moduli Q_i.

5 Conclusion

In this text we have reviewed the toric approach to the evaluation of the maximal cut of Feynman integrals and the derivation of the minimal order differential operator acting on the Feynman integral. On the particular example of the sunset integral we have shown that the Feynman integral can take two different but equivalent forms. One form is an elliptic polylogarithm but it can as well expressed as standard trilogarithm. We have explained that mirror symmetry can be used to evaluate around the point where $p^2 = \infty$. The expressions there makes explicit all the mass parameters. One remarkable fact is that the computation can be done using the existing technology of mirror symmetry developed in other physical [22–24] or mathematics [25] contexts. This analysis extends naturally to the higher loop sunset integrals [55]. The elliptic polylogarithm representation generalises to other two-loop integrals like the kite integral [75–77] or the all equal masses three-loop sunset [61]. This representation leads to fast numerical evaluation [76]. But it has the disadvantage of hiding all the physical parameters in the geometry of the elliptic curve. The expression using the trilogarithm has the advantage of making all the mass parameters explicit and generalising to all loop orders since the expansion of the higher-loop sunset graphs around $p^2 = \infty$ is expected to involve polylogarithms of order l at l-loop order [25, 55].

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Modular and Holomorphic Graph Functions from Superstring Amplitudes

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Abstract We compare two classes of functions arising from genus-one superstring amplitudes: modular and holomorphic graph functions. We focus on their analytic properties, we recall the known asymptotic behaviour of modular graph functions and we refine the formula for the asymptotic behaviour of holomorphic graph functions. Moreover, we give new evidence of a conjecture appeared in [4] which relates these two asymptotic expansions.

1 Introduction

The computation of the perturbative expansion of superstring scattering amplitudes constitutes an extremely fertile field of interaction between mathematicians and theoretical physicists. From a mathematician's viewpoint, this is partly due to the appealing and simple form of the Feynman-like integrals appearing in this expansion, but most remarkably to the fact that the mathematics unveiled is right at the boundary of our present knowledge: it constitutes both an astonishing concrete example of certain new abstract constructions from algebraic geometry, and at the same time it points towards new frontiers to be investigated. In this paper, besides presenting a detailed review of the state of art of number theoretical aspects of superstring amplitudes, we will recall and refine recent results and conjectures presented in [4, 43]. We hope that this will be useful to understand the connection between genus-one superstring

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amplitudes and a new class of functions introduced by Brown in the context of his research on mixed modular motives [14].

It was observed in [4] that the real-analytic single-valued functions arising from genus-one closed-string amplitudes, called modular graph functions, seem to be related in a simple and intriguing way to a seemingly artificial combination of the holomorphic multi-valued functions arising from genus-one open-string amplitudes. This would extend the observation already made at genus zero that closed-string amplitudes seem to be a single-valued version of open-string amplitudes. After introducing some mathematical background and recalling the genus-zero case, we will define modular and holomorphic graph functions, originating from genus-one closed and open-string amplitudes, respectively. Holomorphic graph functions are divided into A-cycle and B-cycle graph functions. The main theorems are the following:

Theorem 1 *The modular graph function associated to a graph Γ with l edges has the asymptotic expansion*

$$D_\Gamma(\tau) = \sum_{k=1-l}^{l} \sum_{m,n\geq 0} d_k^{(m,n)}(\Gamma)\, y^k q^m \overline{q}^n,$$

where $\tau \in \mathbb{H}$, $q = \exp(2\pi i \tau)$, $y = \pi\, Im(\tau)$ and the coefficients $d_k^{(m,n)}(\Gamma)$ are cyclotomic multiple zeta values.

Theorem 2 *The B-cycle graph function associated to a graph Γ with l edges has the asymptotic expansion*

$$B_\Gamma(\tau) = \sum_{k=-l}^{l} \sum_{m\geq 0} b_k^{(m)}(\Gamma)\, T^k q^m,$$

where $T = \pi i \tau$ and the coefficients $b_k^{(m)}(\Gamma)$ are multiple zeta values.

Theorem 1 is a generalization of the main result of [42] and is already contained in the PhD thesis [43], while Theorem 2 builds on previous results contained in [4, 43] but is ultimately new: its novelty consists in the explicit bound on the powers of T in terms of the number of edges l of the graph, which is obtained by exploiting an explicit formula for the open-string propagator.

In [42] it is conjectured that all $d_k^{(m,n)}(\Gamma)$ belong to a small subset of multiple zeta values called single-valued multiple zeta values. One of the main achievements of [4] is to give great evidence of a (partly) stronger statement, which relates open-string amplitudes to closed-string amplitudes:

Conjecture 1 *Let $sv : \zeta(\boldsymbol{k}) \to \zeta_{\mathrm{sv}}(\boldsymbol{k})$. Then for any graph Γ with l edges and all $-l < k < l$ we have*[1]

[1]The reason for the rational coefficient appearing in Eq. (1) is that we want to follow the notation adopted in the modular graph function literature. Setting $y = -2\pi\, Im(\tau)$, which mathematically would be a more natural choice, one would get a cleaner statement.

$$sv(b_k^{(0)}(\Gamma)) = (-2)^{-k} d_k^{(0,0)(\Gamma)}. \tag{1}$$

We call this the (Laurent-polynomial) *esv conjecture*, where the "*e*" stands for elliptic. This is not the only relationship observed in [4] between holomorphic and modular graph functions; in particular, it seems that for graphs with up to six edges one can obtain modular graph function from holomorphic graph functions by applying a very simple set of "*esv* rules". However, we prefer to be cautious and content ourselves to consider here and call conjecture only the Laurent-polynomial version.

In the last section of the paper we will recall the construction due to Brown of a single-valued analogue of certain holomorphic functions on the upper half plane $\mathbb{H}$ (iterated Eichler integrals of modular forms). We will argue that this construction should be related to our *esv* conjecture, and mention various open questions and possible directions originating from this observation.

2 Feynman Periods

One of the origins of the interaction between physicists working on scattering amplitudes and mathematicians is the fact that Feynman integrals of quantum field theories are *period functions* of the kinematic variables (e.g. masses, momenta).

Periods can be defined elementarily as absolutely convergent integrals of algebraic functions over domains given by polynomial inequalities with integer coefficients [31]. When the integrands depend algebraically on parameters, we call the integrals period functions, and for algebraic values of the parameters we get actual periods. Concretely, periods constitute a countable subring $\mathscr{P}$ of $\mathbb{C}$, which contains $\overline{\mathbb{Q}}$ as well as many (often conjecturally) transcendental numbers of geometric or number theoretical interest, such as $\pi = \iint_{x^2+y^2\leq 1} dxdy$ or special values of various kinds of L-functions. It is important to remark that the representation of a period as an integral is far from being unique: for instance, one also has $\pi = \int_{-1\leq x\leq 1}(1-x^2)^{-1/2}dx$. As a consequence of this, it is often very difficult to "recognize" a period, i.e. to notice that a complicated integral can be written in terms of known periods.

The great mathematical relevance of this class of numbers comes from the fact that they can be dubbed, in a precise sense, as the *numbers which come from "geometry"*. Indeed, they can always be obtained from the comparison[2] between algebraic de Rham cohomology (related to algebraic differential forms) of an algebraic variety X and Betti cohomology (related to topological cycles) of the complex points $X(\mathbb{C})$. One of the most important consequences of this fact is that period functions, and therefore Feynman integrals, satisfy special differential equations, called *Picard-Fuchs equations*. Moreover, periods are strictly related to one of Grothendieck's deepest contributions to mathematics: the concept of *motives*. Motives can be thought of as abstract linear algebra structures which encode the same kind of information as (all possible) cohomology theories of an algebraic variety, and which can conjecturally

[2] After tensoring with $\mathbb{C}$, more generally considering "relative cohomologies".

always be obtained as pieces of cohomologies of an actual (non-unique) algebraic variety. Therefore motives come equipped with a "de Rham" and a "Betti" vector space, isomorphic as $\mathbb{C}$-vector spaces, and from this one can define abstract analogues of periods, called *motivic periods*, whose study has surprisingly deep consequences in the computation of Feynman integrals (motivic coaction, motivic f-alphabets..).

Originally, notably after the work of Broadhurst and Kreimer in the 1990s [3], computations of Feynman integrals in the simplest (massless) cases seemed to assign a very special role to certain periods, first considered by Euler and then systematically studied by Zagier [38], called *multiple zeta values* (MZVs). They are defined as the absolutely convergent nested sums

$$\zeta(k_1,\ldots,k_r) = \sum_{0<v_1<\cdots<v_r} \frac{1}{v_1^{k_1}\cdots v_r^{k_r}}, \tag{2}$$

where $\mathbf{k} := (k_1,\ldots,k_r) \in \mathbb{N}^r$ and $k_r \geq 2$. The rational vector space which they span will be denoted by $\mathscr{Z}$. One can easily demonstrate that this vector space is closed under the operation of taking products; in other words, $\mathscr{Z}$ is a $\mathbb{Q}$-algebra, which is conjecturally graded by the *weight* $k_1+\cdots+k_r$. If we call r the *depth* of $\zeta(k_1,\ldots,k_r)$, we can immediately see that depth-one MZVs are nothing but special values of the Riemann zeta function

$$\zeta(s) = \sum_{v\geq 1} \frac{1}{v^s},$$

which are easily shown to be periods, because for each $k \geq 2$, using geometric series,

$$\zeta(k) = \int_{[0,1]^k} \frac{dx_1\cdots dx_k}{1-x_1\cdots x_k}.$$

In fact, similar integral representations allow us to write all MZVs as periods. Physicists very quickly realized the convenience of trying to write down Feynman periods as MZVs, because of a nice explicit (conjectural) description of all relations in $\mathscr{Z}$, and especially because of the astonishing precision to which MZVs can be numerically approximated (thousands of digits within few seconds). The ubiquity of these numbers led to ask deep questions about their nature. Mathematicians realized that they are (geometric) periods of compactified moduli spaces of genus-zero Riemann surfaces with marked points $\overline{\mathfrak{M}}_{0,n}$ and that they can be seen as (real analogues of) motivic periods of a certain class of motives (mixed Tate motives over $\mathbb{Z}$, or $MT(\mathbb{Z})$), which are in some sense the simplest class of motives beyond those described by Grothendieck (called pure motives) [17, 28]. A very good reason for the ubiquity of MZVs was given by Brown, who proved first that all periods of $\overline{\mathfrak{M}}_{0,n}$ belong to $\mathscr{Z}[2\pi i]$ and then that all periods of $MT(\mathbb{Z})$ belong to $\mathscr{Z}[1/2\pi i]$ [9, 10]. Both viewpoints inspired the development of powerful techniques, which can now be used to compute in a surprisingly short time vast classes of Feynman integrals. On the other side, these numbers are not sufficient to describe all interactions of particles, not even in the simplest models (scalar massless φ^4) [2, 11].

Studying Feynman integrals beyond MZVs, studying periods of moduli spaces of Riemann surfaces beyond genus zero and studying motives beyond the mixed Tate case turned out to be different facets of the same problem. The study of superstring amplitudes seems to combine all these themes in a beautiful way.

3 Superstring Amplitudes

Scattering amplitudes in perturbative superstring theory can be approximated by a Feynman-like infinite sum of integrals over compactified moduli spaces of Riemann surfaces[3] with marked points. Each marked point represents a string state, and strings can be roughly divided between *open strings* and *closed strings*: this distinction translates into that between Riemann surfaces with and without boundaries, respectively, as shown in the figure below (Figs. 1 and 2).

To each pair (g, n) given by fixing the genus g and the number of punctures n, one would like to associate a quantity $\mathbf{A}^{\bullet}_{g,n}(\mathbf{s})$: the genus–$g$ amplitude of n open or closed strings ($\bullet$ stands for *op* or *cl*, respectively), i.e. a function of the *Mandelstam variables* $\mathbf{s} = (s_1, s_2, \ldots)$, which are complex numbers encoding the *fundamental string tension* α' and the momenta of the strings. It is important to mention that it is not clear how to define $\mathbf{A}^{\bullet}_{g,n}(\mathbf{s})$ for $g \geq 3$ [26]. This paper is mainly concerned with the study of the mathematics associated with $(g, n) = (1, 4)$. In order to speak of genus one it is useful to recall what is known about the mathematical structure of genus-zero amplitudes, which will be done in the next subsection. We would also

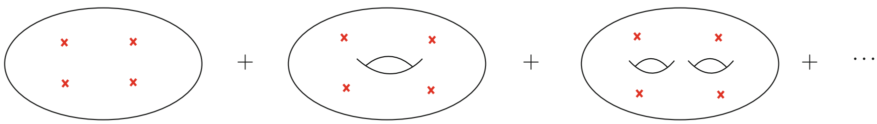


Fig. 1 Four closed strings: Riemann surfaces without boundaries

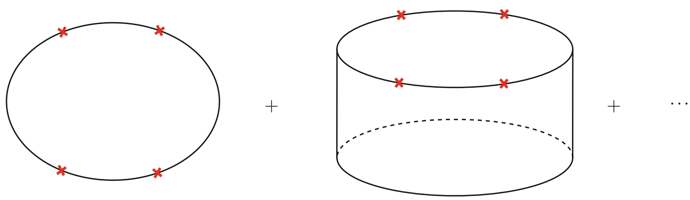


Fig. 2 Four open strings: Riemann surfaces with boundaries, punctures lie on boundaries

[3] More precisely, it should be super-Riemann surfaces, but this does not matter here.

like to mention that very encouraging progress has recently been made in genus two [18–20].

3.1 Genus Zero

Multiple zeta values (see Eq. (2)) can be thought of as special values at $z = 1$ of (one-variable) *multiple polylogarithms*, defined for $|z| < 1$ and $\mathbf{k} \in \mathbb{N}^r$ by

$$\mathrm{Li}_{\mathbf{k}}(z) = \sum_{0<v_1<\cdots<v_r} \frac{z^{k_r}}{v_1^{k_1}\cdots v_r^{k_r}}.$$

These functions can be analytically extended to holomorphic functions on the punctured Riemann sphere $\mathbb{P}^1_{\mathbb{C}} \setminus \{0, 1, \infty\}$ by writing them as iterated integrals on paths from 0 to z, but the analytic continuation depends on the homotopy class of the path. We say that they define *multi-valued functions* on $\mathbb{P}^1_{\mathbb{C}} \setminus \{0, 1, \infty\}$. Using their iterated-integral representation there is a natural way to make sense of their special values at $z = 1$, which gives back our definition of MZVs whenever $k_r \geq 2$. Note that for instance $\mathrm{Li}_1(z) = -\log(1 - z)$ for $|z| < 1$, which obviously extends to a multi-valued holomorphic function on the punctured Riemann sphere. There is a standard way to kill its monodromy and end up with a honest single-valued function: add its complex conjugate $-\log(1 - \overline{z})$ and therefore get $-2Re(\log(1 - z)) = -\log|1 - z|^2$. The price to pay is that we are giving up holomorphicity: we are left with a real analytic function on $\mathbb{P}^1_{\mathbb{C}} \setminus \{0, 1, \infty\}$ (which extends continuously to $\mathbb{C}$). There is a natural generalization of this construction to all multiple polylogarithms $\mathrm{Li}_{\mathbf{k}}(z)$ [12]. We denote the single-valued analogues by $\mathscr{L}_{\mathbf{k}}(z)$, we call them *single-valued multiple polylogarithms* and we call *single-valued multiple zeta values* their (regularized) special values at $z = 1$:

$$\zeta_{\mathrm{sv}}(k_1, \ldots, k_r) := \mathscr{L}_{k_1,\ldots,k_r}(1).$$

It turns out that these special values are contained in $\mathscr{Z}$ [13], and actually form a much smaller sub-algebra, which we denote by $\mathscr{Z}^{\mathrm{sv}}$. For instance, one can prove that $\zeta_{\mathrm{sv}}(2k) = 0$ and $\zeta_{\mathrm{sv}}(2k + 1) = 2\zeta(2k + 1)$ for all $k \geq 1$.

As we have mentioned, string scattering amplitudes should be given by certain integrals over moduli spaces of Riemann surfaces. In practice, it is convenient to think of these integrals as divided into a first integration over all the possible positions of the marked points (string insertions) on a fixed (genus–g) Riemann surface, and then a second integral over all possible (complex structures of) genus–g Riemann surfaces. In genus zero, there is only one possible Riemann surface: the Riemann sphere $\mathbb{P}^1_{\mathbb{C}}$ in the closed-string case and the unit disc in the open-string case, which requires boundaries. The integral needs to be invariant under the $\mathrm{SL}_2(\mathbb{C})$-action ($\mathrm{SL}_2(\mathbb{R})$ for open strings), so we can fix three points and finally think of our genus-zero n-point amplitudes as integrals over possible configurations of $n-3$ points on $\mathbb{P}^1_{\mathbb{C}} \setminus \{0, 1, \infty\}$ in the closed-string case, or as (all possible) integrals of $n-3$ ordered points in the interval [0, 1] in the open-string case.

For what concerns the integrand, we will be even more sketchy. The general idea is that it depends on the Mandelstam variables and on two-variable functions, called *propagators*, that are applied to pairs of marked points on the surface. Propagators are defined in terms of suitable *Green functions*. The closed-string genus-zero propagator is $G_0^{cl}(z_1, z_2) = \log|z_1 - z_2|^2$, while the open-string analogue is given by $G_0^{op}(x_1, x_2) = \log(x_1 - x_2)$ for $0 \leq x_2 < x_1 \leq 1$.

For instance, simplifying a bit, the genus-zero four-point open-string scattering amplitude (or Veneziano amplitude) is given by

$$\int_0^1 \exp((s_1 - 1)\log x + (s_2 - 1)\log(1 - x))\, dx \tag{3}$$

and the closed-string analogue (Virasoro amplitude) is given by

$$-\frac{1}{2\pi i}\int_{\mathbb{P}^1_{\mathbb{C}}} \exp((s_1 - 1)\log|z|^2 + (s_2 - 1)\log|z - 1|^2)\, dz d\overline{z} \tag{4}$$

People are interested in the asymptotic expansion of scattering amplitudes as the Mandelstam variables approach the origin. For instance, one finds that Eqs. (3) and (4) can be written, respectively, as

$$\frac{s_1 + s_2}{s_1 s_2}\, \exp\left(\sum_{n\geq 2} \frac{(-1)^n \zeta(n)}{n}\left(s_1^n + s_2^n - (s_1 + s_2)^n\right)\right), \tag{5}$$

$$\frac{s_1 + s_2}{s_1 s_2}\exp\left(-2\sum_{n\geq 1}\frac{\zeta(2n+1)}{(2n+1)}(s_1^{2n+1} + s_2^{2n+1} - (s_1 + s_2)^{2n+1})\right). \tag{6}$$

These are actually the only cases where we are able to write down a closed formula for the asymptotic expansion in the Mandelstam variables. A simple crucial observation is the following: if we define a *single-valued map*

$$sv : \zeta(\mathbf{k}) \to \zeta_{\mathrm{sv}}(\mathbf{k}),$$

and we extend it to the amplitude by leaving Mandelstam variables and rational numbers untouched, we conclude that the single-valued image of the open-string amplitude (5) is precisely the closed-string amplitude (6). It is known (as a corollary of the work of Brown on the periods of $\mathfrak{M}_{0,n}$ [9]) that, for any number n of string insertions, the coefficients appearing in the asymptotic expansion of genus-zero open-string amplitudes are MZVs [8]. Moreover, extending the trivial four-point observation made above by some "motivic reasoning" and many computer experiments, Schlotterer and Stieberger conjectured that the coefficients of the asymptotic expansion of genus-zero closed-string amplitudes should be given for any number of punctures by single-valued MZVs, and the closed-string amplitude should be (in a precise sense) the single-valued image of the open-string amplitude [36, 37].

3.2 Genus One

In genus one the structure of the moduli spaces gets more complicated, in particular in the open-string case, where we must take into account both oriented and non-oriented Riemann surfaces (cylinders and Möbius strips). In the closed-string case, after fixing one marked point in order to insure translation invariance of the integrals, we are left with a first integration over $n-1$ marked points on a fixed complex torus[4] $\mathscr{E}_\tau = \mathbb{C}/(\tau\mathbb{Z}+\mathbb{Z})$, where $\tau \in \mathbb{H}$, and then a second integration over the (compactification of the) moduli space $\mathfrak{M}_{1,1} = \mathrm{SL}_2(\mathbb{Z}) \setminus \mathbb{H}$ of complex tori. This second integration is not trivial anymore, but in this paper we will only focus on the first integration, whose result will therefore depend on a parameter $\tau \in \mathbb{H}$. For what concerns the open-string case, not only we will focus on the first integral over the position of the insertions, but we furthermore restrict our analysis to the cylinder case with all insertions on one of the two boundary components. The complex structure of the cylinder will depend on a parameter $\tau \in i\mathbb{R}$ (one should think of a cylinder as "half a torus" whose complex parameter τ is purely imaginary). We refer to [5] for more details about the general case.

Once again, the integrands of these amplitudes are written in terms of Mandelstam variables and propagators, i.e. Green functions depending on two marked points on the surface. In the closed-string case the propagator is given by [29]

$$G_1^{cl}(z_1, z_2; \tau) = -\log\left|\frac{\theta(z_1-z_2,\tau)}{\eta(\tau)}\right|^2 + \frac{2\pi(Im(z_1)-Im(z_2))^2}{Im(\tau)}, \qquad (7)$$

where the odd Jacobi θ-function and the Dedekind η-function are defined for $z \in \mathbb{C}$, $\tau \in \mathbb{H}$, $q = \exp(2\pi i\tau)$ and $u = \exp(2\pi i z)$ by

$$\theta(z,\tau) = q^{1/8}(u^{1/2}-u^{-1/2})\prod_{j\geq 1}(1-q^j)(1-q^ju)(1-q^ju^{-1}), \qquad (8)$$

$$\eta(\tau) = q^{1/24}\prod_{j\geq 1}(1-q^j).$$

In the open-string case the propagator is usually defined as a "regularized integral": one can prove that for small ε and $z \in (0,1)$ there exists $K \in \mathbb{Z}_{\geq 0}$ such that

[4] It is well known that any punctured genus-one Riemann surface can be realized as a complex torus.

$$\int_{\varepsilon}^{z} \frac{\theta'(w,\tau)}{\theta(w,\tau)} dw = \sum_{k=0}^{K} g_k(z,\tau) \log^k(2\pi i \varepsilon) + O(\varepsilon). \tag{9}$$

Then one defines[5] the open-string genus-one propagator as [6]

$$G_1^{op}(z_1, z_2; \tau) = -g_0(z_1 - z_2, \tau). \tag{10}$$

The reason in [6] for giving such a non-explicit formula for the open-string propagator is that Eq. (10) is the most convenient form to show that the open-string amplitude can be expressed in terms of *elliptic multiple zeta values* (as defined by Enriquez [27]). It is however useful for our purposes to work out the regularized integral (9), which gives the explicit formula

$$G_1^{op}(z_1, z_2; \tau) = -\log\left(\frac{\theta(z_1 - z_2, \tau)}{\eta^3(\tau)}\right). \tag{11}$$

We will now define the genus-one Feynman-like integrals coming from string amplitudes which inspired the theory of modular and holomorphic graph functions.

The integral over the positions of the marked points on a fixed complex torus contributing to the four-point genus-one closed-string amplitude is given by [29]

$$\begin{aligned}\int_{(\mathscr{E}_\tau)^3} \exp\big(& s_1(G_1^{cl}(z_1, 0; \tau) + G_1^{cl}(z_2, z_3; \tau)) + s_2(G_1^{cl}(z_2, 0; \tau) + G_1^{cl}(z_1, z_3; \tau)) \\ &+ s_3(G_1^{cl}(z_3, 0; \tau) + G_1^{cl}(z_1, z_2; \tau))\big)\, d^2z_1 d^2z_2 d^2z_3,\end{aligned} \tag{12}$$

where we define $d^2z := dz d\overline{z}/Im(\tau)$ and the Mandelstam variables must satisfy the relation $s_1 + s_2 + s_3 = 0$.

On the other side, the integrals over the positions of the ordered marked points on one boundary of the cylinder topology, which contribute to the four-point genus-one open-string amplitude, are given by integrals like [6]

$$\begin{aligned}\int_{0 \le z_1 \le z_2 \le z_3 \le 1} \exp\big(& s_1(G_1^{op}(z_1, 0; \tau) + G_1^{op}(z_2, z_3; \tau)) + s_2(G_1^{op}(z_2, 0; \tau) \\ &+ G_1^{op}(z_1, z_3; \tau)) + s_3(G_1^{op}(z_3, 0; \tau) + G_1^{op}(z_1, z_2; \tau))\big)\, dz_1 dz_2 dz_3,\end{aligned} \tag{13}$$

where again we impose $s_1 + s_2 + s_3 = 0$. Different orderings of the z_i's give rise to different contributions.

The theory of modular and holomorphic graph functions was born out of the study of the expansion of the integrals (12) and (13), respectively, when the Mandelstam variables $s_i \to 0$.

[5]Note that we have changed the sign of the propagator w.r.t. [6], following [4].

4 Modular Graph Functions

Let us consider a connected undirected graph Γ with no self-edges, possibly with multiple edges connecting the same pair of vertices. If we choose a labelling $z_1, \ldots, z_n$ of the n vertices, then for $i < j$ we have $l_{i,j}$ edges between z_i and z_j, with the total number of edges given by the *weight* of the graph

$$l := \sum_{1 \leq i < j \leq n} l_{i,j}.$$

Definition 1 (*D'Hoker–Green–Gürdoğan–Vanhove 2015*) Let Γ be a graph as above. We define its *modular graph function* as

$$D_\Gamma(\tau) = \int_{(\mathscr{E}_\tau)^{n-1}} \prod_{1 \leq i < j \leq n} G_1^{cl}(z_i, z_j; \tau)^{l_{i,j}} \, d^2 z_1 \cdots d^2 z_{n-1}, \tag{14}$$

where $d^2 z_i = dz_i d\bar{z}_i / Im(z_i)$ and we have fixed $z_n \equiv 0$.

It is obvious that this definition does not depend on the labelling. It will often be convenient to write a modular graph function $D_\Gamma(\tau)$ as $\mathbf{D}[\Gamma]$, dropping the dependence of the function on τ and explicitly drawing the graph Γ, as in the following examples: $\mathbf{D}$[], $\mathbf{D}$[], $\mathbf{D}$[], $\mathbf{D}$[] etc..

The definition of this class of functions originated from the study of the contribution to the genus-one four-point closed-string integral given by Eq. (12) [21, 29, 30]. Indeed, if we expand the exponential in the integrand of (12) as a power series in the Mandelstam variables, the coefficients of this expansion are precisely the modular graph functions associated to graphs with at most four vertices. Modular graph functions associated to a higher number of vertices do not suffice to describe higher-point analogues of (12): one must introduce other functions called modular graph forms [22], but for the purpose of this paper it is enough to focus on modular graph functions. As anticipated in the introduction, recent considerations by Brown, contained in [14, 15], seem to assign to this class of functions an important role in the study of mixed motives. We will come back to this in Sect. 6.

So far we have only partially justified the origin of the name of these functions: it is clear that they are related to graphs, but something must be said about the word *modular*. To begin with, one can show [39] that, if we denote $\Lambda_\tau = \mathbb{Z} + \tau\mathbb{Z}$, $\Lambda_\tau^* = \Lambda_\tau \setminus \{(0,0)\}$ and we define for $z \in \mathbb{C}$ the character on Λ_τ given for $\omega \in \Lambda_\tau^*$ by

$$\chi_z(\omega) := \exp\left(\frac{2\pi i(\bar{\omega} z - \omega \bar{z})}{\tau - \bar{\tau}}\right),$$

then

$$G(z_1, z_2; \tau) = \frac{Im(\tau)}{\pi} \sum_{\omega \in \Lambda_\tau^*} \frac{\chi_{z_1 - z_2}(\omega)}{|\omega|^2}. \tag{15}$$

Let us now introduce some more notation attached to the graph Γ. Choosing a labelling $z_1, \ldots, z_n$ of the n vertices induces an orientation on the edges: we orient them from z_i to z_j whenever $i < j$. Therefore we can construct the *incidence matrix*

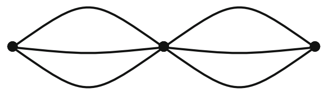
$$(\Gamma_{i,\alpha})_{\substack{1\leq i\leq n\\ 1\leq\alpha\leq l}}$$

of Γ by choosing any labelling e_α on the set of edges, and by setting $\Gamma_{i,\alpha} = 0$ if e_α does not touch z_i, $\Gamma_{i,\alpha} = 1$ if e_α is oriented away from z_i and $\Gamma_{i,\alpha} = -1$ if e_α is oriented towards z_i. It is now not difficult to show that

$$D_\Gamma(\tau) = \left(\frac{Im(\tau)}{\pi}\right)^l \sum_{\omega_1,\ldots,\omega_l\in\Lambda_\tau^*} \prod_{\alpha=1}^{l} |\omega_\alpha|^{-2} \prod_{i=1}^{n} \delta\Big(\sum_{\beta=1}^{l} \Gamma_{i,\beta}\omega_\beta\Big), \tag{16}$$

where $\delta(x) = 1$ if $x = 0$ and $\delta(x) = 0$ otherwise. From Eq. (16) it is easy to see that modular graph functions are indeed modular invariant, i.e. $D_\Gamma(\gamma\tau) = D_\Gamma(\tau)$ for all $\gamma \in \mathrm{SL}_2(\mathbb{Z})$, where $\gamma\tau$ is the Möbius action of the modular group $\mathrm{SL}_2(\mathbb{Z})$ on $\mathbb{H}$.

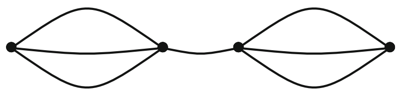
Let us now observe some simple consequences of the graphical nature of these functions. We call *reducible* a graph Γ such that the removal of a vertex would disconnect the graph, as in the figure below.

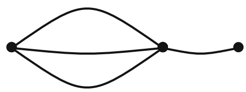


When a graph is reducible, one can prove from the sum representation (16) that the associated modular graph function factors into the product of the irreducible components. For instance, in the case of the figure above the modular graph function associated is $\left(\mathbf{D}\left[\ominus\right]\right)^2$. Note also that the normalization of the Green function given by Eq. (7) is chosen in such a way that

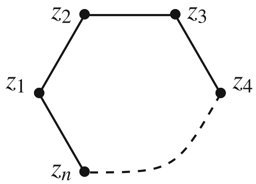
$$\int_{\mathscr{E}_\tau} G_1^{cl}(z, 0; \tau)dz = 0.$$

This, together with the factorization for reducible graphs, implies that $D_\Gamma(\tau) = 0$ whenever there exists any edge whose removal would disconnect the graph (physicists would call such graphs *one-particle reducible*). Below we have pictures of these situations:





Let us now give some concrete examples. For all graphs with n vertices along one cycle, as in the figure



we get by Eq. (16) that

$$D_\Gamma(\tau) = \left(\frac{Im(\tau)}{\pi}\right)^n \sum_{\omega \in \Lambda_\tau^*} \frac{1}{|\omega|^{2n}}.$$

This is precisely the definition of the special values at integers n of the *non-holomorphic Eisenstein series* $E(n, \tau)$. There are two well known results about non-holomorphic Eisenstein series which we want to underline, as some of their features are conjectured to extend to all modular graph functions:

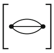
(1) Let $\Delta_\tau := 4(Im(\tau))^2 \frac{\partial^2}{\partial_\tau \partial_{\overline{\tau}}}$ be the hyperbolic Laplacian. Then

$$(\Delta_\tau - n(n-1))E(n, \tau) = 0. \tag{17}$$

(2) Let $y = \pi\, Im(\tau)$, B_k be the kth Bernoulli number and $\sigma_j(k) := \sum_{d|k} d^j$. Then

$$\begin{aligned} E(n, \tau) = \Big[&(-1)^{n-1} \frac{B_{2n}}{(2n)!}(4y)^n + \frac{4(2n-3)!}{(n-2)!(n-1)!}\zeta(2n-1)(4y)^{1-n} \\ &+ \frac{2}{(n-1)!} \sum_{k \geq 1} k^{n-1}\sigma_{1-2n}(k)(q^k + \overline{q}^k) \sum_{m=0}^{n-1} \frac{(n+m-1)!}{m!(n-m-1)!}(4ky)^{-m}\Big]. \end{aligned} \tag{18}$$

Laplace equations like (17) were shown to hold for many other examples of modular graph functions. For instance, we have

$(\Delta_\tau - 6)\,\mathbf{D}\Big[$  $\Big] = 0$ (19)

as well as inhomogeneous equations like

$(\Delta_\tau - 6)\,\mathbf{D}\Big[$  $\Big] = \frac{86}{5}E(5, \tau) - 4E(2, \tau)E(3, \tau) + \frac{\zeta(5)}{10}$

and (infinitely) many others [1, 23, 25]. It is generally believed that the algebra generated by modular graph functions over the ring $\mathscr{Z}$ of multiple zeta values should be closed under the action of Δ_τ.[6]

[6] Recent indications suggest that considering only the action of the Laplace operator we lose some information, and it is instead better to consider the action of the *Cauchy-Riemann derivative* $\nabla_\tau = 2i(Im(\tau))^2\partial_\tau$ and of its complex conjugate $\overline{\nabla}_\tau$ [22, 25].

On the other side, the form of the asymptotic expansion (18) of non-holomorphic Eisenstein series generalizes to all modular graph functions. Indeed, as announced in the introduction, it was shown in [42] for up to four vertices and in [43] in the general case that the asymptotic expansion of a modular graph function has the following form:

Theorem 3 ([43]) *Let $\mathcal{Z}_\infty$ be the $\mathbb{Q}$-algebra generated by all* cyclotomic multiple zeta values*, i.e. all convergent series given for $k_1, \ldots, k_r, N_1, \ldots, N_r \in \mathbb{N}$ by*

$$\sum_{0<v_1<\cdots<v_r} \frac{e^{2\pi i v_1/N_1} \cdots e^{2\pi i v_r/N_r}}{v_1^{k_1} \cdots v_r^{k_r}}.$$

Then for a graph Γ with weight l, setting $y = \pi\, Im(\tau)$, we have

$$D_\Gamma(\tau) = \sum_{k=1-l}^{l} \sum_{m,n\geq 0} d_k^{(m,n)}(\Gamma)\, y^k q^m \overline{q}^n,$$

where $d_k^{(m,n)}(\Gamma) \in \mathcal{Z}_\infty$.

The idea of the proof is to use the alternative representation of the propagator [30]

$$G_1(z,\tau) = 2\pi\, Im(\tau)\overline{B}_2(r) + Q(z,\tau), \tag{20}$$

where $\overline{B}_2(x)$ is the only 1-periodic continuous function coinciding with the second Bernoulli polynomial $B_2(x)$ in the interval $[0, 1]$, $z = s + r\tau$ ($s, r \in [0, 1]$) and

$$Q(z,\tau) = \sum_{\substack{m\in\mathbb{Z}\setminus\{0\}\\ k\in\mathbb{Z}}} \frac{\exp(2\pi i m((k+r)Re(\tau)+s))}{|m|} e^{-2\pi\, Im(\tau)|m||k-r|}. \tag{21}$$

The integral can be thought of as an integral over $r \in [0, 1]$ and $s \in [0, 1]$. One can therefore substitute $\overline{B}_2(r)$ with the polynomial $B_2(r) = r^2 - r + 1/6$. Using the binomial theorem to compute the powers of the propagator in terms of $B_2(r)$ and $Q(z, \tau)$ and interchanging integration with all summations introduced by the functions Q, one is left with integrals that evaluate to an asymptotic expansion of the form

$$\sum_{k=-l}^{l} \sum_{\substack{u\in\mathbb{Z}\\ v\geq 1}} \delta_k^{(u,v)}(\Gamma)\, y^k e^{2\pi i u Re(\tau)} e^{-2\pi v Im(\tau)},$$

where $\delta_k^{(u,v)}(\Gamma)$ are certain explicitly determined complex numbers given in terms of complicated multiple sums and u, v are subject to certain explicit constraints. To conclude the proof, one must first of all do the relatively easy exercise of showing that $\delta_{-l}^{(u,v)}(\Gamma) = 0$, that $v \geq |u|$ and that $u \equiv v$ mod 2: we need the last two conditions because $e^{2\pi i u Re(\tau)} e^{-2\pi v Im(\tau)} = q^m \overline{q}^n$ with $m = (u+v)/2$ and $n = (v-u)/2$, and we want to get $m, n \in \mathbb{Z}_{\geq 0}$. The last step consists in proving that the coefficients are cyclotomic MZVs, but this is non-elementary and relies on a result of Terasoma [35]. The reader can find the details in [43]. However, later we will see that this is (conjecturally) not the best possible result.

The main contribution to this asymptotic expansion as $y \to \infty$ is given by the Laurent polynomial

$$\mathbf{d}[\Gamma] := \sum_{k=1-l}^{l} d_k^{(0,0)}(\Gamma)\, y^k, \tag{22}$$

and great effort was spent on its computation, justified by the fact that all known differential and algebraic relations among modular graph functions can be predicted from its knowledge.[7] The first computations were made in [29, 30]. In particular, in the appendix of [30] Zagier gave a general formula in terms of MZVs for $\mathbf{d}[\Gamma]$ when Γ is a "banana" graph consisting only on two vertices and l edges between them. Later on, Zagier also proved that one can be more precise and write $\mathbf{d}[\Gamma]$ for all banana graphs in terms of odd Riemann zeta values $\zeta(2k+1)$ [40], just like the case of non-holomorphic Eisenstein series. Computations by hands for graphs with three and four vertices seemed to confirm the appearence of odd Riemann zeta values only [30]. A more systematic computation of the Laurent polynomials $\mathbf{d}[\Gamma]$, however, revealed that already for graphs with three vertices one can get MZVs of higher depth [42]. For instance,[8]

$\mathbf{d}\Big[$  $\Big]$

$$= \frac{62}{10945935} y^7 + \frac{2}{243}\zeta(3) y^4 + \frac{119}{324}\zeta(5) y^2 + \frac{11}{27}\zeta(3)^2 y + \frac{21}{16}\zeta(7) + \frac{46}{3}\frac{\zeta(3)\zeta(5)}{y} + \frac{7115\zeta(9) - 3600\zeta(3)^3}{288y^2} + \frac{1245\zeta(3)\zeta(7) - 150\zeta(5)^2}{16y^3} + \frac{288\zeta(3)\zeta(3,5) - 288\zeta(3,5,3) - 5040\zeta(5)\zeta(3)^2 - 9573\zeta(11)}{128y^4} + \frac{2475\zeta(5)\zeta(7) + 1125\zeta(9)\zeta(3)}{32y^5} - \frac{1575}{32}\frac{\zeta(13)}{y^6}.$$

[7] It is however believed that this should not always be true.

[8] There is a typo in the coefficient of y^{-4} in the corresponding formula in [42].

The key observation made in [42] is that one can rewrite

$$\mathbf{d}\Big[$$  $$\Big] = \frac{62}{10945935}y^7 + \frac{1}{243}\zeta_{\mathrm{sv}}(3)y^4 + \frac{119}{648}\zeta_{\mathrm{sv}}(5)y^2 + \frac{11}{108}\zeta_{\mathrm{sv}}(3)^2 y + \frac{21}{32}\zeta_{\mathrm{sv}}(7)$$
$$+ \frac{23}{6}\frac{\zeta_{\mathrm{sv}}(3)\zeta_{\mathrm{sv}}(5)}{y} + \frac{7115\zeta_{\mathrm{sv}}(9) - 900\zeta_{\mathrm{sv}}(3)^3}{576y^2} + \frac{1245\zeta_{\mathrm{sv}}(3)\zeta_{\mathrm{sv}}(7) - 150\zeta_{\mathrm{sv}}(5)^2}{64y^3}$$
$$- \frac{288\zeta_{\mathrm{sv}}(3,5,3) + 1620\zeta_{\mathrm{sv}}(5)\zeta_{\mathrm{sv}}(3)^2 + 9573\zeta_{\mathrm{sv}}(11)}{256y^4}$$
$$+ \frac{2475\zeta_{\mathrm{sv}}(5)\zeta_{\mathrm{sv}}(7) + 1125\zeta_{\mathrm{sv}}(9)\zeta_{\mathrm{sv}}(3)}{128y^5} - \frac{1575}{64}\frac{\zeta_{\mathrm{sv}}(13)}{y^6}. \tag{23}$$

This observation extends to all graphs computed so far. Moreover, it also seems to extend to all other Laurent polynomials appearing in the expansion, and it is consistent with the genus-zero case. This led to the following conjecture (initially stated only in the four-point case [42]):

Conjecture 2 (Z. 2015) *The coefficients $d_k^{(m,n)}(\Gamma)$ given by Theorem 3 belong to the algebra $\mathscr{Z}^{\mathrm{sv}}$ of single-valued MZVs.*

It is important to remark that this conjecture is much stronger than the statement of Theorem 3, which does not even imply that the coefficients of the asymptotic expansion are MZVs. Arguments supporting or proving special cases of this conjecture were given in [21, 24, 40].

We conclude this section by mentioning that an explicit computation of (part of) the asymptotic expansions, together with the differential relations among modular graph functions, allow us to prove algebraic relations such as

$$\mathbf{D}\Big[$$  $$\Big] = \mathbf{D}\Big[$$  $$\Big] + \zeta(3),$$

which can be deduced using the differential Eqs. (17) and (19) and the knowledge of $\mathbf{d}\Big[$  $\Big]$ [23].[9]

5 Holomorphic Graph Functions

Let us consider a graph Γ as in the beginning of Sect. 4. Recall that in genus zero we had (special values of) holomorphic multi-valued multiple polylogarithms on the open-string side and real-analytic single-valued multiple polylogarithms on the closed-string side. These two sides were related by the *sv* map. Since modular graph functions are real-analytic modular functions, i.e. single-valued on

[9]This identity was first proven by Zagier by a complicated direct computation (private communication).

$\mathfrak{M}_{1,1} = \mathrm{SL}_2(\mathbb{Z}) \setminus \mathbb{H}$, in order to make an analogy with genus zero we would like to associate to any graph Γ a holomorphic multi-valued function on $\mathfrak{M}_{1,1}$, together with a map going from one space to the other, which we would like to call *esv* (elliptic single-valued map). Moreover, we would like these holomorphic graph functions to arise from open-string amplitudes, as this would make the analogy with genus zero satisfactory also from the string-theory viewpoint.

A suggestion to achieve all this was given in [4], where not just one but two kinds of holomorphic graph functions, related to each other by a modular transformation, were defined. In order to give the definition, we first need to introduce a modified version of the open-string propagator $G_1^{op}(z_i, z_j; \tau)$:

$$P(z_1, z_2; \tau) := G_1^{op}(z_i, z_j; \tau) - 2\log(\eta(\tau)) + \frac{i\pi\tau}{6} + \frac{i\pi}{2} \tag{24}$$

Definition 2 ([4]) Let $z_1, \ldots, z_n \in [0, 1]$ be the vertices of a graph Γ, let us fix $z_n \equiv 0$ and for $i < j$ let us denote the number of edges between z_i and z_j by $l_{i,j}$. For such Γ we define its *A-cycle graph function* as

$$A_\Gamma(\tau) = \int_{[0,1]^{n-1}} \prod_{1\le i<j\le n} P(z_i, z_j; \tau)^{l_{i,j}}\, dz_1 \cdots dz_{n-1}, \tag{25}$$

and its *B-cycle graph functions* as

$$B_\Gamma(\tau) = A_\Gamma(-1/\tau). \tag{26}$$

We will often make use also of the alternative notations $\mathbf{A}[\Gamma]$ and $\mathbf{B}[\Gamma]$. Note that in general the integral (25) may diverge. In this case we consider instead its ε-regularized version given by the same procedure already explained in the definition of $G_1^{op}(z_1, z_2; \tau)$ (see Eq. (9)).

Without going into details, A-cycle graph functions can be thought of as restrictions of the integral on a torus which defines modular graph functions, given by Eq. (14), to the "A-cycle" $[0, 1]$ of the torus, while B-cycle graph functions as restrictions of (14) to the "B-cycle" $[0, \tau]$. This is a first reason why it is worth introducing both notions, even though one can be obtained from the other by a simple modular transformation. We will see later that another very important reason is given by their radically different asymptotic expansions. However, since Eq. (26) implies that these two classes of functions share many properties, we will sometimes refer to both of them as just *holomorphic graph functions*: indeed, by the definition (24) of $P(z_1, z_2; \tau)$, both A-cycle and B-cycle graph functions are holomorphic functions of $\tau \in \mathbb{H}$.

Let us now see how holomorphic graph functions are related to the four-point open-string integral (13). First of all, note that adding any (z_i, z_j)-independent term to the open-string propagator $G_1^{op}(z_i, z_j; \tau)$ does not modify the open-string integral (13), because of the kinematic condition $s_1 + s_2 + s_3 = 0$ on the Mandelstam variables. Thus considering the modified propagator $P(z_1, z_2; \tau)$ does not affect the amplitude. Let us now define the *abelianization* of (13) as

$$\int_{[0,1]^3} \exp\big(s_1(P(z_1, 0; \tau) + P(z_2, z_3; \tau)) + s_2(P(z_2, 0; \tau) + P(z_1, z_3; \tau)) \\ + s_3(P(z_3, 0; \tau) + P(z_1, z_2; \tau))\big)\, dz_1 dz_2 dz_3. \tag{27}$$

This is nothing but the sum over all possible orderings of the open-string positions on the cylinder's boundary [0, 1] of the integrals of the kind (13); it is called "abelianization" because it would correspond in physics to the amplitude of so-called abelian particle states, like photons, which are however not included in superstring theories. Even though the integral (27) is not "physical", it is clearly related to the open-string amplitude. Expanding (27) as a power series in the Mandelstam variables and allowing $\tau \in \mathbb{H}$, by a computation which is completely similar to that of the closed-string case we find that the coefficients are given by A-cycle graph functions (associated to graphs with at most four vertices), hence the connection between holomorphic graph functions and genus-one open-string amplitudes.

The reason for the normalization (24) of the propagator is given by the fact that

$$\int_0^1 P(z, 0; \tau)\, dz = 0, \tag{28}$$

which implies, as in the case of modular graph functions, that holomorphic graph functions vanish identically whenever they are associated to graphs that can be disconnected by removing one edge. The proof of Eq. (28) using the ε-regularization procedure (9) is left as an exercise to the reader.

In order to talk about non-trivial examples of holomorphic graph functions, we should first of all recall the observation, made in [6], that the coefficients of the power series expansion in the Mandelstam variables of the genus-one open-string integral (13), and therefore also A-cycle graph functions,[10] can be written in terms of *A-elliptic multiple zeta values*. These are holomorphic functions on $\mathbb{H}$ defined by Enriquez which generalize MZVs to genus one [27]. The "A" in their name comes from the fact that A-elliptic MZVs are given by certain iterated integrals over the A-cycle [0, 1] of a torus $\mathscr{E}_\tau$. There exists also a B-cycle version given by iterated integrals over $[0, \tau]$: they are called *B-elliptic multiple zeta values* and they are related to their A-cycle counterparts by the modular transformation $S : \tau \to -1/\tau$. Giving the definition of elliptic MZVs is not necessary here; we will just recall in the next paragraphs the properties needed in our presentation of holomorphic graph functions, and refer the interested reader to [27, 34, 43].

[10] This is only true for graphs with at most four vertices, but there is an obvious n-point version of the integral (27) whose coefficients, i.e. all possible graph functions, must be combinations of A-elliptic MZVs.

The main property that we will need is that elliptic MZVs can be written as (iterated) integrals of Eisenstein series. We recall that Eisenstein series are given for even $k \geq 4$ by

$$G_k(\tau) = \sum_{(r,s)\neq(0,0)} \frac{1}{(r+s\tau)^k} = 2\zeta(k) + \frac{2(2\pi i)^k}{(k-1)!} \sum_{m,n\geq 1} n^{k-1} q^{mn}.$$

They are weight k modular forms w.r.t. the modular group $\mathrm{SL}_2(\mathbb{Z})$, i.e. they are holomorphic functions on $\mathbb{H} \cup i\infty$ such that $G_{2k}(\tau)|_{2k}\,\gamma = G_{2k}(\tau)$, where the weight k right action $|_k\,\gamma$ of the modular group is defined for $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z})$ by

$$f(\tau)|_k\,\gamma = (c\tau+d)^{-k} f\left(\frac{a\tau+b}{c\tau+d}\right).$$

Setting $G_0(\tau) := -1$, *iterated Eisenstein integrals* are defined in [7] for $k_1, \ldots, k_r \in \{0, 4, 6, 8, \ldots\}$[11] by the recursive formula

$$\mathscr{E}(k_1, \ldots, k_r; \tau) = \int_{\tau}^{\vec{1}_\infty} \frac{G_k(z)}{(2\pi i)^{k-1}} \mathscr{E}(k_1, \ldots, k_{r-1}; z)\, dz, \tag{29}$$

where following [16] we define for $f(\tau) = \sum_{j\geq 0} a_j(\tau) q^j$ and $a_j(\tau) \in \mathbb{C}[\tau]$[12]

$$\int_{\tau'}^{\vec{1}_\infty} f(\tau)\, d\tau := \int_{\tau'}^{i\infty} \sum_{j\geq 1} a_j(\tau) q^j\, d\tau - \int_0^{\tau'} a_0(\tau)\, d\tau. \tag{30}$$

Writing down A-cycle graph functions in terms of the iterated integrals $\mathscr{E}(\mathbf{k};\tau)$ is very convenient, because all algebraic relations among the $\mathscr{E}(\mathbf{k};\tau)$'s are known [32] and because their asymptotic expansion can be explicitly worked out [4, 7]. Moreover, most importantly for us, this is a good viewpoint if one is interested in the modular behaviour of A-cycle graph functions, for instance in order to compute B-cycle graph functions [4].

Let us now consider a simple example: one can show by direct computation that

$\mathbf{A}\Big[$  $\Big]$ $= \dfrac{(\pi i\tau)^2}{60} + \dfrac{\zeta(2)}{2} - 6\mathscr{E}(4,0;\tau)$ (31)

$$= \frac{\zeta(2)}{2} + 2q + \frac{9}{2}q^2 + \cdots \tag{32}$$

[11]Here we deviate from [7] and we prefer to exclude the quasi-modular form $G_2(\tau)$.

[12]Since $\mathbb{H}$ is simply connected, we can choose arbitrary paths from τ' to $i\infty$ and from 0 to τ'.

The fact that the first term of the right-hand side of (31) disappears in (32) is not an accident: it is coherent with the fact, proven by Enriquez [27], that A-elliptic MZVs (and therefore A-cycle graph functions) admit an asymptotic expansion

$$\sum_{j\geq 0} a_j q^j, \tag{33}$$

where $a_j \in \mathscr{Z}[(2\pi i)^{-1}]$.[13] As we have mentioned, writing down A-cycle graph functions in terms of iterated Eisenstein integrals is the key to compute B-cycle graph functions. In order to get $\mathbf{B}$[], all we need to do is to compute $\mathscr{E}(4, 0; -1/\tau)$. Let us see some details of this computation, which nicely illustrates various features of the general case. Directly from the definition, one gets

$$\mathscr{E}(4, 0; \tau) = \frac{1}{(2\pi i)^2}\int_{\tau}^{\vec{1}_\infty} (\tau - z) G_4(z)\, dz.$$

Therefore, making use of the change of variables $z \to -1/z$ and of the modular properties of $G_4(\tau)$, we can write

$$\mathscr{E}(4, 0; -1/\tau) = \frac{1}{(2\pi i)^2}\int_{-1/\tau}^{\vec{1}_\infty} \Big(-\frac{1}{\tau} - z\Big) G_4(z)\, dz = \frac{\tau^{-1}}{(2\pi i)^2}\int_{\tau}^{S\vec{1}_\infty} z(\tau - z) G_4(z)\, dz,$$

where $S\vec{1}_\infty$ is the image of the (tangential base point at the) cusp under the modular transformation $S : \tau \to -1/\tau$: one should think of it as the point 0, together with additional informations about the regularization of the integral, similar to those of Eq. (30) [16]. Since these integrals are all homotopy invariant, we can choose a path which passes through the cusp $\vec{1}_\infty$ and split the integral as

$$\mathscr{E}(4, 0; -1/\tau) = \frac{\tau^{-1}}{(2\pi i)^2}\bigg(\int_{\tau}^{\vec{1}_\infty} z(\tau - z) G_4(z)\, dz - \int_{S\vec{1}_\infty}^{\vec{1}_\infty} z(\tau - z) G_4(z)\, dz\bigg) \tag{34}$$

Using the fact that

$$\begin{aligned} 2\mathscr{E}(4, 0, 0; \tau) &= \frac{1}{2\pi i}\int_{\tau}^{\vec{1}_\infty} (\tau - z)^2 G_4(z)\, dz \\ &= \frac{1}{2\pi i}\int_{\tau}^{\vec{1}_\infty} \tau(\tau - z) G_4(z)\, dz - \frac{1}{2\pi i}\int_{\tau}^{\vec{1}_\infty} z(\tau - z) G_4(z)\, dz, \end{aligned}$$

one immediately sees that the first integral of Eq. (34) can be written as $\mathscr{E}(4, 0; \tau) - (\pi i \tau)^{-1}\mathscr{E}(4, 0, 0; \tau)$. The evaluation of the second integral of Eq. (34) can be done

[13] While for A-elliptic MZVs we know that inverting $2\pi i$ is necessary, we suspect that no inverse powers of $2\pi i$ should appear in the asymptotic expansion of A-cycle graph functions.

using the functional equation of the L-functions associated to Eisenstein series: the computation is completely similar to that of period polynomials of Eisenstein series (see [41]). This is not a coincidence, because $\mathscr{E}(4, 0, 0; \tau)$ is essentially an Eichler integral of $G_4(\tau)$. The general theory of *iterated Eichler integrals of modular forms*, developed by Manin and Brown [16, 33], provides the tools to understand the modular behaviour of the functions $\mathscr{E}(\mathbf{k}, \tau)$. It is crucial to remark that not all the $\mathscr{E}(\mathbf{k}, \tau)$'s can be written in terms of iterated Eichler integrals, and indeed not all of them share the same nice modular behaviour of our example $\mathscr{E}(4, 0; \tau)$: it is an instructive exercise to see how the steps of the computations of $\mathscr{E}(4, 0; -1/\tau)$ cannot be repeated for $\mathscr{E}(4, 0, 0, 0; -1/\tau)$. Fortunately, a result by Brown implies that A-cycle graph functions can always be written in terms of the "good $\mathscr{E}(\mathbf{k}, \tau)$'s", i.e. those which are iterated Eichler integrals [15]. We refer to [4] for a detailed analysis of the relationship between the $\mathscr{E}(\mathbf{k}, \tau)$'s and iterated Eichler integrals à la Manin–Brown. The final result is that

$$\begin{aligned}\mathbf{B}\Big[\bigcirc\Big] &= \frac{\zeta(2)}{3} - \frac{\zeta(3)}{T} - \frac{3\zeta(4)}{2T^2} - 6\mathscr{E}(4,0;\tau) + \frac{6}{T}\mathscr{E}(4,0,0;\tau) \\ &= \frac{T^2}{180} + \frac{\zeta(2)}{3} - \frac{\zeta(3)}{T} - \frac{3\zeta(4)}{2T^2} + 2\left(1 - \frac{1}{T}\right)q + \dots,\end{aligned} \tag{35}$$

where $T := \pi i \tau$. We can already see from this simple example that the asymptotic expansion of B-cycle graph functions is substantially different from that of their A-cycle counterpart. In particular, B-cycle graph functions are not invariant under the transformation $\tau \to \tau + 1$. Far from being an issue, this is actually the main reason behind the introduction of B-cycle graph functions in [4]: an expansion like (35), unlike Eq. (33), reminds the asymptotic behaviour of modular graph functions. We will indeed see in the next section that this simple observation has astonishing consequences. The main result of this section is the following refinement of a formula stated in [4] for the asymptotic expansion of B-cycle graph functions.

Theorem 4 *For a graph Γ with weight l, setting $T = \pi i \tau$, we have*

$$B_\Gamma(\tau) = \sum_{k=-l}^{l} \sum_{m \geq 0} b_k^{(m)}(\Gamma)\, T^k q^m,$$

where $b_k^{(m)}(\Gamma) \in \mathscr{Z}$.

Proof It was demonstrated in [4] that

$$B_\Gamma(\tau) = \sum_{k=-K}^{K} \sum_{m \geq 0} b_k^{(m)}(\Gamma)\, T^k q^m \tag{36}$$

for some $K \in \mathbb{N}$, where $b_k^{(m)}(\Gamma) \in \mathscr{Z}$, so all we need to prove is that we can choose $K = l$. In order to do this, let us recall the modular properties of θ and η:

$$\theta(z/\tau, -1/\tau) = -i\sqrt{-i\tau}\,\exp\left(\frac{2\pi i z^2}{2\tau}\right)\theta(z,\tau),$$
$$\eta(-1/\tau) = \sqrt{-i\tau}\,\eta(\tau).$$

Using these transformations together with Eqs. (24) and (8) we deduce that

$$P(z_i, z_j; -1/\tau) = -\frac{\pi i}{6\tau} + \frac{\pi i}{2} - \log\left(i e^{\pi i\tau(z_i-z_j)^2} q^{1/12}\left(\tilde{u}_{ij}^{-1/2} - \tilde{u}_{ij}^{1/2}\right)\prod_{n\geq 1}(1-\tilde{u}_{ij}q^n)(1-\tilde{u}_{ij}^{-1}q^n)\right), \quad (37)$$

where $\tilde{u}_{ij} := \exp(2\pi i\tau(z_i - z_j))$. Therefore, setting $z_{ij} := z_i - z_j$, we can write

$$P(z_i, z_j; -1/\tau) = L(z_{ij}; \tau) + S(z_{ij}; \tau), \quad (38)$$

where we define for $T = \pi i\tau$ and $\tilde{u} = \exp(2\pi i\tau z)$

$$L(z,\tau) = -T\left(z^2 - z + \frac{1}{6}\right) + \frac{\zeta(2)}{T}, \quad (39)$$

$$S(z,\tau) = \sum_{m\geq 1}\frac{\tilde{u}^m}{m} + \sum_{n,m\geq 1}\frac{\tilde{u}^m q^{nm}}{m} + \sum_{n,m\geq 1}\frac{\tilde{u}^{-m}q^{nm}}{m}. \quad (40)$$

In order to compute B-cycle graph functions, we need to take powers of the propagator. We have

$$P(z_i, z_j; -1/\tau)^l = (L(z_{ij};\tau) + S(z_{ij};\tau))^l = \sum_{r+s=l}\frac{l!}{r!s!}L(z_{ij},\tau)^r S(z_{ij},\tau)^s$$
$$= \sum_{a+b+c+d+s=l}\frac{l!}{a!b!c!d!s!}\frac{(-1)^{a+c}}{6^c}\zeta(2)^d z_{ij}^{2a+b} T^{a+b+c-d} S(z_{ij},\tau)^s. \quad (41)$$

Therefore, if for instance we want to know the asymptotic expansion of

$$\int_0^1 P(z, 0; -1/\tau)^l\, dz,$$

i.e. 2-point B-cycle graph functions, we are left with computing integrals of the kind

$$\int_0^1 z^{2a+b} S(z,\tau)^s\, dz.$$

If $s = 0$ this integral evaluates to a rational numbers; thus we get a Laurent polynomial with powers ranging from $-l$ (when $d = l$) to l (when $d = 0$). Now let $s \geq 1$. Since for all $\alpha \in \mathbb{Z}$

$$\int_0^1 z^{2a+b} e^{2\pi i \alpha \tau z}\, dz = \frac{(2a+b)!}{(-2\pi i \alpha \tau)^{2a+b+1}} - \sum_{j=0}^{2a+b} \frac{(2a+b)_j}{(-2\pi i \alpha \tau)^{j+1}} e^{2\pi i \alpha \tau}, \tag{42}$$

where $(k)_j := k(k-1)\cdots(k-j+1)$ is the descending Pochhammer symbol, exchanging integration and summations in (40) we get negative contributions to the powers of T ranging from 1 to $2a+b+1$. The lowest possible power that arises from these contributions is then given, because of Eq. (41), by

$$a+b+c-d-2a-b-1 = c-a-d-1 \geq -l+s-1 \geq -l.$$

This concludes the proof when the graphs Γ has only two vertices. The proof for the general case goes along the same lines and is left to the reader. $\square$

6 The *esv* Conjecture

The main contribution to the asymptotic expansion of B-cycle graph functions $\mathbf{B}[\Gamma]$ when $Im(\tau) \to \infty$ is given by the first Laurent polynomial

$$\mathbf{b}[\Gamma] := \sum_{k=-l}^{l} b_k^{(0)}(\Gamma)\, T^k. \tag{43}$$

For instance, in the case of the weight $l = 2$ B-cycle graph function $\mathbf{B}[\ ]$ we deduce by Eq. (35) that

$$\mathbf{b}[\ ] = \frac{T^2}{180} + \frac{\zeta(2)}{3} - \frac{\zeta(3)}{T} - \frac{3\zeta(4)}{2T^2}.$$

On the other side, we have mentioned in Sect. 4 that$\mathbf{D}[\ ] = E(2,\tau)$, and therefore by Eq. (18) we have

$$\mathbf{d}[\ ] = \frac{y^2}{45} + \frac{\zeta(3)}{y}.$$

Let us now define a map $\mathscr{Z}[T] \to \mathscr{Z}^{\mathrm{sv}}[y]$ by sending $\zeta(\mathbf{k}) \to \zeta_{\mathrm{sv}}(\mathbf{k})$ and $T \to -2y$. We call this map *esv*. Using the fact that $\zeta_{\mathrm{sv}}(2k) = 0$ and $\zeta_{\mathrm{sv}}(2k+1) = 2\zeta(2k+1)$, one can easily check that $esv(\mathbf{b}[\ ]) = \mathbf{d}[\ ]$. This was the starting point of an extensive series of computations, which led to the following apparently surprising statement [4]:

Conjecture 3 (Brödel–Schlotterer-Z. 2018) *For all graphs Γ we have*

$$esv(\boldsymbol{b}[\Gamma]) = \boldsymbol{d}[\Gamma] \tag{44}$$

For the rest of the paper we will refer to this statement as the *esv conjecture*. We would like to remark, in order to avoid possible confusion, that the presentation given here of this conjecture is quite different to that given in [4], because the *esv* "rules" defined in [4] (which contain the *esv* map defined above) act on the whole asymptotic expansion of B-cycle graph functions, while here we will consider only the restriction to the first Laurent polynomial. Note that the *esv* conjecture would imply the part of Conjecture 2 concerning the coefficients $d_k^{(m,n)}(\Gamma)$ of the first Laurent polynomial, i.e. when $(m, n) = (0, 0)$.

The *esv* conjecture was checked for all graphs up to weight six, as well as for the "crucial" weight-seven example[14] (compare with Eq. (23))

$\mathbf{b}\Big[$  $\Big]$

$$\begin{aligned} = &-\frac{31T^7}{700539840} - \frac{5251T^5\zeta_2}{233513280} + \frac{T^4\zeta_3}{3888} - \frac{7405T^3\zeta_4}{598752} + \frac{119T^2\zeta_5}{2592} + \frac{31T^2\zeta_2\zeta_3}{864} \\ &- \frac{11T\zeta_3^2}{216} - \frac{15527T\zeta_6}{10368} + \frac{21\zeta_7}{32} + \frac{67\zeta_2\zeta_5}{27} + \frac{167\zeta_3\zeta_4}{48} - \frac{23\zeta_3\zeta_5}{3T} - \frac{80017\zeta_8}{1296T} + \frac{3\zeta_2\zeta_3^2}{T} \\ &- \frac{25\zeta_3^3}{4T^2} + \frac{7115\zeta_9}{144T^2} + \frac{21\zeta_2\zeta_7}{T^2} + \frac{35\zeta_4\zeta_5}{6T^2} - \frac{6613\zeta_3\zeta_6}{288T^2} + \frac{75\zeta_5^2}{4T^3} - \frac{1245\zeta_3\zeta_7}{8T^3} - \frac{48\zeta_{3,5}\zeta_2}{T^3} \\ &+ \frac{443\zeta_2\zeta_3\zeta_5}{T^3} - \frac{275\zeta_3^2\zeta_4}{8T^3} + \frac{941869\zeta_{10}}{5760T^3} - \frac{9573\zeta_{11}}{16T^4} - \frac{18\zeta_{3,5,3}}{T^4} - \frac{405\zeta_3^2\zeta_5}{4T^4} + \frac{195\zeta_2\zeta_3^3}{2T^4} \\ &+ \frac{27745\zeta_5\zeta_6}{48T^4} - \frac{3795\zeta_4\zeta_7}{16T^4} + \frac{17731\zeta_3\zeta_8}{16T^4} + \frac{15875\zeta_2\zeta_9}{12T^4} - \frac{2475\zeta_5\zeta_7}{4T^5} - \frac{1125\zeta_3\zeta_9}{4T^5} \\ &+ \frac{90\zeta_{3,5}\zeta_4}{T^5} + \frac{450\zeta_{3,7}\zeta_2}{7T^5} - \frac{165\zeta_3\zeta_4\zeta_5}{2T^5} + \frac{3375\zeta_2\zeta_5^2}{7T^5} + \frac{3335\zeta_3^2\zeta_6}{4T^5} + \frac{3960\zeta_2\zeta_3\zeta_7}{7T^5} \\ &+ \frac{93091945\zeta_{12}}{11056T^5} - \frac{1575\zeta_{13}}{T^6} + \frac{13275\zeta_2\zeta_{11}}{4T^6} + \frac{7425\zeta_4\zeta_9}{8T^6} + \frac{129465\zeta_6\zeta_7}{16T^6} \\ &+ \frac{233525\zeta_5\zeta_8}{48T^6} + \frac{160053\zeta_3\zeta_{10}}{64T^6} + \frac{15301285\zeta_{14}}{768T^7} \end{aligned} \tag{45}$$

Let us now make two remarks in order to support the conjecture. First of all, it is straightforward to check that the appearence of the second Bernoulli polynomials in both Eqs. (20) and (38) implies that, for a fixed weight l graph, the coefficient of T^l in (43) is equal to the coefficient of $(-2y)^l$ in (22). Moreover, note that the lowest power of T appearing in the expansion (43) is $-l$, while the lowest power of y appearing in the expansion (22) is $1 - l$. This means that the *esv* conjecture implies that $sv(b_{-l}^{(0)}(\Gamma)) = 0$. We have seen in the proof of Theorem 4 that there are two sources of contribution to the coefficient of T^{-l} in (43). The first one (obtained when $s = 0$) is given by $\prod \zeta(2)^{l_{i,j}}$, while the second one originates from the integrals of products (for all i, j) of the kind

$$L(z_{ij}; \tau)^{l_{i,j}-1} S(z_{ij}; \tau).$$

[14] This case could only be checked numerically, for about five-hundred digits.

From the same kind of computation seen in the proof of Theorem 4 we can conclude that the contribution to the coefficient of T^{-l} (which is given by setting for all i, j $a_{i,j} = l_{i,j} - 1 - d_{i,j}$ in Eq. (42)) is a rational linear combination of $\zeta(2(l-d))\zeta(2)^d$ for $0 \leq d \leq l-1$. This implies that the coefficient of T^{-l} is a rational multiple of $\zeta(2l)$, which is indeed sent to 0 by the sv map. In other words, we have proven:

Proposition 1 *For any weight l graph Γ we have $esv(b_l^{(0)}(\Gamma)\, T^l) = d_l^{(0,0)}(\Gamma)\, y^l$ and $esv(b_{-l}^{(0)}(\Gamma)\, T^{-l}) = 0$.*

We want to conclude by explaining that the esv conjecture should be related to Brown's recent construction of a new class of functions in the context of his research on mixed modular motives [14].

Definition 3 ([15]) Let $f : \mathbb{H} \longrightarrow \mathbb{C}$ be a real analytic function. We call it *modular of weights* (r, s) if for every $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z})$ it satisfies

$$f(\gamma\tau) = (c\tau + d)^r (c\overline{\tau} + d)^s f(\tau). \tag{46}$$

We denote $\mathscr{M}_{r,s}$ the space of modular functions of weights (r, s) which admit an expansion of the form

$$f(q) \in \mathbb{C}[[q, \overline{q}]][y^{\pm 1}], \tag{47}$$

where we recall that $y = \pi\, Im(\tau)$. We also define the bigraded algebra

$$\mathscr{M} = \bigoplus_{r,s} \mathscr{M}_{r,s}.$$

Note that Theorem 3 implies that all modular graph functions belong to $\mathscr{M}_{0,0}$.

The main result of [14] tells us, among other things, that there exists a subalgebra $\mathscr{M}\mathscr{I}^E \subset \mathscr{M}$ generated over $\mathscr{Z}^{\mathrm{sv}}$ by certain computable linear combinations of products of real and imaginary parts of iterated Eichler integrals of Eisenstein series, such that:

- It carries a grading by a certain *M-degree* and a filtration by the length (number of integrations) of the iterated integrals, denoted by $\mathscr{M}\mathscr{I}_k^E \subset \mathscr{M}\mathscr{I}^E$.
- Every element of $\mathscr{M}\mathscr{I}^E$ admits an expansion of the form

$$f(q) \in \mathscr{Z}^{\mathrm{sv}}[[q, \overline{q}]][y^{\pm 1}]$$

- The sub-vector space of elements of fixed modular weights and M-degree $\leq m$ is finite dimensional.
- Every element $F \in \mathscr{M}\mathscr{I}_k^E$ satisfies an inhomogeneous Laplace equation of the form

$$(\Delta + w)F \in (\mathbb{E} + \overline{\mathbb{E}})[y] \times \mathscr{M}\mathscr{I}_{k-1}^E + \mathbb{E}\overline{\mathbb{E}}[y] \times \mathscr{M}\mathscr{I}_{k-2}^E,$$

  where $\mathbb{E}$ denotes the space of holomorphic Eisenstein series for $\mathrm{SL}_2(\mathbb{Z})$.

The elements of this algebra are called *equivariant iterated Eichler integrals of Eisenstein series*. Their properties remind very much the conjectural properties of modular graph functions. In fact, in [14] it is conjectured that modular graph functions should belong to the weight (0, 0) subalgebra of $\mathscr{M}\mathscr{I}^E$ (which would imply that Conjecture 2 is true). This is not surprising, if we think of the general philosophy of string amplitudes: closed-string amplitudes are expected to be a single-valued non-holomorphic version of open-string amplitudes; since genus-one open-string amplitudes can be written in terms of (holomorphic) iterated Eichler integrals of Eisenstein series, we would therefore expect that the closed-string counterpart should be given by real-analytic single-valued (i.e. modular) analogues, and the most natural candidate is given by the elements of the algebra $\mathscr{M}\mathscr{I}^E$. However, the map which associates to a given iterated Eichler integral its equivariant image is rather involved beyond the simplest case of classical Eichler integrals,[15] and this has initially discouraged the first attempts to use it to explicitly relate open-string integrals to closed-string integrals. On the other side, we have seen that by the surprisingly simple *esv* conjecture we can obtain (the asymptotically big part of) modular graph functions from holomorphic graph functions, i.e. from special combinations of iterated Eichler integrals. We believe that, despite their apparently different origin, Brown's "equivariant map" and our *esv* map should be related. Hopefully, understanding this link should pave the way towards proving both Conjecture 2 and the *esv* conjecture.

Finally, we want to remark that all this suggests, as anticipated in Sect. 2, that genus–g superstring amplitudes for $g = 0, 1$ seem to be be related to mixed motives associated to moduli spaces of genus–g Riemann surfaces. It would be extremely interesting to understand whether (and how) this will hold for higher genera, where the analogous mathematical structures have not been understood yet.

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Some Algebraic and Arithmetic Properties of Feynman Diagrams

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Abstract This article reports on some recent progresses in Bessel moments, which represent a class of Feynman diagrams in 2-dimensional quantum field theory. Many challenging mathematical problems on these Bessel moments have been formulated as a vast set of conjectures, by David Broadhurst and collaborators, who work at the intersection of high energy physics, number theory and algebraic geometry. We present the main ideas behind our verifications of several such conjectures, which revolve around linear and non-linear sum rules of Bessel moments, as well as relations between individual Feynman diagrams and critical values of modular L-functions.

1 Introduction

1.1 Bessel Moments and Feynman Diagrams

In perturbative quantum field theory (pQFT), we use *Feynman diagrams* to quantify the interactions among elementary particles [1, 13, 31, 37]. In this survey, we will focus on 2-dimensional pQFT, where the propagator of a free particle with proper mass m_0 takes the following form:

$$\frac{1}{(2\pi)^2}\lim_{\varepsilon\to0^+}\iint_{\mathbb{R}^2}\frac{e^{i\boldsymbol{p}\cdot\boldsymbol{x}-\varepsilon|\boldsymbol{p}|^2}\mathrm{d}^2\boldsymbol{p}}{|\boldsymbol{p}|^2+m_0^2}=\frac{K_0(m_0|\boldsymbol{x}|)}{2\pi}\tag{1}$$

for $\boldsymbol{x}\in\mathbb{R}^2\smallsetminus\{\mathbf{0}\}$. Here, $K_0(t):=\int_0^\infty e^{-t\cosh u}\mathrm{d}u$, $t>0$ is the modified Bessel function of the second kind and zeroth order.

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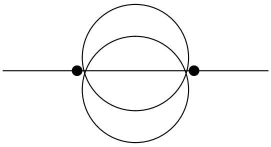
Some results in 2-dimensional pQFT also find their way into the finite part of renormalized perturbative expansions of $(4-\varepsilon)$-dimensional quantum electrodynamics [36]. For example, in Stefano Laporta's recent computation of the 4-loop contribution to electron's magnetic moment [37], one of the master integrals is the 4-loop sunrise diagram for 2-dimensional pQFT:



$$:= 2^4 \int_0^\infty I_0(t)[K_0(t)]^5 t\,\mathrm{d}t$$

$$= \int_0^\infty \frac{\mathrm{d}x_1}{x_1} \int_0^\infty \frac{\mathrm{d}x_2}{x_2} \int_0^\infty \frac{\mathrm{d}x_3}{x_3} \int_0^\infty \frac{\mathrm{d}x_4}{x_4} \frac{1}{\left(1+\sum_{k=1}^4 x_k\right)\left(1+\sum_{k=1}^4 \frac{1}{x_k}\right)-1}. \tag{2}$$

Here, the single integral over the variable t represents the Feynman diagram in configuration space (see [1, §1], [15, §9.2] or [13, (84)]), and $I_0(t) = \frac{1}{\pi}\int_0^\pi e^{t\cos\theta}\mathrm{d}\theta$ is the modified Bessel function of the first kind and zeroth order; alternatively, a quadruple integral over a rational function in the variables x_1, x_2, x_3 and x_4 represents the same Feynman diagram in the Schwinger parameter space (see [15, §9.1] or [44, §8]).

On one hand, Feynman diagrams provide us with many physically meaningful multiple integrals over rational functions, which are special cases of motivic integrals [3, 44], playing prominent rôles in the arena for algebraic geometers. On the other hand, certain Feynman diagrams are (conjecturally or provably) related to arithmetically interesting objects [13, 42, 52], such as special values of modular L-functions inside their critical strips, inviting pilgrims to the pantheon of number theorists.

After high-precision computations of Feynman diagrams, Bailey–Borwein–Broadhurst–Glasser [1], Broadhurst [13, 15], Broadhurst–Schnetz [18] and Broadhurst–Mellit [17] had formulated various conjectures on *Bessel moments*

$$\mathbf{IKM}(a,b;n) := \int_0^\infty [I_0(t)]^a[K_0(t)]^b t^n \mathrm{d}t \tag{3}$$

with $a, b, n \in \mathbb{Z}_{\geq 0}$. The last few years had witnessed rapid progress in these conjectures proposed by David Broadhurst and coworkers. In Sects. 1.2 and 1.3 below, we give precise statements of some recently proven conjectures about Bessel moments, before presenting in Sect. 1.4 a road map for their mathematical understanding.

1.2 Some Algebraic Relations Involving Bessel Moments

The following theorem about linear sum rules for Bessel moments grew out of numerical conjectures by Bailey–Borwein–Broadhurst–Glasser [1, (220)], Broadhurst–

Mellit [17, (7.10)] and Broadhurst–Roberts [9, Conjecture 2]. The first proof appeared in [48].

Theorem 1 (Generalized Bailey–Borwein–Broadhurst–Glasser sum rules and generalized Crandall numbers)

(a) We have

$$\int_0^\infty \frac{[\pi I_0(t)+iK_0(t)]^m+[\pi I_0(t)-iK_0(t)]^m}{i}[K_0(t)]^m t^n \mathrm{d}t=0 \tag{4}$$

for $m\in\mathbb{Z}_{>1}, n\in\mathbb{Z}_{\geq 0}, \frac{m-n}{2}\in\mathbb{Z}_{>0}$, *and*

$$\int_0^\infty \frac{[\pi I_0(t)+iK_0(t)]^m-[\pi I_0(t)-iK_0(t)]^m}{i}[K_0(t)]^m t^n \mathrm{d}t=0 \tag{5}$$

for $m\in\mathbb{Z}_{>0}, n\in\mathbb{Z}_{\geq 0}, \frac{m-n-1}{2}\in\mathbb{Z}_{>0}$, *which generalize the Bailey–Borwein–Broadhurst–Glasser sum rule [1, (220)].*

(b) The Crandall numbers (OEIS `A262961` *[43])*

$$A(n):=\left(\frac{2}{\pi}\right)^4\int_0^\infty \left\{[\pi I_0(t)]^2-[K_0(t)]^2\right\} I_0(t)[K_0(t)]^5\,(2t)^{2n-1}\mathrm{d}t \tag{6}$$

are integers for all $n\in\mathbb{Z}_{>0}$. *More generally, the integral*

$$C_{m,n}=\frac{2^{1+2(n-1)[1-(-1)^m]}}{\pi^{m+1}}\int_0^\infty \frac{[\pi I_0(t)+iK_0(t)]^m-[\pi I_0(t)-iK_0(t)]^m}{i}\times \\ \times [K_0(t)]^m(2t)^{2n+m-3}\mathrm{d}t \tag{7}$$

evaluates to a positive integer for each $m,n\in\mathbb{Z}_{>0}$.

The next theorem includes two sets of non-linear sum rules, which were originally discovered by Broadhurst–Mellit [17, (6.12) and (7.13)] through numerical experiments on moderate-sized determinants. An analytic proof has recently been found [53] for Broadhurst–Mellit determinants that come in arbitrary sizes.

Theorem 2 (Broadhurst–Mellit determinant formulae) *Define* $\mathbf{M}_k$ *and* $\mathbf{N}_k$ *as* $k\times k$ *matrices with elements*

$$(\mathbf{M}_k)_{a,b}:=\int_0^\infty [I_0(t)]^a[K_0(t)]^{2k+1-a}t^{2b-1}\mathrm{d}t, \tag{8}$$

$$(\mathbf{N}_k)_{a,b}:=\int_0^\infty [I_0(t)]^a[K_0(t)]^{2k+2-a}t^{2b-1}\mathrm{d}t. \tag{9}$$

Then we have the following determinant formulae:

$$\det \mathbf{M}_k = \prod_{j=1}^{k} \frac{(2j)^{k-j}\pi^j}{\sqrt{(2j+1)^{2j+1}}}, \tag{10}$$

$$\det \mathbf{N}_k = \frac{2\pi^{(k+1)^2/2}}{\Gamma((k+1)/2)} \prod_{j=1}^{k+1} \frac{(2j-1)^{k+1-j}}{(2j)^j}, \tag{11}$$

where Euler's gamma function[1] *is defined by* $\Gamma(x) := \int_0^\infty t^{x-1}e^{-t}\mathrm{d}t$ *for* $x > 0$.

1.3 Some Arithmetic Properties of Bessel Moments

In what follows, we write $f_{k,N}$ for a *modular form* (see Sect. 2.3 for technical details) of weight k and level N, and define its L-function through a Mellin transform:

$$L(f_{k,N}, s) := \frac{(2\pi)^s}{\Gamma(s)} \int_0^\infty f_{k,N}(iy)y^{s-1}\mathrm{d}y. \tag{12}$$

A special L-value $L(f_{k,N}, s)$ is said to be *critical*, if $s \in \mathbb{Z} \cap (0, k)$. In this survey, we will be interested in the following three special modular forms:

$$f_{3,15}(z) = [\eta(3z)\eta(5z)]^3 + [\eta(z)\eta(15z)]^3, \tag{13}$$

$$f_{4,6}(z) = [\eta(z)\eta(2z)\eta(3z)\eta(6z)]^2, \tag{14}$$

$$f_{6,6}(z) = \frac{[\eta(2z)\eta(3z)]^9}{[\eta(z)\eta(6z)]^3} + \frac{[\eta(z)\eta(6z)]^9}{[\eta(2z)\eta(3z)]^3}, \tag{15}$$

where the Dedekind eta function is defined as $\eta(z) := e^{\pi iz/12}\prod_{n=1}^\infty(1 - e^{2\pi inz})$ for complex numbers z satisfying $\operatorname{Im} z > 0$. For $y > 0$, one can deduce

$$f_{k,N}\left(\frac{i}{Ny}\right) = (\sqrt{N}y)^k f_{k,N}(iy) \tag{16}$$

from the modular transformation $\eta(-1/\tau) = \sqrt{\tau/i}\,\eta(\tau)$ for $\tau/i > 0$. Consequently, the L-functions attached to these three modular forms satisfy the following reflection formulae [13, (95), (106), (138)]:

$$\Lambda(f_{k,N}, s) := \left(\frac{\sqrt{N}}{\pi}\right)^s \Gamma\left(\frac{s}{2}\right)\Gamma\left(\frac{s+1}{2}\right)L(f_{k,N}, s) = \Lambda(f_{k,N}, k - s). \tag{17}$$

[1] Throughout this survey, we reserve the upright Γ for Euler's gamma function, and write $\mathit{\Gamma}$ in slanted typeface for congruence subgroups (to be introduced in Sect. 2.3).

The studies of the Bessel moments $\mathbf{IKM}(1,4;1)$ and $\mathbf{IKM}(2,3;1)$ had been initiated by Bailey–Borwein–Broadhurst–Glasser [1, §5]. Back in 2008, it was analytically confirmed that

$$\mathbf{IKM}(2,3;1)=\frac{\sqrt{15}\pi}{2}C \tag{18}$$

where

$$C=\frac{1}{240\sqrt{5}\pi^2}\Gamma\left(\frac{1}{15}\right)\Gamma\left(\frac{2}{15}\right)\Gamma\left(\frac{4}{15}\right)\Gamma\left(\frac{8}{15}\right) \tag{19}$$

is the *Bologna constant* attributed to Broadhurst [1, 16] and Laporta [36]. Later on, it was realized that (18) can be rewritten as $\mathbf{IKM}(2,3;1)=\frac{3}{4}L(f_{3,15},2)=\frac{3\pi}{2\sqrt{15}}L(f_{3,15},1)$ [13, (96)–(97)], thanks to the work of Rogers–Wan–Zucker [41, Theorem 5]. An innocent-looking conjecture $\mathbf{IKM}(1,4;1)=\frac{2\pi}{\sqrt{15}}\mathbf{IKM}(2,3;1)$ was proposed in 2008 [1, (95)], but was not resolved until Bloch–Kerr–Vanhove carried out a *tour de force* in motivic cohomology during 2015 [3], and Samart elucidated the computations of special gamma values in 2016 [42]. We have recently simplified [52, Theorem 2.2.2] the result of Bloch–Kerr–Vanhove and Samart, as stated in the theorem below.

Theorem 3 (3-loop sunrise via Bologna constant) *We have*

$$\mathbf{IKM}(1,4;1)=\pi^2C=\frac{\pi^2}{5}L(f_{3,15},1)=\frac{3\pi}{2\sqrt{15}}L(f_{3,15},2). \tag{20}$$

Based on a discussion with Francis Brown at Les Houches in 2010, and encouraged by a result of Zhiwei Yun published in 2015 [47], David Broadhurst discovered some relations between $\mathbf{IKM}(a,6-a;1)$ and $L(f_{4,6},s)$ [13, §7.3], as well as between $\mathbf{IKM}(a,8-a;1)$ and $L(f_{6,6},s)$ [13, §7.6]. All these conjectures have been verified recently [52, §§4–5], so they are included in the theorem below.

Theorem 4 (Critical L-values for 6-Bessel and 8-Bessel problems)

(a) We have

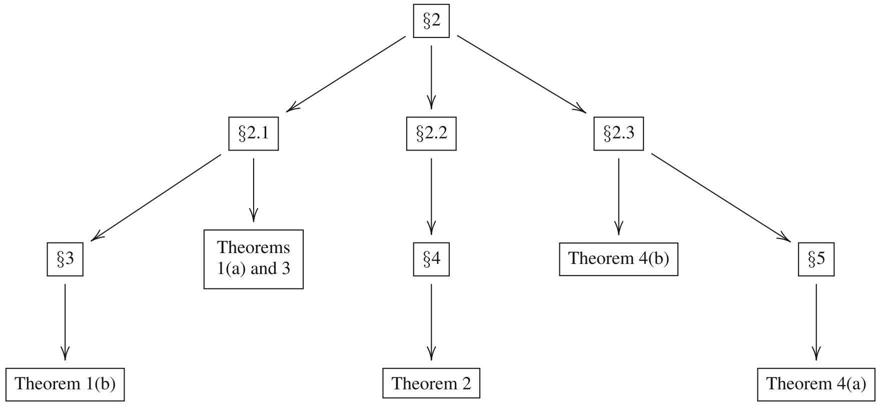
$$\frac{3}{\pi^2}\mathbf{IKM}(1,5;1)=\mathbf{IKM}(3,3;1)=\frac{3}{2}L(f_{4,6},2), \tag{21}$$

$$\mathbf{IKM}(2,4;1)=\frac{\pi^2}{2}L(f_{4,6},1)=\frac{3}{2}L(f_{4,6},3), \tag{22}$$

where the first equality in (21) comes from Theorem 1(a), and the last equality in (22) descends from (17).

(b) We have

Table 1 Organizational chart



$$\mathbf{IKM}(4,4;1)=L(f_{6,6},3), \tag{23}$$

$$\frac{1}{\pi^2}\mathbf{IKM}(1,7;1)=\mathbf{IKM}(3,5;1)=\frac{9}{4}L(f_{6,6},4), \tag{24}$$

$$\mathbf{IKM}(2,6;1)=\frac{27}{4}L(f_{6,6},5), \tag{25}$$

where the first equality in (24) *follows from Theorem 1(a),*

1.4 Plan of Proofs

To help our readers navigate through this survey, we present the *Leitfaden* in Table 1.

In Sect. 2.1, we begin with a summary of useful analytic properties for Bessel functions, which result in a proof of Theorem 1(a). We then present Wick rotations, which are special contour deformations connecting moment problems for $\mathbf{IKM}(a, b; n)$ to those for

$$\mathbf{JYM}(\alpha,\beta;n):=\int_0^\infty [J_0(t)]^\alpha [Y_0(t)]^\beta t^n \mathrm{d}t, \tag{26}$$

where $a+b=\alpha+\beta$, and $J_0(x):=\frac{2}{\pi}\int_0^{\pi/2}\cos(x\cos\varphi)\mathrm{d}\varphi$, $Y_0(x):=-\frac{2}{\pi}\int_0^\infty \cos(x\cosh u)\mathrm{d}u$ are Bessel functions of the zeroth order, defined for $x>0$. The **JYM** problems have some desirable properties [6, 51], which lead us to a quick proof of Theorem 3. Further applications of Wick rotations are given in Sect. 3, in the context of Theorem 1.

In Sect. 2.2, we give a brief overview of Vanhove's differential equations [44, §9], and compute certain Wrońskian determinants involving Bessel moments. These preparations allow us to present the main ideas behind the proof of Theorem 2, in Sect. 4.

In Sect. 2.3, we describe how to obtain critical L-values via integrations over products of certain modular forms, illustrating our general procedures with the proof of Theorem 4(b). Some extensions in Sect. 5 then lead to a sketched proof of all the statements in Theorem 4.

In Sect. 6, we wrap up this survey with some open questions on Bessel moments.

2 Toolkit

2.1 Wick Rotations of Bessel Moments

As we may recall, for $\nu \in \mathbb{C}$, $-\pi < \arg z < \pi$, the Bessel functions J_ν and Y_ν are defined by

$$J_\nu(z) := \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(k+\nu+1)} \left(\frac{z}{2}\right)^{2k+\nu}, \quad Y_\nu(z) := \lim_{\mu\to\nu} \frac{J_\mu(z)\cos(\mu\pi) - J_{-\mu}(z)}{\sin(\mu\pi)}, \tag{27}$$

which may be compared to the modified Bessel functions I_ν and K_ν:

$$I_\nu(z) := \sum_{k=0}^{\infty} \frac{1}{k!\Gamma(k+\nu+1)} \left(\frac{z}{2}\right)^{2k+\nu}, \quad K_\nu(z) := \frac{\pi}{2} \lim_{\mu\to\nu} \frac{I_{-\mu}(z) - I_\mu(z)}{\sin(\mu\pi)}. \tag{28}$$

Here, the fractional powers of complex numbers are defined through $w^\beta = \exp(\beta \log w)$ for $\log w = \log|w| + i \arg w$, where $|\arg w| < \pi$.

The cylindrical Hankel functions $H_0^{(1)}(z) = J_0(z) + iY_0(z)$ and $H_0^{(2)}(z) = J_0(z) - iY_0(z)$ are both well defined for $-\pi < \arg z < \pi$. In view of (27) and (28), we can verify

$$J_0(ix) = I_0(x) \quad \text{and} \quad \frac{\pi i}{2} H_0^{(1)}(ix) = K_0(x) \tag{29}$$

along with

$$H_0^{(1)}(\pm x + i0^+) = \pm J_0(x) + iY_0(x) \tag{30}$$

for $x > 0$.

As $|z| \to \infty$, $-\pi < \arg z < \pi$, we have the following asymptotic expansions [46, §7.2]:

$$\begin{cases} H_0^{(1)}(z) = \sqrt{\dfrac{2}{\pi z}} e^{i\left(z-\frac{\pi}{4}\right)} \left\{1 + \sum_{n=1}^{N} \dfrac{\left[\Gamma\left(n+\frac{1}{2}\right)\right]^2}{(2iz)^n \pi n!} + O\left(\dfrac{1}{|z|^{N+1}}\right)\right\}, \\ H_0^{(2)}(z) = \sqrt{\dfrac{2}{\pi z}} e^{i\left(\frac{\pi}{4}-z\right)} \left\{1 + \sum_{n=1}^{N} \dfrac{\left[\Gamma\left(n+\frac{1}{2}\right)\right]^2}{(-2iz)^n \pi n!} + O\left(\dfrac{1}{|z|^{N+1}}\right)\right\}, \end{cases} \tag{31}$$

which allow us to establish a vanishing identity

$$\int_{-i\infty}^{i\infty} [H_0^{(1)}(z) H_0^{(2)}(z)]^m z^n \mathrm{d}z = 0, \quad n \in \mathbb{Z} \cap [0, m-1) \tag{32}$$

by closing the contour rightwards. One can transcribe the last vanishing integral into the statements in Theorem 1(a), bearing in mind that

$$H_0^{(1)}(it) H_0^{(2)}(it) = \frac{4K_0(|t|)}{\pi^2} \left[K_0(|t|) - \frac{\pi i t}{|t|} I_0(|t|)\right], \quad \forall t \in (-\infty, 0) \cup (0, \infty). \tag{33}$$

Lemma 1 (An application of Wick rotation) *We have the following relation between* **IKM** *and* **JYM***:*

$$\left(\frac{2}{\pi}\right)^4 \mathbf{IKM}(1, 4; 1) = -\mathbf{JYM}(5, 0; 1) + 6\mathbf{JYM}(3, 2; 1) - \mathbf{JYM}(1, 4; 1). \tag{34}$$

Proof From (29), we know that

$$\left(\frac{2}{\pi}\right)^4 \mathbf{IKM}(1, 4; 1) = -\mathrm{Re} \int_0^{i\infty} J_0(z) [H_0^{(1)}(z)]^4 z \mathrm{d}z, \tag{35}$$

where the contour runs along the positive $\mathrm{Im}\, z$-axis.

Noting that the asymptotic behavior of $J_0(z) = [H_0^{(1)}(z) + H_0^{(2)}(z)]/2$ can be inferred from (31), we can rotate the contour 90° clockwise, from the positive $\mathrm{Im}\, z$-axis to the positive $\mathrm{Re}\, z$-axis (see Fig. 1a), thereby equating (35) with

$$-\mathrm{Re} \int_0^{\infty} J_0(x) [H_0^{(1)}(x)]^4 x \mathrm{d}x = -\mathrm{Re} \int_0^{\infty} J_0(x) [J_0(x) + iY_0(x)]^4 x \mathrm{d}x, \tag{36}$$

hence the right-hand side of (34). □

Proposition 1 (Evaluation of **IKM**(1, 4; 1)) *We have*

$$\mathbf{IKM}(1, 4; 1) = \frac{\pi^4}{30} \mathbf{JYM}(5, 0; 1) = \pi^2 C, \tag{37}$$

where C is the Bologna constant defined in (19).

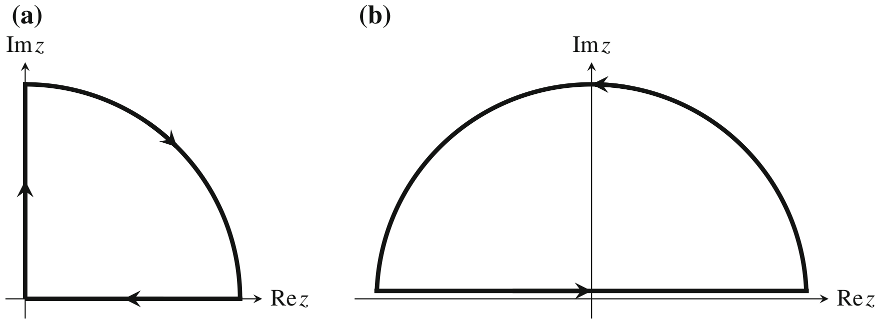


Fig. 1 **a** Wick rotation that turns an **IKM** to a sum of several **JYM**'s. Note that the contribution from the circular arc tends to zero as $|z| \to \infty$, thanks to Jordan's lemma being applicable to the asymptotic behavior of Hankel functions. **b** Contour of integration that leads to a cancelation formula for **JYM**'s

Proof For $\ell, m, n \in \mathbb{Z}_{\geq 0}$ satisfying either $\ell - (m+n)/2 < 0$; $m < n$ or $\ell - m = \ell - n < -1$, we can prove

$$\int_{i0^+-\infty}^{i0^++\infty} [J_0(z)]^m [H_0^{(1)}(z)]^n z^\ell \mathrm{d}z := \lim_{\varepsilon\to 0^+} \lim_{R\to\infty} \int_{i\varepsilon-R}^{i\varepsilon+R} [J_0(z)]^m [H_0^{(1)}(z)]^n z^\ell \mathrm{d}z = 0, \tag{38}$$

by considering the contour in Fig. 1b. According to (30) and $J_0(-x) = J_0(x)$, we may reformulate (38) as

$$\int_0^\infty [J_0(x)]^m \left\{[J_0(x) + iY_0(x)]^n + (-1)^\ell[-J_0(x) + iY_0(x)]^n\right\} x^\ell \mathrm{d}x = 0, \tag{38$'$}$$

which is a convenient cancelation formula for **JYM**'s.

With $J(J^4-6J^2Y^2+Y^4) - \frac{2J^2}{3}[(J+iY)^3 - (-J+iY)^3] - \frac{(J+iY)^5-(-J+iY)^5}{10} = -\frac{8J^5}{15}$ in hand, we can identify the right-hand side of (34) with $\frac{8}{15}$**JYM**$(5, 0; 1)$. This proves the first equality in (37). The second equality can be directly deduced from [6, (5.2)]. □

So far, we have recapitulated an analytic proof of Theorem 3, as originally given in [52, §2]. It is worth pointing out that Kluyver's function [35]

$$p_n(x) = \int_0^\infty J_0(xt)[J_0(t)]^n xt\mathrm{d}t \tag{39}$$

characterizes the probability density of the distance x traveled by a rambler, who walks in the Euclidean plane, taking n consecutive steps of unit lengths, aiming at uniformly distributed random directions. The analytic properties of such probability densities have been extensively studied [5–8, 49]. Recently, we have shown

Table 2 The first few Vanhove differential operators (abridged from [44, §9, Table 1])

n	$\widetilde{L}_n$
1	$u(u-4)D^1+(u-2)D^0$
2	$u(u-1)(u-9)D^2+(3u^2-20u+9)D^1+(u-3)D^0$
3	$u^2(u-4)(u-16)D^3+6u(u^2-15u+32)D^2+(7u^2-68u+64)D^1+(u-4)D^0$
4	$u^2(u-1)(u-9)(u-25)D^4+2u(5u^3-140u^2+777u-450)D^3+(25u^3-518u^2+1839u-450)D^2+(3u-5)(5u-57)D^1+(u-5)D^0$

[49, Theorem 5.1] that $p_n(x)$ is expressible through Feynman diagrams when n is odd, as stated in the theorem below.

Theorem 5 ($p_{2j+1}(x)$ as Feynman diagrams) *For each $j\in\mathbb{Z}_{>1}$, the function $p_{2j+1}(x)$, $0\le x\le 1$ is a unique $\mathbb{Q}$-linear combination of*

$$\int_0^\infty I_0(xt)[I_0(t)]^{2m+1}\left[\frac{K_0(t)}{\pi}\right]^{2(j-m)}xt\mathrm{d}t,\quad \textit{where } m\in\mathbb{Z}\cap\left[0,\frac{j-1}{2}\right].\tag{40}$$

(When $j=1$, the same is true for $0\le x<1$.)

2.2 Vanhove's Differential Equations and Wrońskians of Bessel Moments

In [44, §9], Vanhove has constructed nth order differential operators $\widetilde{L}_n$ (written in the variable u in this survey) so that the relation

$$\widetilde{L}_n\int_0^\infty I_0(\sqrt{u}t)[K_0(t)]^{n+1}t\mathrm{d}t=\text{const}\tag{41}$$

holds for all $n\in\mathbb{Z}_{>0}$ and $u\in(0,(n+1)^2)$. The first few Vanhove operators $\widetilde{L}_n$ are listed in Table 2, where $D^n=\partial^n/\partial u^n$ for $n\in\mathbb{Z}_{>0}$ and D^0 is the identity operator.

In general, for each $n\in\mathbb{Z}_{\ge1}$, Vanhove's operator $\widetilde{L}_n$ satisfies

$$\begin{cases} t\widetilde{L}_nI_0(\sqrt{u}t)=\frac{(-1)^n}{2^n}L^*_{n+2}\frac{I_0(\sqrt{u}t)}{t},\\ t\widetilde{L}_nK_0(\sqrt{u}t)=\frac{(-1)^n}{2^n}L^*_{n+2}\frac{K_0(\sqrt{u}t)}{t},\end{cases}\tag{42}$$

where L^*_{n+2} is the formal adjoint to the Borwein–Salvy operator L_{n+2} [4], the latter of which is the $(n+1)$-st symmetric power of the Bessel differential operator $(t\partial/\partial t)^2-t^2$ that annihilates both $I_0(t)$ and $K_0(t)$. Using the Bronstein–Mulders–Weil algorithm [19] for symmetric powers, we have shown [53, Lemma 4.2] that the following homogeneous differential equations

$$\widetilde{L}_n\left[\int_0^\infty I_0(\sqrt{u}t)[K_0(t)]^{n+1}t\mathrm{d}t+(n+1)\int_0^\infty K_0(\sqrt{u}t)I_0(t)[K_0(t)]^n t\mathrm{d}t\right]=0, \tag{43}$$

$$\widetilde{L}_n\int_0^\infty I_0(\sqrt{u}t)[I_0(t)]^{j-1}[K_0(t)]^{n+2-j}t\mathrm{d}t=0,\quad\forall j\in\mathbb{Z}\cap\left[2,\frac{n}{2}+1\right], \tag{44}$$

$$\widetilde{L}_n\int_0^\infty K_0(\sqrt{u}t)[I_0(t)]^{j}[K_0(t)]^{n+1-j}t\mathrm{d}t=0,\quad\forall j\in\mathbb{Z}\cap\left[2,\frac{n+1}{2}\right] \tag{45}$$

hold for $u\in(0,1)$.

For $N\in\mathbb{Z}_{>1}$, we write $W[f_1(u),\dots,f_N(u)]$ for the Wrońskian determinant $\det(D^{i-1}f_j(u))_{1\le i,j\le N}$. In [53, §4.1], we have constructed some Wrońskians as precursors to Broadhurst–Mellit determinants $\det\mathbf{M}_k$ and $\det\mathbf{N}_k$ (see Theorem 2). Concretely speaking, for each $k\in\mathbb{Z}_{\ge2}$, we set

$$\begin{cases}\mu_{k,1}^{\ell}(u)=\frac{1}{2k+1}\int_0^\infty\{I_0(\sqrt{u}t)K_0(t)+2kK_0(\sqrt{u}t)I_0(t)\}[K_0(t)]^{2k-1}t^{2\ell-1}\mathrm{d}t,\\ \mu_{k,j}^{\ell}(u)=\int_0^\infty I_0(\sqrt{u}t)[I_0(t)]^{j-1}[K_0(t)]^{2k+1-j}t^{2\ell-1}\mathrm{d}t,\forall j\in\mathbb{Z}\cap[2,k],\\ \mu_{k,j}^{\ell}(u)=\int_0^\infty K_0(\sqrt{u}t)[I_0(t)]^{j-k+1}[K_0(t)]^{3k-1-j}t^{2\ell-1}\mathrm{d}t,\forall j\in\mathbb{Z}\cap[k+1,2k-1],\end{cases} \tag{46}$$

and

$$\begin{cases}\nu_{k,1}^{\ell}(u)=\frac{1}{2(k+1)}\int_0^\infty\{I_0(\sqrt{u}t)K_0(t)+(2k+1)K_0(\sqrt{u}t)I_0(t)\}[K_0(t)]^{2k}t^{2\ell-1}\mathrm{d}t,\\ \nu_{k,j}^{\ell}(u)=\int_0^\infty I_0(\sqrt{u}t)[I_0(t)]^{j-1}[K_0(t)]^{2k+2-j}t^{2\ell-1}\mathrm{d}t,\forall j\in\mathbb{Z}\cap[2,k+1],\\ \nu_{k,j}^{\ell}(u)=\int_0^\infty K_0(\sqrt{u}t)[I_0(t)]^{j-k}[K_0(t)]^{3k+1-j}t^{2\ell-1}\mathrm{d}t,\forall j\in\mathbb{Z}\cap[k+2,2k],\end{cases} \tag{47}$$

and consider the Wrońskian determinants $\Omega_{2k-1}(u):=W[\mu_{k,1}^1(u),\dots,\mu_{k,2k-1}^1(u)]$, $\omega_{2k}(u):=W[\nu_{k,1}^1(u),\dots,\nu_{k,2k}^1(u)]$. For $k\in\mathbb{Z}_{\ge2}$, Vanhove's operators $\widetilde{L}_{2k-1}$ and $\widetilde{L}_{2k}$ take the following forms [44, (9.11)–(9.12)]:

$$\widetilde{L}_{2k-1}=\mathfrak{m}_{2k-1}(u)D^{2k-1}+\frac{2k-1}{2}\frac{\mathrm{d}\mathfrak{m}_{2k-1}(u)}{\mathrm{d}u}D^{2k-2}+L.O.T., \tag{48}$$

$$\widetilde{L}_{2k}=\mathfrak{n}_{2k}(u)D^{2k}+k\frac{\mathrm{d}\mathfrak{n}_{2k}(u)}{\mathrm{d}u}D^{2k-1}+L.O.T., \tag{49}$$

where

$$\mathfrak{m}_{2k-1}(u)=u^k\prod_{j=1}^{k}[u-(2j)^2],\quad\mathfrak{n}_{2k}(u)=u^k\prod_{j=1}^{k+1}[u-(2j-1)^2], \tag{50}$$

and "$L.O.T.$" stands for "lower order terms". Therefore, we have the following evolution equations for Wrońskians:

$$D^1\Omega_{2k-1}(u)=\frac{2k-1}{2}\Omega_{2k-1}(u)D^1\log\frac{1}{u^k\prod_{j=1}^{k}[(2j)^2-u]},\tag{51}$$

$$D^1\omega_{2k}(u)=k\omega_{2k}(u)D^1\log\frac{1}{u^k\prod_{j=1}^{k+1}[(2j-1)^2-u]},\tag{52}$$

where $0<u<1$. These differential equations will play crucial rôles in the proof of Theorem 2 in Sect. 4.

2.3 Modular Forms and Their Integrations

Let

$$\varGamma_0(N):=\left\{\left.\begin{pmatrix}a&b\\c&d\end{pmatrix}\right|a,b,c,d\in\mathbb{Z};ad-bc=1;c\equiv0\,(\operatorname{mod}N)\right\}\tag{53}$$

be the Hecke congruence group of level $N\in\mathbb{Z}_{>0}$. For a given Dirichlet character χ, a modular form $M_{k,N}(z)$ of weight k, level N and multiplier χ is a holomorphic[2] function that transforms like[3]

$$M_{k,N}\left(\frac{az+b}{cz+d}\right)=(cz+d)^k\chi(d)M_{k,N}(z),\tag{54}$$

where $\left(\begin{smallmatrix}a&b\\c&d\end{smallmatrix}\right)$ runs over all the members of $\varGamma_0(N)$, and z is an arbitrary point in the upper half-plane $\mathfrak{H}:=\{w\in\mathbb{C}|\operatorname{Im}w>0\}$. Modular forms of weight 0 (relaxing the requirement on holomorphy at cusps) are called modular functions. These $\varGamma_0(N)$-invariant modular functions are effectively defined on the moduli space $Y_0(N)(\mathbb{C})=\varGamma_0(N)\backslash\mathfrak{H}$ (see Fig. 2) for isomorphism classes of complex elliptic curves.

Following the notation of Chan–Zudilin [20], we write $\hat{W}_3=\frac{1}{\sqrt{3}}\left(\begin{smallmatrix}3&-2\\6&-3\end{smallmatrix}\right)$ and construct a group $\varGamma_0(6)_{+3}=\langle\varGamma_0(6),\hat{W}_3\rangle$ by adjoining $\hat{W}_3$ to $\varGamma_0(6)$. This group is of particular importance to the following motivic integral [3, §2]:

$$\begin{aligned}&\int_0^\infty I_0(\sqrt{u}t)[K_0(t)]^4t\,\mathrm{d}t\\&=\frac18\int_0^\infty\frac{\mathrm{d}X}{X}\int_0^\infty\frac{\mathrm{d}Y}{Y}\int_0^\infty\frac{\mathrm{d}Z}{Z}\frac{1}{(1+X+Y+Z)\left(1+\frac1X+\frac1Y+\frac1Z\right)-u}.\end{aligned}\tag{55}$$

[2]For technical requirements on holomorphy at $i\infty$ (more precisely, the $\varGamma_0(N)$ images of $i\infty$, namely, the cusps $\varGamma_0(N)\backslash\mathbb{P}^1(\mathbb{Q})=\varGamma_0(N)\backslash(\mathbb{Q}\cup\{i\infty\})$), see [23, Definition 1.2.3].

[3]For the modular forms $f_{4,6}(z)$ in (14) and $f_{6,6}(z)$ in (15), the multiplier is the trivial Dirichlet character $\chi(d)\equiv1$. For the modular form $f_{3,15}(z)$ in (13), we have $\chi(d)=\left(\frac{d}{15}\right)$ [38, Proposition 5.1], where the Dirichlet character is defined through a Jacobi–Kronecker symbol.

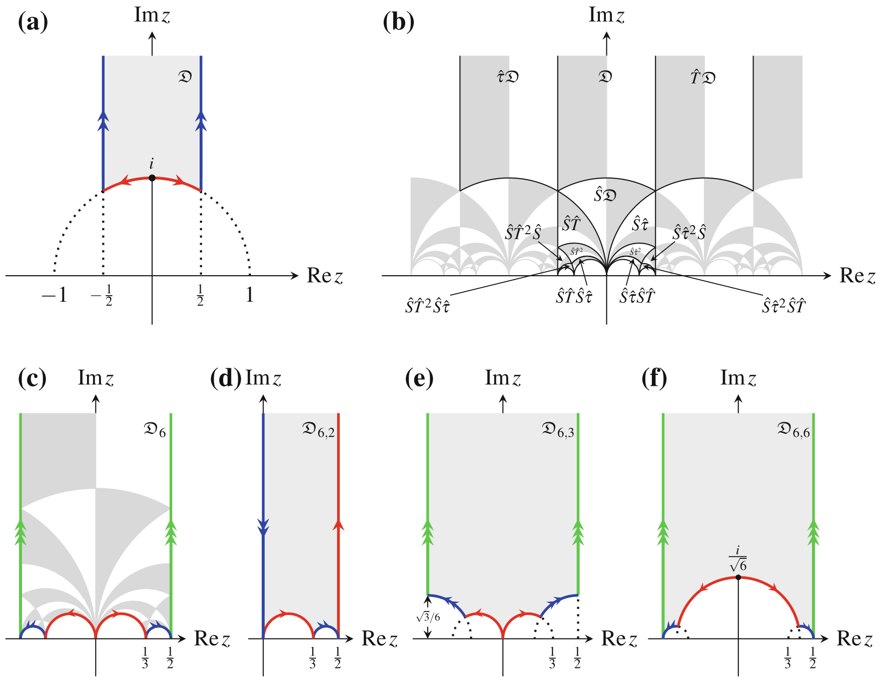


Fig. 2 (Adapted from [26, Fig. 61].) **a** Fundamental domain $\mathfrak{D}$ of $\varGamma_0(1) = SL(2,\mathbb{Z})$. The moduli space $Y_0(1)(\mathbb{C}) = SL(2,\mathbb{Z})\backslash\mathfrak{H}$ is a quotient space of $\mathfrak{D}$ that identifies the corresponding sides of the boundary $\partial\mathfrak{D}$ along the *arrows*. **b** Tessellation of the upper half-plane $\mathfrak{H}$ by successive translations [generator $\hat{T} = \hat{\tau}^{-1} : z \mapsto z+1$] and inversions [generator $\hat{S} = \hat{S}^{-1} : z \mapsto -1/z$] of the fundamental domain $\mathfrak{D}$. Each tile is subdivided and painted in *gray* or *white* according as the pre-image satisfies $\operatorname{Re} z < 0$ or $\operatorname{Re} z > 0$ in the fundamental domain $\mathfrak{D}$. **c** Fundamental domain $\mathfrak{D}_6$ of $\varGamma_0(6)$, dissected with $SL(2,\mathbb{Z})$-tiles (cf. panel **b**). Gluing the three pairs of boundary sides of $\mathfrak{D}_6$ along the *arrows*, one obtains the moduli space $Y_0(6)(\mathbb{C}) = \varGamma_0(6)\backslash\mathfrak{H}$. **d**–**f** Fundamental domains $\mathfrak{D}_{6,k}$ for the Chan–Zudilin groups $\varGamma_0(6)_{+k} = \langle \varGamma_0(6), \hat{W}_k \rangle$, where $\hat{W}_2 z = (2z-1)/(6z-2)$, $\hat{W}_3 z = (3z-2)/(6z-3)$, and $\hat{W}_6 z = -1/(6z)$

As pointed out in Verrill's thesis [45, Theorems 1 and 2], the differential equation $\widetilde{L}_3 f(u) = 0$ (cf. Table 2) is the Picard–Fuchs equation for a pencil of $K3$ surfaces:

$$\mathscr{X}_{A_3} : (1+X+Y+Z)\left(1+\frac{1}{X}+\frac{1}{Y}+\frac{1}{Z}\right) = u, \tag{56}$$

whose monodromy group is isomorphic to $\overline{\varGamma_0(6)_{+3}}$, the image of $\varGamma_0(6)_{+3}$ after quotienting out by scalars. As a consequence, the general solutions to $\widetilde{L}_3 f(u) = 0$ admit a modular parametrization

$$f(u) = Z_{6,3}(z)(c_0 + c_1 z + c_2 z^2), \tag{57}$$

where $c_0, c_1, c_2 \in \mathbb{C}$ are constants, and

$$u = -64X_{6,3}(z) := -\left[\frac{2\eta(2z)\eta(6z)}{\eta(z)\eta(3z)}\right]^6, \tag{58}$$

$$Z_{6,3}(z) := \frac{[\eta(z)\eta(3z)]^4}{[\eta(2z)\eta(6z)]^2}. \tag{59}$$

Here, $X_{6,3}(z)$ is a modular function on $\varGamma_0(6)_{+3}$ [20, (2.2)], while $Z_{6,3}(z)$ is a modular form of weight 2 and level 6 [20, (2.5)].

Since $\int_0^\infty J_0(\sqrt{-u}t)I_0(t)[K_0(t)]^3 t\mathrm{d}t$ is annihilated by Vanhove's operator $\widetilde{L}_3$, we can establish the following modular parametrization

$$\int_0^\infty J_0\left(8\sqrt{X_{6,3}(z)}t\right) I_0(t)[K_0(t)]^3 t\mathrm{d}t = \frac{\pi^2}{16} Z_{6,3}(z) \tag{60}$$

through asymptotic analysis of both sides near the infinite cusp $z \to i\infty$ [whereupon the left-hand side tends to $\int_0^\infty I_0(t)[K_0(t)]^3 t\mathrm{d}t = \mathbf{IKM}(1, 3; 1)$ and the right-hand side tends to $\frac{\pi^2}{16} = \mathbf{IKM}(1, 3; 1)$]. Here, the positive $\operatorname{Im} z$-axis corresponds to $\sqrt{-u} = 8\sqrt{X_{6,3}(z)} \in (0, \infty)$. In a similar fashion, one can show that

$$\int_0^\infty J_0\left(8\sqrt{X_{6,3}(z)}t\right) [I_0(t)]^2[K_0(t)]^2 t\mathrm{d}t = \frac{\pi z}{4i} Z_{6,3}(z) \tag{61}$$

holds for $z/i > 0$. Now, we can prove Theorem 4(b) by throwing (60)–(61) into the Parseval–Plancherel identity for Hankel transforms [1, (16)]

$$\int_0^\infty f(t)g(t)t\mathrm{d}t = \int_0^\infty \left[\int_0^\infty J_0(xt)f(t)t\mathrm{d}t\right]\left[\int_0^\infty J_0(x\tau)g(\tau)\tau\mathrm{d}\tau\right]x\mathrm{d}x, \tag{62}$$

and noting that [52, Theorem 5.1.1]

$$[Z_{6,3}(z)]^2 \frac{\mathrm{d}X_{6,3}(z)}{\mathrm{d}z} = 2\pi i f_{6,6}(z). \tag{63}$$

Actually, we can say a little more about the 8-Bessel problem than what has been stated in Theorem 4(b). With heavy use of Wick rotations and integrations of $f_{6,6}(z)z^n$, $n \in \{0, 1, 2, 3, 4\}$ over the boundary $\partial\mathfrak{D}_{6,3}$ of the fundamental domain $\mathfrak{D}_{6,3}$ (Fig. 2e), one may show that [52, §5]

$$\frac{L(f_{6,6}, 5)}{L(f_{6,6}, 3)} = \frac{2\pi^2}{21}. \tag{64}$$

Comparing this to Theorem 4(b), one confirms a sum rule $9\pi^2\mathbf{IKM}(4, 4; 1) = 14\mathbf{IKM}(2, 6; 1)$, which was originally proposed in 2008 [1, at the end of §6.3, between (228) and (229)].

3 Some Linear Sum Rules of Feynman Diagrams

The contour integral in (32) is no longer convergent when $n \in \mathbb{Z} \cap [m, \infty)$, so the methods in Sect. 2.1 do not directly apply to Theorem 1(b), which involves Bessel moments $\mathbf{IKM}(a, b; n)$ with high orders $n \geq (a + b - 2)/2$. In [48, §3], I used a real-analytic approach (based on Hilbert transforms), to circumvent divergent contour integrals while handling Theorem 1(b). After email exchanges with Mark van Hoeij on Oct. 24, 2017, about the asymptotic expansion of $[I_0(x)K_0(x)]^4$ for large and positive x (see van Hoeij's update on [43], dated Oct. 23, 2017), I realized that the divergence problem in the complex-analytic approach can be amended by subtracting Laurent polynomials from $[H_0^{(1)}(z)H_0^{(2)}(z)]^m$. This amendment is described in the lemma below.

Lemma 2 (Asymptotic expansions and Bessel moments) *We have the following asymptotic expansion as* $|z| \to \infty$, $-\pi < \arg z < \pi$*:*

$$\begin{aligned}&\left(\frac{\pi}{2}\right)^{2m}[H_0^{(1)}(z)H_0^{(2)}(z)]^m\\&=\sum_{n=1}^{N}\frac{(-1)^{n+1}}{z^{2n+m-2}}\int_0^\infty\frac{[\pi I_0(t)+iK_0(t)]^m-[\pi I_0(t)-iK_0(t)]^m}{\pi i}[K_0(t)]^m t^{2n+m-3}\mathrm{d}t\\&\quad+O\left(\frac{1}{|z|^{2N+m}}\right),\end{aligned}\tag{65}$$

where $m, N \in \mathbb{Z}_{>0}$.

Proof From (31), we know that as $|z| \to \infty$, $-\pi < \arg z < \pi$, there exist certain constant coefficients $a_{m,n}$ such that the following relation holds:

$$F_{m,N}(z) := [H_0^{(1)}(z)H_0^{(2)}(z)]^m - \sum_{n=1}^{N}\frac{a_{m,n}}{z^{2n+m-2}} = O\left(\frac{1}{|z|^{2N+m}}\right).\tag{66}$$

To determine $a_{m,N}$, we consider

$$\lim_{\varepsilon\to0^+}\lim_{T\to\infty}\left(\int_{-iT}^{-i\varepsilon}+\int_{C_\varepsilon}+\int_{i\varepsilon}^{iT}\right)F_{m,N}(z)z^{2N+m-3}\mathrm{d}z,\tag{67}$$

where C_ε is a semi-circular arc in the right half-plane, joining $-i\varepsilon$ to $i\varepsilon$. For each fixed $\varepsilon > 0$, the contour integral in question tends to zero, as $T \to \infty$, because we can close the contour to the right. Recalling (33), and integrating the Laurent polynomial over C_ε, we arrive at the claimed result. □

Before moving onto the proof of Theorem 1(b) in the next proposition, we point out that one can also generalize the method in the last lemma into other cancelation formulae. For example, in [50, Lemma 3.3], we used a vanishing contour integral

$$\lim_{T\to\infty}\int_{-iT}^{iT} H_0^{(1)}(z)H_0^{(2)}(z)\left\{[H_0^{(1)}(z)H_0^{(2)}(z)]^2-\frac{4}{\pi^2 z^2}\right\}z^3\mathrm{d}z=0 \tag{68}$$

to prove

$$\int_0^\infty I_0(t)[K_0(t)]^5t^3\mathrm{d}t=\frac{\pi^2}{3}\int_0^\infty I_0(t)K_0(t)\left\{[I_0(t)]^2[K_0(t)]^2-\frac{1}{4t^2}\right\}t^3\mathrm{d}t, \tag{69}$$

which paved way for the verification of a conjecture [50, (1.11)] due to Laporta [37, (29)] and Broadhurst (private communication on Nov. 10, 2017).

Thanks to van Hoeij's observation that led to Lemma 2, we see that the expression $C_{m,n}$ in (7) evaluates to a rational number [cf. (31)], and these sequences of rational numbers satisfy a discrete convolution relation with respect to the power m. To show that $C_{m,n}$ is in fact a positive integer, it now suffices to prove that, for each $\ell\in\mathbb{Z}_{>0}$,

$$C_{1,\ell}=\frac{[(2\ell-2)!]^3}{2^{2\ell-2}[(\ell-1)!]^4}=[(2\ell-3)!!]^2\binom{2\ell-2}{\ell-1} \tag{70}$$

and

$$C_{2,\ell}=\frac{1}{2^{4(\ell-1)}}\sum_{k=1}^{\ell}\frac{[(2\ell-2k)!]^3}{[(\ell-k)!]^4}\frac{[(2k-2)!]^3}{[(k-1)!]^4} \tag{71}$$

are both integers. Here, we have $\binom{n}{k}:=\frac{n!}{k!(n-k)!}\in\mathbb{Z}$ for $n\in\mathbb{Z}_{\geq0}$, $k\in\mathbb{Z}\cap[0,n]$, and $(2n-1)!!:=(2n)!/(n!2^n)\in\mathbb{Z}$ for $n\in\mathbb{Z}_{\geq0}$, so the statement $C_{1,\ell}\in\mathbb{Z}$ holds true. The integrality of $C_{2,\ell}$ will be explained below.

Proposition 2 (An integer sequence) *For each $\ell\in\mathbb{Z}_{>0}$, the number $\alpha_\ell:=C_{2,\ell}$ is a positive integer.*

Proof In [40, Theorem 3.1], Mathew Rogers has effectively shown that the following identity holds for $|u|$ sufficiently small:

$$\sum_{\ell=1}^{\infty}\frac{\alpha_{\ell+1}-\ell^2\alpha_\ell}{(\ell!)^2}u^\ell=3\sum_{n=1}^{\infty}[(2n-1)!!]^2\binom{3n-1}{2n}\frac{1}{(n!2^n)^2}\frac{u^{2n}}{(1-u)^{3n}}. \tag{72}$$

Comparing the coefficients of u^n on both sides, we see that, for each $n\in\mathbb{Z}_{>0}$, the expression $\alpha_{n+1}-n^2\alpha_n$ equals a sum of finitely many terms, each of which is an integer multiple of $(k!!)^2\in\mathbb{Z}$ for a certain odd positive integer k less than n. Therefore, we have $\alpha_1=1$, $\alpha_{\ell+1}-\ell^2\alpha_\ell\in\mathbb{Z}$ for $\ell\in\mathbb{Z}_{>0}$, which entails the claimed result. □

4 Some Non-linear Sum Rules of Feynman Diagrams

As we did in Sect. 3, we will build non-linear sum rules of Feynman diagrams without evaluating individual Bessel moments in closed form. In what follows, we describe a key step towards the proof of Broadhurst–Mellit determinant formulae (Theorem 2), namely, the asymptotic analysis of the Wrońskians $\varOmega_{2k-1}(u)$ and $\omega_{2k}(u)$ introduced in Sect. 2.2.

As in [53, §4], we differentiate (46) with respect to u and define

$$\acute{\mu}^{\ell}_{k,j}(u) := 2\sqrt{u}D^1\mu^{\ell}_{k,j}(u), \quad \forall j \in \mathbb{Z}\cap[1,2k-1]. \tag{73}$$

Through iterated applications of the Bessel differential equations $(uD^2 + D^1)$ $I_0(\sqrt{u}t) = \frac{t^2}{4}I_0(\sqrt{u}t)$ and $(uD^2 + D^1)K_0(\sqrt{u}t) = \frac{t^2}{4}K_0(\sqrt{u}t)$, we can verify

$$(2\sqrt{u})^{(k-1)(2k-1)}\varOmega_{2k-1}(u) = \det\begin{pmatrix} \mu^1_{k,1}(u) & \cdots & \mu^1_{k,2k-1}(u) \\ \acute{\mu}^1_{k,1}(u) & \cdots & \acute{\mu}^1_{k,2k-1}(u) \\ \cdots & \cdots & \cdots \\ \mu^k_{k,1}(u) & \cdots & \mu^k_{k,2k-1}(u) \end{pmatrix}, \tag{74}$$

where the μ (resp. $\acute{\mu}$) terms occupy the odd-numbered (resp. even-numbered) rows. Since $W[I_0(u), K_0(u)] = -I_0(u)K_1(u) - K_0(u)I_1(u) = -1/u$, we can show that

$$\begin{cases} \mu^{\ell}_{k,j}(1) = \mu^{\ell}_{k,k+j-1}(1), \\ \acute{\mu}^{\ell}_{k,k+j-1}(1) - \acute{\mu}^{\ell}_{k,j}(1) = -\mu^{\ell}_{k-1,j-1}(1) \end{cases} \tag{75}$$

for all $j \in \mathbb{Z}\cap[2,k]$. Thus, we obtain, after column eliminations and row bubble sorts,

$$\begin{aligned} & 2^{(k-1)(2k-1)}\varOmega_{2k-1}(1) \\ &= \det\begin{pmatrix} \mu^1_{k,1}(1) \cdots \mu^1_{k,k}(1) & 0 & \cdots & 0 \\ \acute{\mu}^1_{k,1}(1) \cdots \acute{\mu}^1_{k,k}(1) & -\mu^1_{k-1,1}(1) & \cdots & -\mu^1_{k-1,k-1}(1) \\ \cdots\cdots\cdots & \cdots & \cdots & \cdots \\ \mu^k_{k,1}(1) \cdots \mu^k_{k,k}(1) & 0 & \cdots & 0 \end{pmatrix} \\ &= (-1)^{\frac{k(k-1)}{2}} \det\left(\begin{array}{c|c} \mathbf{M}_k^{\mathrm{T}} & \mathbf{O} \\ \hline \begin{matrix} \acute{\mu}^1_{k,1}(1) & \cdots & \acute{\mu}^1_{k,k}(1) \\ \cdots & \cdots & \cdots \\ \acute{\mu}^{k-1}_{k,1}(1) & \cdots & \acute{\mu}^{k-1}_{k,k}(1) \end{matrix} & -\mathbf{M}_{k-1}^{\mathrm{T}} \end{array}\right), \end{aligned} \tag{76}$$

which factorizes into

$$\Omega_{2k-1}(1)=(-1)^{\frac{(k-1)(k-2)}{2}}\frac{\det\mathbf{M}_{k-1}}{2^{(k-1)(2k-1)}}\det\mathbf{M}_k \tag{77}$$

for each $k\in\mathbb{Z}_{\geq 2}$. By a similar procedure (see [53, Proposition 4.4] for detailed asymptotic analysis), one can show that

$$\lim_{u\to 0^+}u^{k(2k-1)/2}\Omega_{2k-1}(u)=(-1)^{\frac{(k-1)(k-2)}{2}}\frac{k[\Gamma(k/2)]^2}{(2k+1)}\frac{(\det\mathbf{N}_{k-1})^2}{2^{(k-1)(2k-1)+1}}. \tag{78}$$

Consequently, the evolution equation in (51) admits a solution

$$\Omega_{2k-1}(u)=\frac{(-1)^{\frac{(k-1)(k-2)}{2}}k[\Gamma(k/2)]^2}{u^{k(2k-1)/2}(2k+1)}\frac{(\det\mathbf{N}_{k-1})^2}{2^{(k-1)(2k-1)+1}}\prod_{j=1}^{k}\left[\frac{(2j)^2}{(2j)^2-u}\right]^{k-\frac{1}{2}} \tag{79}$$

for $u\in(0,1]$.

Comparing (77) and (79), we arrive at

$$\det\mathbf{M}_{k-1}\det\mathbf{M}_k=\frac{k[\Gamma(k/2)]^2(\det\mathbf{N}_{k-1})^2}{2(2k+1)}\prod_{j=1}^{k}\left[\frac{(2j)^2}{(2j)^2-1}\right]^{k-\frac{1}{2}}, \tag{80}$$

for all $k\in\mathbb{Z}_{\geq 2}$. A similar service [53, §4.3] on $\omega_{2k}(u)$ then brings us

$$\det\mathbf{N}_{k-1}\det\mathbf{N}_k=\frac{2k+1}{k+1}\frac{(\det\mathbf{M}_k)^2}{(k-1)!}\prod_{j=2}^{k+1}\left[\frac{(2j-1)^2}{(2j-1)^2-1}\right]^{k}. \tag{81}$$

The last pair of equations, together with the initial conditions $\det\mathbf{M}_1=\mathbf{IKM}(1,2;1)=\frac{\pi}{3\sqrt{3}}$ [1, (23)] and $\det\mathbf{N}_1=\mathbf{IKM}(1,3;1)=\frac{\pi^2}{2^4}$ [1, (55)], allow us to prove Theorem 2 by induction.

As a by-product, we see from (79) that $\Omega_{2k-1}(u)=W[\mu^1_{k,1}(u),\dots,\mu^1_{k,2k-1}(u)]$ is non-vanishing for $u\in(0,1]$. Therefore, the functions $\mu^1_{k,1}(u),\dots,\mu^1_{k,2k-1}(u)$ (restricted to the interval $(0,1]$) form a basis for the kernel space of $\widetilde{L}_{2k-1}$. Consequently, for each $k\in\mathbb{Z}_{\geq 2}$, the function $p_{2k}(\sqrt{u})/\sqrt{u}$, $0<u\leq 1$ (where $p_{2k}(x)=\int_0^\infty J_0(xt)[J_0(t)]^{2k}xt\,\mathrm{d}t$ is Kluyver's probability density) is an $\mathbb{R}$-linear combination of the functions $\mu^1_{k,1}(u),\dots,\mu^1_{k,2k-1}(u)$. Unlike our statement in Theorem 5, where the Bessel moment representation of $p_{2j+1}(x)$, $j\in\mathbb{Z}_{\geq 2}$ leaves a convergent Taylor expansion for $0\leq x\leq 1$, the representation of $p_{2k}(x)$, $0\leq x\leq 1$ through a linear combination of Bessel moments may involve $O(x\log x)$ singularities in the $x\to 0^+$ regime, attributable to the Bessel function K_0. Such logarithmic singularities had been previously studied by Borwein–Straub–Wan–Zudilin [6].

5 Critical Values of Modular L-Functions and Multi-loop Feynman Diagrams

As in the proof of Theorem 4(b) in Sect. 2.3, we need to fuse Hankel transforms in the Parseval–Plancherel identity to prove (22).

Fusing the following Hankel transform (cf. [52, (4.1.16)])

$$\int_0^\infty J_0\left(\frac{3[\eta(w)]^2[\eta(6w)]^4}{[\eta(3w)]^2[\eta(2w)]^4}it\right)I_0(t)[K_0(t)]^2t\mathrm{d}t=\frac{\pi}{3\sqrt{3}}\frac{\eta(3w)[\eta(2w)]^6}{[\eta(w)]^3[\eta(6w)]^2} \tag{82}$$

(where $w=\frac{1}{2}+iy$, $y>0$ corresponds to $0<\frac{3[\eta(w)]^2[\eta(6w)]^4}{[\eta(3w)]^2[\eta(2w)]^4}i<\infty$) with itself, we obtain (cf. [52, Proposition 4.2.1])

$$\mathbf{IKM}(2,4;1)=\frac{\pi^3 i}{3}\int_{\frac{1}{2}}^{\frac{1}{2}+i\infty}f_{4,6}(w)\mathrm{d}w. \tag{83}$$

This is not quite the statement in (22) yet, as the integration path still sits on the "wrong" portion of $\partial\mathfrak{D}_{6,2}$ (Fig. 2d). To compensate for this, we need another Hankel fusion, together with some modular transforms on the Chan–Zudilin group $\varGamma_0(6)_{+2}$, to construct an identity [52, Proposition 4.2.2]:

$$\mathbf{JYM}(6,0;1)=\frac{12}{\pi i}\int_0^{i\infty}f_{4,6}(w)\mathrm{d}w-\frac{6}{\pi i}\int_{\frac{1}{2}}^{\frac{1}{2}+i\infty}f_{4,6}(w)\mathrm{d}w. \tag{84}$$

Now that Wick rotation brings us $\mathbf{IKM}(2,4;1)=\frac{\pi^4}{30}\mathbf{JYM}(6,0;1)$ [52, (4.1.1)], we can deduce (22) from the last two displayed equations.

It takes slightly more effort to verify (21). Towards this end, we need a "Hilbert cancelation formula" [52, Lemma 4.2.4]

$$\int_0^\infty\left[\int_0^\infty J_0(xt)F(t)t\mathrm{d}t\right]\left[\int_0^\infty Y_0(x\tau)F(\tau)\tau\mathrm{d}\tau\right]x\mathrm{d}x=0 \tag{85}$$

for functions $F(t), t>0$ satisfying certain growth bounds, along with modular parametrizations of some generalized Hankel transforms, such as (cf. [52, (4.1.31)])

$$\begin{aligned}&\int_0^\infty J_0\left(\frac{3[\eta(w)]^2[\eta(6w)]^4}{[\eta(3w)]^2[\eta(2w)]^4}it\right)[K_0(t)]^3t\mathrm{d}t\\&-\frac{3\pi}{2}\int_0^\infty Y_0\left(\frac{3[\eta(w)]^2[\eta(6w)]^4}{[\eta(3w)]^2[\eta(2w)]^4}it\right)I_0(t)[K_0(t)]^2t\mathrm{d}t\\=&\frac{\pi^2(2w-1)}{2\sqrt{3}i}\frac{\eta(3w)[\eta(2w)]^6}{[\eta(w)]^3[\eta(6w)]^2}\end{aligned} \tag{86}$$

for $w=\frac{1}{2}+iy$, $y>0$. We refer our readers to [52, Proposition 4.1.3 and Theorem 4.2.5] for detailed computations that lead to (21).

6 Outlook

6.1 Broadhurst's p-adic Heuristics

In Sect. 1.3, the modular forms $f_{3,15}$, $f_{4,6}$ and $f_{6,6}$ were not picked randomly, but were discovered by Broadhurst via some deep insights into p-adic analysis and étale cohomology [21, 32]. In short, Broadhurst's computations of Bessel moments over finite fields led him to local factors in the Hasse–Weil zeta functions, which piece together into the modular L-functions, namely, $L(f_{3,15}, s)$ for the 5-Bessel problem, $L(f_{4,6}, s)$ for the 6-Bessel problem, and $L(f_{6,6}, s)$ for the 8-Bessel problem.

On the arithmetic side, Broadhurst investigated Kloosterman moments ("Bessel moments over finite fields"), with extensive numerical experiments [13, §§2–6]. A Bessel function over a finite field [39], with respect to the variable $a \in \mathbb{F}_q = \mathbb{F}_{p^k}$, is defined by the following Kloosterman sum:

$$\mathrm{Kl}_2(\mathbb{F}_{p^k}, a) := \sum_{x_1,x_2\in\mathbb{F}_q^\times, x_1x_2=a} e^{\frac{2\pi i}{p}\mathrm{Tr}_{\mathbb{F}_q/\mathbb{F}_p}(x_1+x_2)} = \sum_{x\in\mathbb{F}_q^\times} e^{\frac{2\pi i}{p}\mathrm{Tr}_{\mathbb{F}_q/\mathbb{F}_p}\left(x+\frac{a}{x}\right)} \tag{87}$$

where the Frobenius trace $\mathrm{Tr}_{\mathbb{F}_q/\mathbb{F}_p}$ acts on an element $z \in \mathbb{F}_q$ as $\mathrm{Tr}_{\mathbb{F}_q/\mathbb{F}_p}(z) := \sum_{j=0}^{k-1} z^{p^j}$. Writing $\mathrm{Kl}_2(\mathbb{F}_{p^k}, a) = -\alpha_a - \beta_a$ where $\alpha_a\beta_a = q$, and introducing the n-th symmetric power $\mathrm{Kl}_2^n := \mathrm{Sym}^n(\mathrm{Kl}_2)$ as $\mathrm{Kl}_2^n(\mathbb{F}_{p^k}, a) := \sum_{j=0}^n \alpha_a^j\beta_a^{n-j}$, we may further define Bessel moments over a finite field as the following Kloosterman moments:

$$S_n(q) := \sum_{a\in\mathbb{F}_q^\times} \mathrm{Kl}_2^n(\mathbb{F}_{p^k}, a) = \sum_{a\in\mathbb{F}_q^\times}\sum_{j=0}^n \alpha_a^j\beta_a^{n-j}. \tag{88}$$

With $c_n(q) = -\frac{1+S_n(q)}{q^2}$ for a prime power $q = p^k$, one defines the Hasse–Weil local factor by a formula

$$Z_n(p, T) := \exp\left(-\sum_{k=0}^\infty \frac{c_n(p^k)}{k}T^k\right). \tag{89}$$

Following the notations of Fu–Wan [28], we set $L_p(\mathbb{P}^1_{\mathbb{F}_p} \smallsetminus \{0, \infty\}, \mathrm{Sym}^n(\mathrm{Kl}_2), s) = 1/Z_n(p, p^{-s})$, and define the Hasse–Weil zeta function

$$\zeta_{n,1}(s) := \prod_p L_p(\mathbb{P}^1_{\mathbb{F}_p} \smallsetminus \{0, \infty\}, \mathrm{Sym}^n(\mathrm{Kl}_2), s) = \prod_p \frac{1}{Z_n(p, p^{-s})}, \tag{90}$$

where the product runs over all the primes. It is known that $\zeta_{5,1}(s) = L(f_{3,15}, s)$ [38] and $\zeta_{6,1}(s) = L(f_{4,6}, s)$ [34]. The structure of $\zeta_{7,1}(s)$, which involves a Hecke eigenform of weight 3 and level 525, had been conjectured by Evans [25, Conjecture 1.1], before being completely verified by Yun [47, §4.7.7]. The story for the 8-Bessel problem is much more convoluted (see [47, Theorem 4.6.1 and Appendix B] as well as [13, §7.6]).

On the geometric side, Broadhurst's L-functions $L(f_{3,15}, s)$ and $L(f_{4,6}, s)$ are closely related to the étale cohomologies of certain Calabi–Yau manifolds. Concretely speaking, one may regard the 4-loop sunrise [quadruple integral in (2)] as a motivic integral over the Barth–Nieto quintic variety [2, 30, 34], which is defined through a complete intersection

$$N := \left\{ [u_0 : u_1 : u_2 : u_3 : u_4 : u_5] \in \mathbb{P}^5 \left| \sum_{k=0}^{5} u_k = \sum_{k=0}^{5} \frac{1}{u_k} = 0 \right.\right\}. \tag{91}$$

The projective variety N has a smooth Calabi–Yau model Y. Its third étale cohomology group $H^3_{\text{ét}}(Y)$ is related to 2-dimensional representations of $\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$ [34, §3], so that for each prime $p \geq 5$, one has $L_p(H^3_{\text{ét}}(Y), s) = [1 - a_p(Y)p^{-s} + p^{3-2s}]^{-1}$ for

$$a_p(Y) = \mathrm{tr}(\mathrm{Frob}_p^*, H^3_{\text{ét}}(Y)) = 1 + 50p + 50p^2 + p^3 - \#Y(\mathbb{F}_p), \tag{92}$$

where $\#Y(\mathbb{F}_p)$ counts the number of points within Y over the finite field $\mathbb{F}_p$. The modular L-function $L(f_{4,6}, s)$ coincides with $L(H^3_{\text{ét}}(Y), s) = \prod_p L_p(H^3_{\text{ét}}(Y), s)$ for all the local factors $L_p(\cdot, s)$ corresponding to primes $p \geq 5$ and $\mathrm{Re}\, s$ sufficiently large. A similar p-adic reinterpretation for $L(f_{3,15}, s)$ also exists. Let A_n be the Fourier coefficient in $f_{3,15}(z) = \sum_{n=1}^{\infty} A_n e^{2\pi i n z}$, and $\left(\frac{p}{3}\right)$ be the Legendre symbol for a prime p other than 3 and 5, then [38, Theorem 5.3]

$$1 + p^2 + p\left(16 + 4\left(\frac{p}{3}\right)\right) + A_p \tag{93}$$

counts the number of $\mathbb{F}_p$-rational points of a $K3$ surface that is the minimal resolution of singularities of

$$\left\{ [u_0 : u_1 : u_2 : u_3 : u_4] \in \mathbb{P}^4 \left| \sum_{k=0}^{4} u_k = \sum_{k=0}^{4} \frac{1}{u_k} = 0 \right.\right\}. \tag{94}$$

Behind the aforementioned results on p-adic Bessel moments is a long and heroic tradition of algebraic geometry. Back in the 1970s, building upon the theories of Dwork [24] and Grothendieck [32, 33], Deligne interpreted Hasse–Weil L-functions as Fredholm determinants of Frobenius maps [22, (1.5.4)]. This tradition has been continued by Robba [39], Fu–Wan [27–29] and Yun [47], in their studies of p-adic Bessel functions and Kloosterman sheaves.

While Broadhurst's p-adic heuristics give strong hints that $L(f_{3,15}, s)$, $L(f_{4,6}, s)$ and $L(f_{6,6}, s)$ are appropriate mathematical models for 5-, 6- and 8-Bessel problems, our proofs of Theorems 3 and 4 described in this survey do not touch upon the p-adic structure. It is perhaps worthwhile to rework these proofs from the Hasse–Weil perspective, using local-global correspondence. We call for this effort because there are still many conjectures of Broadhurst (see Sect. 6.2 for a partial list) that go beyond the reach of this survey, but might appear tractable to specialists in p-adic analysis and étale cohomology.

6.2 Open Questions

There are three outstanding problems involving 5-, 6- and 8-Bessel factors, originally formulated by Broadhurst–Mellit [17, (4.3), (5.8), (7.15)] and Broadhurst [13, (101), (114), (160)].

Conjecture 1 (Broadhurst–Mellit) *The following determinant formulae hold:*

$$\det\begin{pmatrix}\mathbf{IKM}(0,5;1) & \mathbf{IKM}(0,5;3)\\ \mathbf{IKM}(2,3;1) & \mathbf{IKM}(2,3;3)\end{pmatrix} \overset{?}{=} \frac{45}{8\pi^2}L(f_{3,15},4), \tag{95}$$

$$\det\begin{pmatrix}\mathbf{IKM}(0,6;1) & \mathbf{IKM}(0,6;3)\\ \mathbf{IKM}(2,4;1) & \mathbf{IKM}(2,4;3)\end{pmatrix} \overset{?}{=} \frac{27}{4\pi^2}L(f_{4,6},5), \tag{96}$$

$$\det\begin{pmatrix}\mathbf{IKM}(0,8;1) & \mathbf{IKM}(0,8;3)-2\mathbf{IKM}(0,8;5)\\ \mathbf{IKM}(2,6;1) & \mathbf{IKM}(2,6;3)-2\mathbf{IKM}(2,6;5)\end{pmatrix} \overset{?}{=} \frac{6075}{128\pi^2}L(f_{6,6},7). \tag{97}$$

Here, one might wish to compare the last conjectural determinant evaluation to the following proven result:

$$\begin{aligned}\frac{5\pi^8}{2^{19}3} = \det\mathbf{N}_3 &= \det\begin{pmatrix}\mathbf{IKM}(1,7;1) & \mathbf{IKM}(1,7;3) & \mathbf{IKM}(1,7;5)\\ \mathbf{IKM}(2,6;1) & \mathbf{IKM}(2,6;3) & \mathbf{IKM}(2,6;5)\\ \mathbf{IKM}(3,5;1) & \mathbf{IKM}(3,5;3) & \mathbf{IKM}(3,5;5)\end{pmatrix}\\ &= \frac{\pi^2}{2^8}\det\begin{pmatrix}\mathbf{IKM}(1,7;1) & \mathbf{IKM}(1,7;3)-2\mathbf{IKM}(1,7;5)\\ \mathbf{IKM}(2,6;1) & \mathbf{IKM}(2,6;3)-2\mathbf{IKM}(2,6;5)\end{pmatrix}.\end{aligned} \tag{98}$$

To arrive at the last step, we have used the Crandall number relations [Theorem 1(b)] $\mathbf{IKM}(3,5;1)-\frac{\mathbf{IKM}(1,7;1)}{\pi^2}=0$, $\mathbf{IKM}(3,5;3)-\frac{\mathbf{IKM}(1,7;3)}{\pi^2}=\frac{\pi^2}{2^7}$, $\mathbf{IKM}(3,5;5)-\frac{\mathbf{IKM}(1,7;5)}{\pi^2}=\frac{\pi^2}{2^8}$, along with row and column eliminations.

The special L-values $L(f_{k,N},s)$ in Conjecture 1 all lie outside the critical strip $0<\operatorname{Re}s<k$, so they do not yield to the methods given in Sect. 2.3 or Sect. 5.

Working with Anton Mellit at Mainz, David Broadhurst has discovered a numerical connection (see [17, (6.8)] or [13, (129)]) between $\zeta_{7,1}(s)=\prod_p\frac{1}{Z_7(p,p^{-s})}$ and the 7-Bessel problem, which still awaits a proof.

Conjecture 2 (Broadhurst–Mellit) *We have*

$$\mathbf{IKM}(2,5;1) \overset{?}{=} \frac{5\pi^2}{24}\zeta_{7,1}(2). \tag{99}$$

In a recent collaboration with David Roberts [9–12, 14], David Broadhurst has discovered a lot more empirical formulae relating determinants of Bessel moments to special values of Hasse–Weil L-functions, which are outside the scope of the current exposition. Nevertheless, we believe that one day such determinant formulae will reveal deep p-adic structures of Bessel moments, as foreshadowed by pioneering works on Hasse–Weil L-functions and Fredholm determinants for Frobenius maps [22, 27–29, 34, 38, 39, 47].

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