

GENERALIZED POLYLOGARITHMS IN
PERTURBATIVE QUANTUM FIELD THEORY

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Introduction

The Standard Model (SM) of particle physics settled into its current form in the 1970s and has since proved a resounding success. A large array of precision measurements has confirmed SM predictions, in some cases to an astounding degree. For example, the theoretical and experimental values for the anomalous magnetic dipole moment of the electron agree to better than one part in a billion. Furthermore, with the recent discovery of the Higgs boson at the Large Hadron Collider (LHC) at CERN, the entire particle content of the SM has now been observed.

The guiding principles that govern the structure of the SM are the presence of a continuous local internal symmetry, known as gauge symmetry, and renormalizability, which guarantees that the theory will have predictive power. Together these principles highly constrain the set of operators that may appear in the SM Lagrangian. In fact, except for a few unresolved subtleties, these principles uniquely determine the form of the Lagrangian, provided that the fundamental fields and their internal symmetries are specified.

The matter content of the SM consists of three generations of up- and down-type quarks, three generations of charged and uncharged leptons, and the Higgs boson. Additionally, there are gauge bosons that mediate the three forces. The gauge group of the SM is the Lie group $SU(3)_C \times SU(2)_L \times U(1)_Y$, where $SU(3)_C$ is the color symmetry of Quantum Chromodynamics (QCD), and $SU(2)_L \times U(1)_Y$ is the electroweak symmetry, which is spontaneously broken to a single $U(1)_{\text{EM}}$ by the Higgs mechanism.

Despite the great success of the SM, it is almost certainly not the entire story. At the very least, it must be augmented to account for nonzero neutrino masses.

It has not yet been determined if neutrinos have Dirac or Majorana masses, but in either case the adjustments to the SM are essentially cosmetic. A more substantive modification of the SM will be necessary to account for the presence of dark matter. Furthermore, explaining other cosmological observations like dark energy and baryon asymmetry require additional modifications of the SM.

The SM also suffers from various internal deficiencies not rooted in experimental measurements. For example, the Higgs mass receives large quantum corrections that must cancel against its bare mass to very high precision. What is the reason for this large degree of fine-tuning? Moreover, the SM does not offer an explanation for why the θ angle in QCD should be small or zero, which it must be in order to agree with the fact that no CP violation has been observed in pure QCD. There are many other open questions concerning particular values of parameters in the SM. Why are the neutrino masses so small? Why is the top quark mass so large? Do the gauge couplings unify at some energy scale?

Answering questions like these is an important driving force in high-energy physics research. Currently there are not many answers, but the large supply of unresolved questions is a clear indication that the SM is not a complete theory. This last statement represents the seeds of a paradigm shift that has resulted in the modern viewpoint that the SM should be thought of as an effective field theory, valid up to some energy scale Λ , above which new physics effects must be included. From this perspective, renormalizability is no longer considered strictly necessary because there is a physical cutoff, Λ , that regulates any potential ultraviolet (UV) divergences. Relaxing the renormalizability constraint opens the door for a large number of new operators and a corresponding set of new phenomena awaiting detection.

On the other hand, there is no indication that the other main guiding principle in the formulation of the SM — gauge symmetry — is anything but a fundamental property of the universe. To the extent that quantum field theory is a good description of nature, it is widely believed that any inadequacies of the SM can be resolved by adding new particles and interactions that entirely respect the principles of gauge symmetry. Of course, any theory of particle physics must ultimately be reconciled with gravity and the theory of general relativity. Even still, there is no reason to

suspect that the principles of gauge theories should be abandoned. In fact, gauge theories play an important role in string theory, as they are intimately related to D-brane geometry.

With this in mind, it is not surprising that the vast majority of recent research in quantum field theory has focused on gauge theories. Happily, an enormous amount of progress has been made across the wide spectrum of this research. Some of the most intriguing developments have been in the study of perturbative scattering amplitudes. A significant step forward came in 2003, when Witten discovered that a transformation of tree-level amplitudes into twistor space endows them with a simple geometrical description. This led to the introduction of MHV diagrams and subsequently to the Britto-Cachazo-Feng-Witten (BCFW) recursions relations, which exhibit an intricate iterative structure between scattering amplitudes with differing numbers of external particles.

The BCFW recursions relations are just one of several distinct types of recursion relations, including Berends-Giele, Cachazo, Svrcek, Witten (CSW), and Risager recursion relations. It has recently been argued that these various types of recursion relations may be understood as particular consequences of a larger structure based on the Grassmannian. In general, these recursion relations allow for extremely efficient computations of tree-level scattering amplitudes, giving access to results that previously seemed unattainable, owing to the very large number of Feynman diagrams required to compute them using conventional techniques.

One of the most striking features of these calculations has been the remarkable simplicity of the final results. In certain cases, this simplicity was anticipated. For example, the extremely compact form for maximally helicity-violating (MHV) amplitudes in pure Yang-Mills,

$$A_{\text{MHV}}(1^-, 2^+, \dots, j^-, \dots, n^+) = i(2\pi)^4 \delta^{(4)} \left(\sum_{i=1}^n \lambda_i^\alpha \tilde{\lambda}_i^{\dot{\alpha}} \right) \frac{\langle 1j \rangle^4}{\langle 12 \rangle \langle 23 \rangle \langle 34 \rangle \cdots \langle n1 \rangle}, \quad (0.0.1)$$

where $\langle ij \rangle = \lambda_i^\alpha \lambda_{j\alpha}$, was conjectured by Parke and Taylor in 1986. Generically, the introduction of matter fields complicates the structure of the resulting amplitudes. On

the other hand, if the additional matter is constrained by some symmetry principles, one might expect the results to maintain some simplicity. Indeed, as first observed by Nair, MHV amplitudes with maximal ($\mathcal{N} = 4$) supersymmetry are given by a simple generalization of the Parke-Taylor formula,

$$\mathcal{A}_{\text{MHV}}(\lambda, \tilde{\lambda}, \eta) = i(2\pi)^4 \frac{\delta^{(4)}\left(\sum_{i=1}^n \lambda_i^\alpha \tilde{\lambda}_i^{\dot{\alpha}}\right) \delta^{(8)}\left(\sum_{i=1}^n \lambda_i^a \eta_i^A\right)}{\langle 12 \rangle \langle 23 \rangle \langle 34 \rangle \cdots \langle n1 \rangle}, \quad (0.0.2)$$

where the Grassmann variables η keep track of the various constituents of the super-amplitude.

Owing to its high degree of symmetry, $\mathcal{N} = 4$ super Yang-Mills theory exhibits many extraordinary properties. It possesses a conformal symmetry that holds even at the quantum level. It has only two free parameters: the coupling $a = g_{YM}^2 N_c / (32\pi)^2$ and the number of colors N_c . In the planar limit of a large number colors, in which $N_c \rightarrow \infty$ with a held fixed, the coupling constant is the only parameter. For large values of the coupling, the AdS/CFT correspondence conjectures a duality to weakly-coupled type IIB string theory on the curved background $\text{AdS}_5 \times S^5$. Finally, many lines of reasoning suggest that the theory is integrable, and that an exact solution for the scattering matrix of the theory might be achievable, at least in the planar sector.

Another noteworthy property of $\mathcal{N} = 4$ super Yang-Mills is that the BCFW recursion relations may be generalized and extended to this maximally supersymmetric setting. Remarkably, these recursion relations were solved, yielding an explicit formulation for all tree-level scattering amplitudes in $\mathcal{N} = 4$ super Yang-Mills. The solution contains the solution for pure Yang-Mills theory as a special case, and has even been extended to the less-symmetric case of QCD.

So far we have only discussed tree-level amplitudes, but there has also been substantial progress in the understanding of loop amplitudes. A key technique is the unitarity method, which leverages the unitarity of the S matrix to express the imaginary part of a given loop amplitude in terms of products of lower-loop amplitudes. Indeed, writing $S = 1 + T$, the condition that $S^\dagger S = 1$ implies that $2 \text{Im } T = T^\dagger T$. Expanding this equation perturbatively yields the desired interpretation. The imaginary part is understood as the discontinuity across a branch cut, which may be

associated with any given momentum channel. By examining such “unitarity cuts” in all possible channels, it is possible to reconstruct the amplitude, at least up to contributions that have no branch cuts. These contributions are known as rational terms, and they must be fixed by other means, such as with recursion relations or d -dimensional unitarity cuts.

It is useful to generalize the unitarity method to include multi-particle cuts. Such cuts are not necessarily in physical momentum channels, and they cannot be related to the unitarity of the S matrix. Moreover, in order to reveal such cuts, it is necessary to consider complex external momenta. Nevertheless, this analysis exposes more fully the analytic properties of the scattering amplitude and can capture information to which the traditional unitarity method is insensitive.

A particularly enlightening calculation made possible by these techniques was the evaluation of the three-loop four-point scattering amplitude in $\mathcal{N} = 4$ super Yang-Mills. This computation revealed an iterative structure relating the three-loop contribution to the lower-loop contributions. This observation inspired an ansatz, known as the BDS ansatz, for the exponentiation of the full n -point MHV amplitude. It is generally true that for any gauge theory, the infrared (IR) divergences exponentiate; the content of the ansatz is that the finite pieces also exponentiate. This ansatz was subsequently confirmed for $n < 6$, but for more external particles it requires modification,

$$A_n^{\text{MHV}} = A_n^{\text{BDS}} \times \exp(R_n), \quad (0.0.3)$$

where the function R_n is known as the *remainder function*.

In constructing the integrand for the four-point amplitude at three and four loops, it was observed that the individual integrands all obey a conformal symmetry in a dual momentum space, whose coordinates x_i^μ are related to the original momenta k_i^μ by $k_i = x_i - x_{i+1}$. This dual conformal symmetry is completely distinct from the conformal symmetry of $\mathcal{N} = 4$ super Yang-Mills in position space. Moreover, it is only present at the level of the integrand, since IR divergences break the symmetry.

Meanwhile, using the AdS/CFT correspondence, an analysis at strong coupling confirmed the BDS ansatz at four points. The computation also used the change of

variables $k_i = x_i - x_{i+1}$, which was interpreted as a T-duality transformation on the string world-sheet. In terms of the variables x_i , the calculation proceeds in a manner very similar to that of the expectation value of a polygonal Wilson loop with vertices x_i . This observation motivated explicit computations at weak coupling, which, quite remarkably, supported the existence of a new duality in which n -particle scattering amplitudes are dual to n -sided Wilson loops. The coordinates of the Wilson loop are identified with the dual momentum variables x_i , and the UV divergences generated at the cusps of the Wilson loop correspond to the IR divergences of the amplitude.

In the Wilson loop setting, the breaking of conformal symmetry is a UV effect, and it is governed by an anomalous Ward identity. The most general solution to the Ward identity is given by the BDS ansatz times an arbitrary conformally invariant function. From the amplitude perspective, the Ward identity implies the validity of eq. (0.0.3), provided that the remainder function is dual-conformally invariant.

For the four- and five-gluon scattering amplitudes, the only dual-conformally invariant functions are constants, and because of this fact the BDS ansatz is exact and the remainder function vanishes to all loop orders, $R_4 = R_5 = 0$. For six-gluon amplitudes, dual conformal invariance restricts the functional dependence to have the form $R_6(u_1, u_2, u_3)$, where the u_i are the unique invariant cross ratios constructed from distances x_{ij}^2 in the dual space:

$$u_1 = \frac{x_{13}^2 x_{46}^2}{x_{14}^2 x_{36}^2} = \frac{s_{12} s_{45}}{s_{123} s_{345}}, \quad u_2 = \frac{x_{24}^2 x_{15}^2}{x_{25}^2 x_{14}^2} = \frac{s_{23} s_{56}}{s_{234} s_{456}}, \quad u_3 = \frac{x_{35}^2 x_{26}^2}{x_{36}^2 x_{25}^2} = \frac{s_{34} s_{61}}{s_{345} s_{561}}. \quad (0.0.4)$$

Furthermore $R_6(u_1, u_2, u_3)$ is not entirely arbitrary since, among other conditions, it must be totally symmetric under permutations of the u_i and vanish in the collinear limit [1, 2].

In the absence of an explicit computation, it remained a possibility that $R_6 = 0$, despite the fact that all known symmetries allow for a non-zero function $R_6(u_1, u_2, u_3)$. However, a series of calculations have since been performed and they showed definitively that $R_6 \neq 0$.

The first evidence of a non-vanishing remainder function came from an analysis at strong coupling, where a deviation from the BDS ansatz was found for a large number

of gluons [3]. Shortly afterwards, a computation of the hexagonal light-like Wilson loop at two loops indicated a breakdown of either the BDS ansatz or the Wilson loop/amplitude duality for six gluons [4]. The multi-Regge limits of $2 \rightarrow 4$ gluon scattering amplitudes at two loops suggested that it was the BDS ansatz that required corrections [5]. Numerical evidence at specific kinematic points showed definitively that R_6 was non-zero at two loops [1, 2], and an explicit calculation of R_6 at two loops for general kinematics eventually followed [6, 7].

The limit of multi-Regge kinematics (MRK) has received considerable attention in the context of $\mathcal{N} = 4$ super-Yang Mills theory [5, 8–20]. One reason for this is that multi-leg scattering amplitudes become considerably simpler in MRK while still maintaining a non-trivial analytic structure. Taking the multi-Regge limit at six points, for example, essentially reduces the amplitude to a function of just two variables, w and w^* , which are complex conjugates of each other. This latter point will play a prominent role in chapters 1 and 2, in which we study the six-point remainder function in MRK.

The remainder function captures all of the non-iterating structure of MHV scattering amplitudes in planar $\mathcal{N} = 4$ super Yang-Mills. For this reason, it has been the subject of considerable study, both at weak and strong coupling, and in general and specific kinematic regimes. Assuming the Wilson loop/amplitude duality, we present a calculation of R_6 at three loops for general kinematics in chapter 4 and at four loops for general kinematics in chapter 5. Like the vast majority of Feynman integrals calculated to date, the results can be expressed in terms of multiple polylogarithms.

Multiple polylogarithms are a general class of iterated integrals and are reviewed in appendix C.1. Ordinary logarithms, polylogarithms, Nielsen polylogarithms, and harmonic polylogarithms are all special cases of multiple polylogarithms. It is known that more complicated types of functions, such as elliptic functions, are necessary to describe Feynman integrals in general, but most phenomenologically relevant quantities do not require these exotic functions. In this thesis, we will be focusing on situations where such functions do not appear, though it would of course be interesting to investigate how our analysis might be generalized to include them.

A very useful tool for classifying polylogarithmic functions is the concept of transcendentality. The transcendental weight may be defined as the number of iterated integrations in a multiple polylogarithm. For example, the logarithm is generated by one integral over a rational function, and therefore has transcendental weight one; the dilogarithm requires two integrations and has weight two, etc. When these functions are evaluated at particular values, the resulting constants have the same weight as the original function. For example, the transcendentality of $i\pi = \log(-1)$ is one, and the transcendentality of $\zeta_n = \text{Li}_n(1)$ is n .

Every calculation so far indicates that $\mathcal{N} = 4$ super Yang-Mills obeys the principle of uniform maximal transcendentality. For example, at loop order ℓ , a scattering amplitude in $\mathcal{N} = 4$ super Yang-Mills is expected to be a homogeneous combination of transcendental functions of weight 2ℓ . This property is not obeyed by less symmetric theories, like QCD, for which results contain functions of mixed transcendental weight. In many cases, the maximal-transcendental piece of a QCD calculation is given precisely by the $\mathcal{N} = 4$ super Yang-Mills result. This can be taken as another motivation for studying $\mathcal{N} = 4$, since calculations might give some direct insight into QCD.

The observation that $\mathcal{N} = 4$ super Yang-Mills obeys the principle of maximal transcendentality, together with the conjecture that the MHV sector is free of elliptic integrals, provides a rough outline of the space of functions that might appear in a given ℓ -loop calculation: it should be a subset of the space of all multiple polylogarithms of weight 2ℓ . This space is infinitely large because we have not yet specified the variables upon which the multiple polylogarithms can depend. On the other hand, if we can somehow specify the variables, the space of functions will become finite and we can use it as a basis. The entire calculation would thereby reduce to a problem in linear algebra. The only task left is to construct a sufficiently large set of physical and mathematical constraints so as to fix the free coefficients of the basis. This is exactly the approach that we will pursue throughout this thesis.

We will consider two collections of computations, distinguished by the number of independent variables upon which the resulting polylogarithmic functions depend.

In Part I, we examine functions of two variables. As argued above, in the limit

of multi-Regge kinematics, the six-point remainder function depends on only two relevant variables, w and w^* , which are complex conjugates of one another. Moreover, we will argue in chapter 3 that the off-shell dual-conformal integrals also depend on just two similarly-defined variables, z and \bar{z} ; such integrals arise in the computation of the four-point correlation function of stress-tensor multiplets in $\mathcal{N} = 4$ super Yang-Mills.

In Part II, we consider functions of three variables. These functions are relevant for the study of conformal six-point integrals. In particular, they are sufficient to describe the six-point remainder function. In chapter 4, we complete the calculation of R_6 at three loops. The calculation is not direct, as it uses physical information from the Wilson loop/amplitude duality to help fix coefficients in the basis of multiple polylogarithms. We evaluate the function numerically on a variety of interesting one- and two-dimensional subspaces of the full three-dimensional space of cross ratios. Remarkably, the two- and three-loop remainder functions are quantitatively very similar (up to an overall multiplicative rescaling) for large swaths of parameter space, and only differ significantly in regions where the functions diverge at different rates. In chapter 5, we extend this analysis to four loops, computing first the symbol and then ultimately the full function. We evaluate the four-loop remainder function numerically on several one-dimensional subspaces and compare it to the functions at two- and three-loops, and, in one case, to a result at strong coupling. In all cases there is excellent qualitative agreement, and, up to an overall rescaling, the quantitative agreement observed at three loops continues to four loops as well.

Part I

Functions of two variables

Chapter 1

Single-valued harmonic polylogarithms and the multi-Regge limit

1.1 Introduction

Enormous progress has taken place recently in unraveling the properties of relativistic scattering amplitudes in four-dimensional gauge theories and gravity. Perhaps the most intriguing developments have been in maximally supersymmetric $\mathcal{N} = 4$ Yang-Mills theory, in the planar limit of a large number of colors. Many lines of evidence suggest that it should be possible to solve for the scattering amplitudes in this theory to all orders in perturbation theory. There are also semi-classical results based on the AdS/CFT duality to match to at strong coupling [21]. The scattering amplitudes in the planar theory can be expressed in terms of a set of dual (or region) variables x_i^μ , which are related to the usual external momentum four-vectors k_i^μ by $k_i = x_i - x_{i+1}$. Remarkably, the planar $\mathcal{N} = 4$ super-Yang-Mills amplitudes are governed by a dual conformal symmetry acting on the x_i [3, 21–26]. This symmetry can be extended to a dual superconformal symmetry [27], which acts on supermultiplets of amplitudes that are packaged together by using an $\mathcal{N} = 4$ on-shell superfield and associated Grassmann coordinates [28–31].

Due to infrared divergences, amplitudes are not invariant under dual conformal transformations. Rather, there is an anomaly, which was first understood in terms of polygonal Wilson loops rather than amplitudes [26]. (For such Wilson loops the anomaly is ultraviolet in nature.) A solution to the anomalous Ward identity for maximally-helicity violating (MHV) amplitudes is to write them in terms of the BDS ansatz [32],

$$A_n^{\text{MHV}} = A_n^{\text{BDS}} \times \exp(R_n), \quad (1.1.1)$$

where R_n is the so-called *remainder function* [1, 2, 2], which is fully dual-conformally invariant.

For the four- and five-gluon scattering amplitudes, the only dual-conformally invariant functions are constants, and because of this fact the BDS ansatz is exact and the remainder function vanishes to all loop orders, $R_4 = R_5 = 0$. For six-gluon amplitudes, dual conformal invariance restricts the functional dependence to have the form $R_6(u_1, u_2, u_3)$, where the u_i are the unique invariant cross ratios constructed from distances x_{ij}^2 in the dual space:

$$u_1 = \frac{x_{13}^2 x_{46}^2}{x_{14}^2 x_{36}^2} = \frac{s_{12} s_{45}}{s_{123} s_{345}}, \quad u_2 = \frac{x_{24}^2 x_{15}^2}{x_{25}^2 x_{14}^2} = \frac{s_{23} s_{56}}{s_{234} s_{456}}, \quad u_3 = \frac{x_{35}^2 x_{26}^2}{x_{36}^2 x_{25}^2} = \frac{s_{34} s_{61}}{s_{345} s_{561}} \quad (1.1.2)$$

The need for a nonzero remainder function R_n for Wilson loops was first indicated by the strong-coupling behavior of polygonal loops corresponding to amplitudes with a large number of gluons n [3]. At the six-point level, investigation of the multi-Regge limits of $2 \rightarrow 4$ gluon scattering amplitudes led to the conclusion that R_6 must be nonvanishing at two loops [5]. Numerical evidence was found soon thereafter for a nonvanishing two-loop coefficient $R_6^{(2)}$ for generic nonsingular kinematics [1, 2], in agreement with the numerical values found simultaneously for the corresponding hexagonal Wilson loop [2].

Based on the Wilson line representation [2], and using dual conformal invariance to take a quasi-multi-Regge limit and simplify the integrals, an analytic result for $R_6^{(2)}$ was derived [6, 7, 7] in terms of Goncharov's multiple polylogarithms [33]. Making use of properties of the *symbol* [34–37, 147] associated with iterated integrals, the analytic

result for $R_6^{(2)}$ was then simplified to just a few lines of classical polylogarithms [36].

A powerful constraint on the structure of the remainder function at higher loop order is provided by the operator product expansion (OPE) for polygonal Wilson loops [38–40]. At three loops, this constraint, together with symmetries, collinear vanishing, and an assumption about the final entry of the symbol, can be used to determine the symbol of $R_6^{(3)}$ up to just two constant parameters [14]. Another powerful technique for determining the remainder function is to exploit an infinite-dimensional Yangian invariance [41, 42] which includes the dual superconformal generators. These symmetries are anomalous at the loop level (or alternatively one can say that the algebra has to be deformed) [43]. However, the symmetries imply a first order linear differential equation for the ℓ -loop n -point amplitude, and the anomaly dictates the inhomogeneous term in the differential equation, in terms of an integral over an $(\ell - 1)$ -loop $(n + 1)$ -point amplitude [44, 45]. Using this differential equation, a number of interesting results were obtained in ref. [45]. In particular, the result for the symbol of $R_6^{(3)}$ found in ref. [14] was recovered and the two previously-undetermined constants were fixed.

In principle, the method of refs. [44, 45] works to arbitrary loop order. However, it requires knowing lower-loop amplitudes with an increasing number of external legs, for which the number of kinematic variables (the dual conformal cross ratios) steadily increases. Although the symbol of the two-loop remainder function $R_n^{(2)}$ is known for arbitrary n [46], the same is not true of the three-loop seven-point remainder function, which would feed into the four-loop six-point remainder function — one of the subjects of this paper.

In this article, we focus on features of the six-point kinematics that allow us to push directly to higher loop orders for this amplitude, without having to solve for amplitudes with more legs. In fact, most of our paper is concerned with a special limit of the kinematics in which we can make even more progress: multi-Regge kinematics (MRK), a limit which has already received considerable attention in the context of $\mathcal{N} = 4$ super-Yang-Mills theory [5, 8–10, 12–18]. In the MRK limit of $2 \rightarrow 4$ gluon scattering, the four outgoing gluons are widely-spaced in rapidity. In other words, two of the four gluons are emitted far forward, with almost the same energies and

directions of the two incoming gluons. The other two outgoing gluons are also well-separated from each other, and have smaller energies than the two far-forward gluons.

The MHV amplitude possesses a unique limit of this type. For definiteness, we will take legs 3 and 6 to be incoming, legs 1 and 2 to be the far-forward outgoing gluons, and legs 4 and 5 to be the other two outgoing gluons. Neglecting power-suppressed terms, helicity must be conserved along the high-energy lines. In the usual all-outgoing convention for labeling helicities, the helicity configuration can be taken to be $(++-+-)$. For generic $2 \rightarrow 4$ scattering in four dimensions there are eight kinematic variables. Dual conformal invariance reduces the eight variables down to just the three dual conformal cross ratios u_i . Taking the multi-Regge limit essentially reduces the amplitude to a function of just two variables, w and w^* , which turn out to be the complex conjugates of each other.

We will argue that the function space relevant for this limit has been completely characterized by Brown [47]. We call the functions *single-valued harmonic polylogarithms* (SVHPLs). They are built from the analytic functions of a single complex variable that are known as harmonic polylogarithms (HPLs) in the physics literature [48]. These functions have branch cuts at $w = 0$ and $w = -1$. However, bilinear combinations of HPLs in w and in w^* can be constructed [47] to cancel the branch cuts, so that the resulting functions are single-valued in the (w, w^*) plane. The single-valued property matches perfectly a physical constraint on the remainder function in the multi-Regge limit. SVHPLs, like HPLs, are equipped with an integer transcendental *weight*. The required weight increases with the loop order. However, at any given weight there is only a finite-dimensional vector space of available functions. Thus, once we have identified the proper function space, the problem of solving for the remainder function in MRK reduces simply to determining a set of rational numbers, namely the coefficients multiplying the allowed SVHPLs at a given weight.

In order to further appreciate the simplicity of the multi-Regge limit, we recall that for generic six-point kinematics there are nine possible choices for the entries in the symbol for the remainder function $R_6(u_1, u_2, u_3)$ [14, 36]:

$$\{u_1, u_2, u_3, 1 - u_1, 1 - u_2, 1 - u_3, y_1, y_2, y_3\}, \quad (1.1.3)$$

where

$$y_i = \frac{u_i - z_+}{u_i - z_-}, \quad (1.1.4)$$

$$z_{\pm} = \frac{-1 + u_1 + u_2 + u_3 \pm \Delta}{2}, \quad (1.1.5)$$

$$\Delta = (1 - u_1 - u_2 - u_3)^2 - 4u_1u_2u_3. \quad (1.1.6)$$

The first entry of the symbol is actually restricted to the set $\{u_1, u_2, u_3\}$ due to the location of the amplitude's branch cuts [40]; the integrability of the symbol restricts the second entry to the set $\{u_i, 1 - u_i\}$ [14, 40]; and a “final-entry condition” [14, 46] implies that there are only six, not nine, possibilities for the last entry. However, the remaining entries are unrestricted. The large number of possible entries, and the fact that the y_i variables are defined in terms of square-root functions of the cross ratios (although the u_i can be written as rational functions of the y_i [14]), complicates the task of identifying the proper function space for this problem.

So in this paper we will solve a simpler problem. The MRK limit consists of taking one of the u_i , say u_1 , to unity, and letting the other two cross ratios vanish at the same rate that $u_1 \rightarrow 1$: $u_2 \approx x(1 - u_1)$ and $u_3 \approx y(1 - u_1)$ for two fixed variables x and y . To reach the Minkowski version of the MRK limit, which is relevant for $2 \rightarrow 4$ scattering, it is necessary to analytically continue u_1 from the Euclidean region according to $u_1 \rightarrow e^{-2\pi i}|u_1|$, before taking this limit [5]. Although the square-root variables y_2 and y_3 remain nontrivial in the MRK limit, all of the square roots can be rationalized by a clever choice of variables [12]. We define w and w^* by

$$x \equiv \frac{1}{(1 + w)(1 + w^*)}, \quad y \equiv \frac{w w^*}{(1 + w)(1 + w^*)}. \quad (1.1.7)$$

Then the MRK limit of the other variables is

$$u_1 \rightarrow 1, \quad y_1 \rightarrow 1, \quad y_2 \rightarrow \tilde{y}_2 = \frac{1 + w^*}{1 + w}, \quad y_3 \rightarrow \tilde{y}_3 = \frac{(1 + w)w^*}{w(1 + w^*)}. \quad (1.1.8)$$

Neglecting terms that vanish like powers of $(1 - u_1)$, we expand the remainder function in the multi-Regge limit in terms of coefficients multiplying powers of the large

logarithm $\log(1 - u_1)$ at each loop order, following the conventions of ref. [14],

$$R_6(u_1, u_2, u_3)|_{\text{MRK}} = 2\pi i \sum_{\ell=2}^{\infty} \sum_{n=0}^{\ell-1} a^\ell \log^n(1 - u_1) \left[g_n^{(\ell)}(w, w^*) + 2\pi i h_n^{(\ell)}(w, w^*) \right], \quad (1.1.9)$$

where the coupling constant for planar $\mathcal{N} = 4$ super-Yang-Mills theory is $a = g^2 N_c / (8\pi^2)$.

The remainder function R_6 is a transcendental function with weight 2ℓ at loop order ℓ . Therefore the coefficient functions $g_n^{(\ell)}$ and $h_n^{(\ell)}$ have weight $2\ell - n - 1$ and $2\ell - n - 2$ respectively. As a consequence of eqs. (1.1.7) and (1.1.8), their symbols have only four possible entries,

$$\{w, 1 + w, w^*, 1 + w^*\}. \quad (1.1.10)$$

Furthermore, w and w^* are independent complex variables. Hence the problem of determining the coefficient functions factorizes into that of determining functions of w whose symbol entries are drawn from $\{w, 1 + w\}$ — a special class of HPLs — and the complex conjugate functions of w^* .

On the other hand, not every combination of HPLs in w and HPLs in w^* will appear. When the symbol is expressed in terms of the original variables $\{x, y, \tilde{y}_2, \tilde{y}_3\}$, the first entry must be either x or y , reflecting the branch-cut behavior and first-entry condition for general kinematics. Also, the full function must be a single-valued function of x and y , or equivalently a single-valued function of w and w^* . These conditions imply that the coefficient functions belong to the class of SVHPLs defined by Brown [47].

The MRK limit (1.1.9) is organized hierarchically into the leading-logarithmic approximation (LLA) with $n = \ell - 1$, the next-to-leading-logarithmic approximation (NLLA) with $n = \ell - 2$, and in general the $N^k\text{LL}$ terms with $n = \ell - k - 1$. Just as the problem of DGLAP evolution in x space is diagonalized by transforming to the space of Mellin moments N , the MRK limit can be diagonalized by performing a Fourier-Mellin transform from (w, w^*) to a new space labeled by (ν, n) . In fact, Fadin, Lipatov and Prygarin [12, 15] have given an all-loop-order formula for R_6 in the multi-Regge

limit, in terms of two functions of (ν, n) : The eigenvalue $\omega(\nu, n)$ of the BFKL kernel in the adjoint representation, and the (regularized) MHV impact factor $\Phi_{\text{Reg}}(\nu, n)$. Each function can be expanded in a , and each successive order in a corresponds to increasing k by one in the $N^k\text{LLA}$. It is possible that the assumption that was made in refs. [12, 15], of single Reggeon exchange through NLL, breaks down beyond that order, due to Reggeon-number changing interactions or other possible effects [49]. In this paper we will assume that it holds through $N^3\text{LL}$ (for the impact factor); the three quantities we extract beyond NLL could be affected if this assumption is wrong.

The leading term in the impact factor is just one, while the leading BFKL eigenvalue $E_{\nu, n}$ was found in ref. [8]. The NLL term in the impact factor was found in ref. [12], and the NLL contribution to the BFKL eigenvalue in ref. [15].

With this information it is possible to compute the LLA functions $g_{\ell-1}^{(\ell)}$, NLLA functions $g_{\ell-2}^{(\ell)}$ and $h_{\ell-2}^{(\ell)}$, and even the real part at NNLLA, $h_{\ell-3}^{(\ell)}$. All one needs to do is perform the inverse Fourier-Mellin transform back to the (w, w^*) variables. At the three-loop level, this was carried out at LLA for $g_2^{(3)}$ and $h_1^{(3)}$ in ref. [12], and at NLLA for $g_1^{(3)}$ and $h_0^{(3)}$ in ref. [15]. Here we will use the SVHPL basis to make this step very simple. The inverse transform contains an explicit sum over n , and an integral over ν which can be evaluated via residues in terms of a sum over a second integer m . For low loop orders we can perform the double sum analytically using harmonic sums [50–55]. For high loop orders, it is more efficient to simply truncate the double sum. In the (w, w^*) plane this truncation corresponds to truncating the power series expansion in $|w|$ around the origin. We know the answer is a linear combination of a finite number of SVHPLs with rational-number coefficients. In order to determine the coefficients, we simply compute the power series expansion of the generic linear combination of SVHPLs and match it against the truncated double sum over m and n . We can now perform the inverse Fourier-Mellin transform, in principle to all orders, and in practice through weight 10, corresponding to 10 loops for LLA and 9 loops for NLLA.

Furthermore, we can bring in additional information at fixed loop order, in order to obtain more terms in the expansion of the BFKL eigenvalue and the MHV impact factor. In ref. [15], the NLLA results for $g_1^{(3)}$ and $h_0^{(3)}$ confirmed a previous

prediction [14] based on an analysis of the multi-Regge limit of the symbol for $R_6^{(3)}$. In this limit, the two free symbol parameters mentioned above dropped out. The symbol could be integrated back up into a function, but a few more “beyond-the-symbol” constants entered at this stage. One of the constants was fixed in ref. [15] using the NLLA information. As noted in ref. [15], the result from ref. [14] for $g_0^{(3)}$ can be used to determine the NNLLA term in the impact factor. In this paper, we will use our knowledge of the space of functions of (w, w^*) (the SVHPLs) to build up a dictionary of the functions of (ν, n) (special types of harmonic sums) that are the Fourier-Mellin transforms of the SVHPLs. From this dictionary and $g_0^{(3)}$ we will determine the NNLLA term in the impact factor.

We can go further if we know the four-loop remainder function $R_6^{(4)}$. In separate work [56], we have heavily constrained the symbol of $R_6^{(4)}(u_1, u_2, u_3)$ for generic kinematics, using exactly the same constraints used in ref. [14]: integrability of the symbol, branch-cut behavior, symmetries, the final-entry condition, vanishing of collinear limits, and the OPE constraints (which at four loops are a constraint on the triple discontinuity). Although there are millions of possible terms before applying these constraints, afterwards the symbol contains just 113 free constants (112 if we apply the overall normalization for the OPE constraints). Next we construct the multi-Regge limit of this symbol, and apply all the information we have about this limit:

- Vanishing of the super-LLA terms $g_n^{(4)}$ and $h_n^{(4)}$ for $n = 4, 5, 6, 7$;
- LLA and NLLA predictions for $g_n^{(4)}$ and $h_n^{(4)}$ for $n = 2, 3$;
- the NNLLA real part $h_1^{(4)}$, which is also predicted by the NLLA formula;
- a consistency condition between $g_1^{(4)}$ and $h_0^{(4)}$.

Remarkably, these conditions determine all but one of the symbol-level parameters in the MRK limit. (The one remaining free parameter seems highly likely to vanish, given the complicated way it enters various formulas, but we have not yet proven that to be the case.)

We then extract the remaining four-loop coefficient functions, $g_1^{(4)}$, $h_0^{(4)}$ and $g_0^{(4)}$, introducing some additional beyond-the-symbol parameters at this stage. We use this

information to determine the NNLLA BFKL eigenvalue and the N^3 LLA MHV impact factor, up to these parameters. Although our general dictionary of functions of (ν, n) contains various multiple harmonic sums, we find that the key functions entering the multi-Regge limit can all be expressed just in terms of certain rational combinations of ν and n , together with the polygamma functions ψ , ψ' , ψ'' , etc. (derivatives of the logarithm of the Γ function) with arguments $1 \pm i\nu + |n|/2$.

As a by-product, we find that the SVHPLs also describe the multi-Regge limit of the one remaining helicity configuration for six-gluon scattering in $\mathcal{N} = 4$ super-Yang-Mills theory, namely the next-to-MHV (NMHV) configuration with three negative and three positive gluon helicities. It was shown recently [18] that in LLA the NMHV and MHV remainder functions are related by a simple integro-differential operator. This operator has a natural action in terms of the SVHPLs, allowing us to easily extend the NMHV LLA results of ref. [18] from three loops to 10 loops.

This article is organized as follows. In section 1.2 we review the structure of the six-point MHV remainder function in the multi-Regge limit. Section 1.3 reviews Brown's construction of single-valued harmonic polylogarithms. In section 1.4 we exploit the SVHPL basis to determine the functions $g_n^{(\ell)}$ and $h_n^{(\ell)}$ at LLA through 10 loops and at NNLLA through 9 loops. Section 1.5 determines the NMHV remainder function at LLA through 10 loops. In section 1.6 we describe our construction of the functions of (ν, n) that are the Fourier-Mellin transforms of the SVHPLs. Section 1.7 applies this knowledge, plus information from the four-loop remainder function [56], in order to determine the NNLLA MHV impact factor and BFKL eigenvalue, and the N^3 LLA MHV impact factor, in terms of a handful of (mostly) beyond-the-symbol constants. In section 1.8 we report our conclusions and discuss directions for future research.

We include two appendices. Appendix A.1 collects expressions for the SVHPLs (after diagonalizing the action of a $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry), in terms of HPLs through weight 5. It also gives expressions before diagonalizing one of the two \mathbb{Z}_2 factors. Appendix A.2 gives a basis for the function space in (ν, n) through weight 5, together with the Fourier-Mellin map to the SVHPLs. In addition, for the lengthier formulae, we provide separate computer-readable text files as ancillary material. In particular,

we include files (in `Mathematica` format) that contain the expressions for the SVHPLs in terms of ordinary HPLs up to weight six, decomposed into an eigenbasis of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry, as well as the analytic results up to weight ten for the imaginary parts of the MHV remainder function at LLA and NLLA and for the NMHV remainder function at LLA. Furthermore, we include the expressions for the NNLL BFKL eigenvalue and impact factor and the N³LL impact factor in terms of the building blocks in the variables (ν, n) constructed in section 1.6, as well as a dictionary between these building blocks and the SVHPLs up to weight five.

1.2 The six-point remainder function in the multi-Regge limit

The principal aim of this paper is to study the six-point MHV amplitude in $\mathcal{N} = 4$ super Yang-Mills theory in multi-Regge kinematics. This limit is defined by the hierarchy of scales,

$$s_{12} \gg s_{345}, s_{456} \gg s_{34}, s_{45}, s_{56} \gg s_{23}, s_{61}, s_{234}. \quad (1.2.1)$$

In this limit the cross ratios (1.1.2) behave as

$$1 - u_1, u_2, u_3 \sim 0, \quad (1.2.2)$$

together with the constraint that the following ratios are held fixed,

$$x \equiv \frac{u_2}{1 - u_1} = \mathcal{O}(1) \quad \text{and} \quad y \equiv \frac{u_3}{1 - u_1} = \mathcal{O}(1). \quad (1.2.3)$$

In the following it will be convenient [12] to parametrize the dependence on x and y by a single complex variable w ,

$$x \equiv \frac{1}{(1 + w)(1 + w^*)} \quad \text{and} \quad y \equiv \frac{w w^*}{(1 + w)(1 + w^*)}. \quad (1.2.4)$$

Any function of the three cross ratios can then develop large logarithms $\log(1 - u_1)$ in the multi-Regge limit, and we can write generically,

$$F(u_1, u_2, u_3) = \sum_i \log^i(1 - u_1) f_i(w, w^*) + \mathcal{O}(1 - u_1). \quad (1.2.5)$$

Let us make at this point an important observation which will be a recurrent theme in the rest of the paper: If $F(u_1, u_2, u_3)$ represents a physical quantity like a scattering amplitude, then F should only have cuts in physical channels, corresponding to branch cuts starting at points where one of the cross ratios vanishes. Rotation around the origin in the complex w plane, i.e. $(w, w^*) \rightarrow (e^{2\pi i} w, e^{-2\pi i} w^*)$, does not correspond to crossing any branch cut. As a consequence, the functions $f_i(w, w^*)$ should not change under this operation. More generally, the functions $f_i(w, w^*)$ must be *single-valued* in the complex w plane.

Let us start by reviewing the multi-Regge limit of the MHV remainder function $R(u_1, u_2, u_3) \equiv R_6(u_1, u_2, u_3)$ introduced in eq. (1.1.1). It can be shown that, while in the Euclidean region the remainder function vanishes in the multi-Regge limit, there is a Mandelstam cut such that we obtain a non-zero contribution in MRK after performing the analytic continuation [5]

$$u_1 \rightarrow e^{-2\pi i} |u_1|. \quad (1.2.6)$$

After this analytic continuation, the six-point remainder function can be expanded into the form given in eq. (1.1.9), which we repeat here for convenience,

$$R|_{\text{MRK}} = 2\pi i \sum_{\ell=2}^{\infty} \sum_{n=0}^{\ell-1} a^\ell \log^n(1 - u_1) [g_n^{(\ell)}(w, w^*) + 2\pi i h_n^{(\ell)}(w, w^*)]. \quad (1.2.7)$$

The functions $g_n^{(\ell)}(w, w^*)$ and $h_n^{(\ell)}(w, w^*)$ will in the following be referred to as the *coefficient functions* for the logarithmic expansion in the MRK limit. The imaginary part $g_n^{(\ell)}$ is associated with a single discontinuity, and the real part $h_n^{(\ell)}$ with a double discontinuity, although both functions also include information from higher discontinuities, albeit with accompanying explicit factors of π^2 .

The coefficient functions are single-valued pure transcendental functions in the complex variable w , of weight $2\ell - n - 1$ for $g_n^{(\ell)}$ and weight $2\ell - n - 2$ for $h_n^{(\ell)}$. They are left invariant by a $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry acting via complex conjugation and inversion,

$$w \leftrightarrow w^* \quad \text{and} \quad (w, w^*) \leftrightarrow (1/w, 1/w^*). \quad (1.2.8)$$

The complex conjugation symmetry arises because the MHV remainder function has a parity symmetry, or invariance under $\Delta \rightarrow -\Delta$, which inverts \tilde{y}_2 and \tilde{y}_3 in eq. (1.1.8). The inversion symmetry is a consequence of the fact that the six-point remainder function is a totally symmetric function of the three cross ratios u_1 , u_2 and u_3 . In particular, exchanging $\tilde{y}_2 \leftrightarrow \tilde{y}_3$ is the product of conjugation and inversion. The inversion symmetry is sometimes referred to as target-projectile symmetry [10]. Finally, the vanishing of the six-point remainder function in the collinear limit implies the vanishing of $g_n^{(\ell)}(w, w^*)$ and $h_n^{(\ell)}(w, w^*)$ in the limit where $(w, w^*) \rightarrow 0$. Clearly the functions $g_n^{(\ell)}$ and $h_n^{(\ell)}$ are already highly constrained on general grounds.

In ref. [12, 15] an all-loop integral formula for the six-point amplitude in MRK was presented¹,

$$\begin{aligned} e^{R+i\pi\delta}|_{\text{MRK}} &= \cos \pi\omega_{ab} \\ &+ i \frac{a}{2} \sum_{n=-\infty}^{\infty} (-1)^n \left(\frac{w}{w^*}\right)^{\frac{n}{2}} \int_{-\infty}^{+\infty} \frac{d\nu |w|^{2i\nu}}{\nu^2 + \frac{n^2}{4}} \Phi_{\text{Reg}}(\nu, n) \left(-\frac{1}{\sqrt{u_2 u_3}}\right)^{\omega(\nu, n)}. \end{aligned} \quad (1.2.9)$$

The first term is the Regge pole contribution, with

$$\omega_{ab} = \frac{1}{8} \gamma_K(a) \log \frac{u_3}{u_2} = \frac{1}{8} \gamma_K(a) \log |w|^2, \quad (1.2.10)$$

and $\gamma_K(a)$ is the cusp anomalous dimension, known to all orders in perturbation

¹There is a difference in conventions regarding the definition of the remainder function. What we call R is called $\log(R)$ in refs. [12, 15]. Apart from the zeroth order term, the first place this makes a difference is at four loops, in the real part.

theory [57],

$$\gamma_K(a) = \sum_{\ell=1}^{\infty} \gamma_K^{(\ell)} a^\ell = 4a - 4\zeta_2 a^2 + 22\zeta_4 a^3 - \left(\frac{219}{2}\zeta_6 + 4\zeta_3^2\right) a^4 + \dots \quad (1.2.11)$$

The second term in eq. (1.2.9) arises from a Regge cut and is fully determined to all orders by the BFKL eigenvalue $\omega(\nu, n)$ and the (regularized) impact factor $\Phi_{\text{Reg}}(\nu, n)$. The function δ appearing in the exponent on the left-hand side is the contribution from a Mandelstam cut present in the BDS ansatz, and is given to all loop orders by

$$\delta = \frac{1}{8} \gamma_K(a) \log(xy) = \frac{1}{8} \gamma_K(a) \log \frac{|w|^2}{|1+w|^4}. \quad (1.2.12)$$

In addition, we have

$$\frac{1}{\sqrt{u_2 u_3}} = \frac{1}{1-u_1} \frac{|1+w|^2}{|w|}. \quad (1.2.13)$$

The BFKL eigenvalue and the impact factor can be expanded perturbatively,

$$\begin{aligned} \omega(\nu, n) &= -a \left(E_{\nu, n} + a E_{\nu, n}^{(1)} + a^2 E_{\nu, n}^{(2)} + \mathcal{O}(a^3) \right), \\ \Phi_{\text{Reg}}(\nu, n) &= 1 + a \Phi_{\text{Reg}}^{(1)}(\nu, n) + a^2 \Phi_{\text{Reg}}^{(2)}(\nu, n) + a^3 \Phi_{\text{Reg}}^{(3)}(\nu, n) + \mathcal{O}(a^4). \end{aligned} \quad (1.2.14)$$

The BFKL eigenvalue is known to the first two orders in perturbation theory [8, 15],

$$E_{\nu, n} = -\frac{1}{2} \frac{|n|}{\nu^2 + \frac{n^2}{4}} + \psi \left(1 + i\nu + \frac{|n|}{2} \right) + \psi \left(1 - i\nu + \frac{|n|}{2} \right) - 2\psi(1) \quad (1.2.15)$$

$$\begin{aligned} E_{\nu, n}^{(1)} &= -\frac{1}{4} \left[\psi'' \left(1 + i\nu + \frac{|n|}{2} \right) + \psi'' \left(1 - i\nu + \frac{|n|}{2} \right) \right. \\ &\quad \left. - \frac{2i\nu}{\nu^2 + \frac{n^2}{4}} \left(\psi' \left(1 + i\nu + \frac{|n|}{2} \right) - \psi' \left(1 - i\nu + \frac{|n|}{2} \right) \right) \right] \\ &\quad - \zeta_2 E_{\nu, n} - 3\zeta_3 - \frac{1}{4} \frac{|n| \left(\nu^2 - \frac{n^2}{4} \right)}{\left(\nu^2 + \frac{n^2}{4} \right)^3}, \end{aligned} \quad (1.2.16)$$

where $\psi(z) = \frac{d}{dz} \log \Gamma(z)$ is the digamma function, and $\psi(1) = -\gamma_E$ is the Euler-Mascheroni constant. The NLL contribution to the impact factor is given by [10]

$$\Phi_{\text{Reg}}^{(1)}(\nu, n) = -\frac{1}{2}E_{\nu,n}^2 - \frac{3}{8} \frac{n^2}{(\nu^2 + \frac{n^2}{4})^2} - \zeta_2. \quad (1.2.17)$$

The BFKL eigenvalues and impact factor in eqs. (1.2.15), (1.2.16) and (1.2.17) are enough to compute the six-point remainder function in the Regge limit in the leading and next-to-leading logarithmic approximations (LLA and NLLA). Indeed, we can interpret the integral in eq. (1.2.9) as a contour integral in the complex ν plane and close the contour at infinity. By summing up the residues we then obtain the analytic expression of the remainder function in the LLA and NLLA in MRK. This procedure will be discussed in greater detail in section 1.4. Some comments are in order about the integral in eq. (1.2.9):

1. The contribution coming from $n = 0$ is ill-defined, as the integral in eq. (1.2.9) diverges. After closing the contour at infinity, our prescription is to take only half of the residue at $\nu = n = 0$ into account.
2. We need to specify the Riemann sheet of the exponential factor in the right-hand side of eq. (1.2.9). We find that the replacement

$$\left(-\frac{1}{\sqrt{u_2 u_3}}\right)^{\omega(\nu,n)} \rightarrow e^{-i\pi\omega(\nu,n)} \left(\frac{1}{\sqrt{u_2 u_3}}\right)^{\omega(\nu,n)} \quad (1.2.18)$$

gives the correct result.

The $i\pi$ factor in the right-hand side of eq. (1.2.18) generates the real parts $h_n^{(\ell)}$ in eq. (1.2.7). It is easy to see that the $g_n^{(\ell)}$ and $h_n^{(\ell)}$ functions are not independent, but

they are related. For example, at LLA and NLLA we have,

$$\begin{aligned}
 h_{\ell-1}^{(\ell)}(w, w^*) &= 0, \\
 h_{\ell-2}^{(\ell)}(w, w^*) &= \frac{\ell-1}{2} g_{\ell-1}^{(\ell)}(w, w^*) + \frac{1}{16} \gamma_K^{(1)} g_{\ell-2}^{(\ell-1)}(w, w^*) \log \frac{|1+w|^4}{|w|^2} \\
 &\quad - \frac{1}{2} \sum_{k=2}^{\ell-2} g_{k-1}^{(k)} g_{\ell-k-1}^{(\ell-k)}, \quad \ell > 2,
 \end{aligned} \tag{1.2.19}$$

where $\gamma_K^{(1)} = 4$ from eq. (1.2.11). (Note that the sum over k in the formula for $h_{\ell-2}^{(\ell)}$ would not have been present if we had used the convention for R in refs. [12, 15].) Similar relations can be derived beyond NLLA, i.e. for $n < \ell - 2$.

So far we have only considered $2 \rightarrow 4$ scattering. In ref. [13] it was shown that if the remainder function is analytically continued to the region corresponding to $3 \rightarrow 3$ scattering, then it takes a particularly simple form. The analytic continuation from $2 \rightarrow 4$ to $3 \rightarrow 3$ scattering can be obtained easily by performing the replacement

$$\log(1 - u_1) \rightarrow \log(u_1 - 1) - i\pi \tag{1.2.20}$$

in eq. (1.2.9). After analytic continuation the real part of the remainder function only gets contributions from the Regge pole and is given by [13]

$$\text{Re} \left(e^{R_{3 \rightarrow 3} - i\pi\delta} \right) = \cos \pi\omega_{ab}. \tag{1.2.21}$$

It is manifest from eq. (1.2.9) that eq. (1.2.21) is automatically satisfied if the relations among the coefficient functions derivable by tracking the $i\pi$ from eq. (1.2.18) (e.g. eq. (1.2.19)) are satisfied in $2 \rightarrow 4$ kinematics.

So far we have only reviewed some general properties of the six-point remainder function in MRK, but we have not yet given explicit analytic expressions for the coefficient functions. The two-loop contributions to eq. (1.2.9) in LLA and NLLA were computed in refs. [10, 12], while the three-loop contributions up to the NNLLA were found in refs. [10, 14]. In all cases the results have been expressed as combinations of classical polylogarithms in the complex variable w and its complex conjugate w^* , with

potential branching points at $w = 0$ and $w = -1$. As discussed at the beginning of this section, all the branch cuts in the complex w plane must cancel, i.e., the function must be single-valued in w . The class of functions satisfying these constraints has been studied in full generality in the mathematical literature, as will be reviewed in the next section.

1.3 Harmonic polylogarithms and their single-valued analogues

1.3.1 Review of harmonic polylogarithms

In this section we give a short review of the classical and harmonic polylogarithms, one of the main themes in the rest of this paper. The simplest possible polylogarithmic functions are the so-called *classical* polylogarithms, defined inside the unit circle by a convergent power series,

$$\text{Li}_m(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^m}, \quad |z| < 1. \quad (1.3.1)$$

They can be continued to the cut plane $\mathbb{C} \setminus [1, \infty)$ by an iterated integral representation,

$$\text{Li}_m(z) = \int_0^z dz' \frac{\text{Li}_{m-1}(z')}{z'}. \quad (1.3.2)$$

For $m = 1$, the polylogarithm reduces to the ordinary logarithm, $\text{Li}_1(z) = -\log(1-z)$, a fact that dictates the location of the branch cut for all m (along the real axis for $z > 1$). It also determines the discontinuity across the cut,

$$\Delta \text{Li}_m(z) = 2\pi i \frac{\log^{m-1} z}{(m-1)!}. \quad (1.3.3)$$

It is possible to define more general classes of polylogarithmic functions by allowing for different kernels inside the iterated integral in eq. (1.3.2). The *harmonic* polylogarithms (HPLs) [48] are a special class of generalized polylogarithms whose

properties and construction we review in the remainder of this section. To begin, let w be a word formed from the letters x_0 and x_1 , and let e be the empty word. Then, for each w , define a function $H_w(z)$ which obeys the differential equations,

$$\frac{\partial}{\partial z} H_{x_0 w}(z) = \frac{H_w(z)}{z} \quad \text{and} \quad \frac{\partial}{\partial z} H_{x_1 w}(z) = \frac{H_w(z)}{1-z}, \quad (1.3.4)$$

subject to the following conditions,

$$H_e(z) = 1, \quad H_{x_0^n}(z) = \frac{1}{n!} \log^n z, \quad \text{and} \quad \lim_{z \rightarrow 0} H_{w \neq x_0^n}(z) = 0. \quad (1.3.5)$$

There is a unique family of solutions to these equations, and it defines the HPLs. Note that we use the term ‘‘HPL’’ in a restricted sense² – we only consider poles in the differential equations (1.3.4) at $z = 0$ and $z = 1$. (In our MRK application, we will let $z = -w$, so that the poles are at $w = 0$ and $w = -1$.)

The *weight* of an HPL is the length of the word w , and its *depth* is the number of x_1 ’s³. HPLs of depth one are simply the classical polylogarithms, $H_n(z) = \text{Li}_n(z)$. Like the classical polylogarithms, the HPLs can be written as iterated integrals,

$$H_{x_0 w}(z) = \int_0^z dz' \frac{H_w(z')}{z'} \quad \text{and} \quad H_{x_1 w} = \int_0^z dz' \frac{H_w(z')}{1-z'}. \quad (1.3.7)$$

The structure of the underlying iterated integrals endows the HPLs with an important property: they form a *shuffle algebra*. The shuffle relations can be written,

$$H_{w_1}(z) H_{w_2}(z) = \sum_{w \in w_1 \amalg w_2} H_w(z), \quad (1.3.8)$$

²In the mathematical literature, these functions are sometimes referred to as *multiple polylogarithms in one variable*.

³For ease of notation, we will often impose the replacement $\{x_0 \rightarrow 0, x_1 \rightarrow 1\}$ in subscripts. In some cases, we will use the collapsed notation where a subscript m denotes $m - 1$ zeroes followed by a single 1. For example, if $w = x_0 x_0 x_1 x_0 x_1$,

$$H_w(z) = H_{x_0 x_0 x_1 x_0 x_1}(z) = H_{0,0,1,0,1}(z) = H_{3,2}(z). \quad (1.3.6)$$

In the collapsed notation, the *weight* is the sum of the indices, and the *depth* is the number of nonzero indices.

Weight	Lyndon words	Dimension
1	0, 1	2
2	01	1
3	001, 011	2
4	0001, 0011, 0111	3
5	00001, 00011, 00101, 00111, 01011, 01111	6

 Table 1.1: All Lyndon words $\text{Lyndon}(x_0, x_1)$ through weight five

where $w_1 \sqcup w_2$ is the set of mergers of the sequences w_1 and w_2 that preserve their relative ordering. Equation (1.3.8) may be used to express all HPLs of a given weight in terms of a relatively small set of basis functions and products of lower-weight HPLs. One convenient such basis [58] of irreducible functions is the *Lyndon* basis, defined by $\{H_w(z) : w \in \text{Lyndon}(x_0, x_1)\}$. The Lyndon words $\text{Lyndon}(x_0, x_1)$ are those words w such that for every decomposition into two words $w = uv$, the left word is lexicographically smaller than the right, $u < v$. Table 1.1 gives the first few examples of Lyndon words.

All HPLs are real whenever the argument z is less than 1, and so, in particular, the HPLs are analytic in a neighborhood of $z = 0$. The Taylor expansion around $z = 0$ is particularly simple and involves only a special class of harmonic numbers [48, 52] (hence the name *harmonic* polylogarithm),

$$H_{m_1, \dots, m_k}(z) = \sum_{l=1}^{\infty} \frac{z^l}{l^{m_1}} Z_{m_2, \dots, m_k}(l-1), \quad m_i > 0, \quad (1.3.9)$$

where $Z_{m_1, \dots, m_k}(n)$ denote the so-called Euler-Zagier sums [50, 51], defined recursively by

$$Z_{m_1}(n) = \sum_{l=1}^n \frac{1}{l^{m_1}} \quad \text{and} \quad Z_{m_1, \dots, m_k}(n) = \sum_{l=1}^n \frac{1}{l^{m_1}} Z_{m_2, \dots, m_k}(l-1). \quad (1.3.10)$$

Note that the indexing of the weight vectors m_1, \dots, m_k in eqs. (1.3.9) and (1.3.10) is in the collapsed notation.

Another important property of HPLs is that they are closed under certain transformations of the arguments [48]. In particular, using the integral representation (1.3.7),

it is easy to show that the set of all HPLs is closed under the following transformations,

$$z \mapsto 1 - z, \quad z \mapsto 1/z, \quad z \mapsto 1/(1 - z), \quad z \mapsto 1 - 1/z, \quad z \mapsto z/(z - 1). \quad (1.3.11)$$

If we add to these mappings the identity map $z \mapsto z$, we can identify the transformations in eq. (1.3.11) as forming a representation of the symmetric group S_3 . In other words, the vector space spanned by all HPLs is endowed with a natural action of the symmetric group S_3 .

Finally, it is evident from the iterated integral representation (1.3.7) that HPLs can have branch cuts starting at $z = 0$ and/or $z = 1$, i.e., HPLs define in general multi-valued functions on the complex plane. In the next section we will define analogues of HPLs without any branch cuts, thus obtaining a single-valued version of the HPLs.

1.3.2 Single-valued harmonic polylogarithms

Before reviewing the definition of single-valued harmonic polylogarithms in general, let us first review the special case of single-valued classical polylogarithms. The knowledge of the discontinuities of the classical polylogarithms, eq. (1.3.3), can be leveraged to construct a sequence of real analytic functions on the punctured plane $\mathbb{C} \setminus \{0, 1\}$. The idea is to consider linear combinations of (products of) classical polylogarithms and ordinary logarithms such that all the branch cuts cancel. Although the space of single-valued functions is unique, the choice of basis is not unique, and there have been several versions proposed in the literature. As an illustration, consider the functions of Zagier [59],

$$D_m(z) = \Re_m \left\{ \sum_{k=1}^m \frac{(-\log |z|)^{m-k}}{(m-k)!} \text{Li}_k(z) + \frac{\log^m |z|}{2^m m!} \right\}, \quad (1.3.12)$$

where \Re_m denotes the imaginary part for m even and the real part for m odd. The discontinuity of the function inside the curly brackets is given by

$$2\pi i \sum_{k=1}^m \frac{(-\log |z|)^{m-k}}{(m-k)!} \frac{\log^{k-1} z}{(k-1)!} = 2\pi \frac{i^m}{(m-1)!} (\arg z)^{m-1}. \quad (1.3.13)$$

Since eq. (1.3.13) is real for even m and pure imaginary for odd m , $D_m(z)$ is indeed single-valued. For the special case $m = 2$, we reproduce the famous Bloch-Wigner dilogarithm [60],

$$D_2(z) = \text{Im}\{\text{Li}_2(z)\} + \arg(1-z) \log |z|. \quad (1.3.14)$$

Just as there have been numerous proposals in the literature for single-valued versions of the classical polylogarithms, there are many potential choices of bases for single-valued HPLs. On the other hand, if we choose to demand some reasonable properties, it turns out that a unique set of functions emerges. Following ref. [47], we require the single-valued HPLs to be built entirely from holomorphic and anti-holomorphic HPLs. Specifically, they should be a linear combination of terms of the form $H_{w_1}(z)H_{w_2}(\bar{z})$, where w_1 and w_2 are words in x_0 and x_1 or the empty word e . The single-valued classical polylogarithms obey an analogous property, and it can be understood as the condition that the single-valued functions are the proper extensions of the original functions. The remaining requirements are simply the analogues of the conditions used to construct the ordinary HPLs.

Define a function $\mathcal{L}_w(z)$, which is a linear combination of functions $H_{w_1}(z)H_{w_2}(\bar{z})$ and which obeys the differential equations

$$\frac{\partial}{\partial z} \mathcal{L}_{x_0 w}(z) = \frac{\mathcal{L}_w(z)}{z} \quad \text{and} \quad \frac{\partial}{\partial z} \mathcal{L}_{x_1 w}(z) = \frac{\mathcal{L}_w(z)}{1-z}, \quad (1.3.15)$$

subject to the conditions,

$$\mathcal{L}_e(z) = 1, \quad \mathcal{L}_{x_0^n}(z) = \frac{1}{n!} \log^n |z|^2 \quad \text{and} \quad \lim_{z \rightarrow 0} \mathcal{L}_{w \neq x_0^n}(z) = 0. \quad (1.3.16)$$

In ref. [47] Brown showed that there is a unique family of solutions to these equations that is single-valued in the complex z plane, and it defines the single-valued HPLs

(SVHPLs). The functions $\mathcal{L}_w(z)$ are linearly independent and span the space. That is to say, every single-valued linear combination of functions of the form $H_{w_1}(z)H_{w_2}(\bar{z})$ can be written in terms of the $\mathcal{L}_w(z)$. In ref. [47] an algorithm was presented that allows for the explicit construction of all SVHPLs as linear combinations of (products of) ordinary HPLs. We present a short review of this algorithm in section 1.3.3.

The SVHPLs of ref. [47] share all the nice features of their multi-valued analogues. First, like the ordinary HPLs, they obey shuffle relations,

$$\mathcal{L}_{w_1}(z) \mathcal{L}_{w_2}(z) = \sum_{w \in w_1 \amalg w_2} \mathcal{L}_w(z), \quad (1.3.17)$$

where again $w_1 \amalg w_2$ represents the shuffles of w_1 and w_2 . As a consequence, we may again choose to solve eq. (1.3.17) in terms of a Lyndon basis. It follows that if we want the full list of all SVHPLs of a given weight, it is enough to know the corresponding Lyndon basis up to that weight.

Furthermore, the space of SVHPLs is also closed under the S_3 action defined by eq. (1.3.11). Indeed, if we extend the action to the complex conjugate variable \bar{z} , then the closure of the space of all ordinary HPLs implies the closure of the space spanned by all products of the form $H_{w_1}(z)H_{w_2}(\bar{z})$, and, in particular, the closure of the subspace of SVHPLs. For the SVHPLs, it is possible to enlarge the symmetry group to $\mathbb{Z}_2 \times S_3$, where the \mathbb{Z}_2 subgroup acts by complex conjugation, $z \leftrightarrow \bar{z}$.

It turns out that the functions $\mathcal{L}_w(z)$ can generically be decomposed as

$$\mathcal{L}_w(z) = (H_w(z) - (-1)^{|w|} H_w(\bar{z})) + [\text{products of lower weight}], \quad (1.3.18)$$

where $|w|$ denotes the weight. As such, it is convenient to consider the even and odd projections, i.e., the decomposition into eigenfunctions of the \mathbb{Z}_2 action,

$$\begin{aligned} L_w(z) &= \frac{1}{2} (\mathcal{L}_w(z) - (-1)^{|w|} \mathcal{L}_w(\bar{z})) , \\ \bar{L}_w(z) &= \frac{1}{2} (\mathcal{L}_w(z) + (-1)^{|w|} \mathcal{L}_w(\bar{z})) . \end{aligned} \quad (1.3.19)$$

The basis defined by $\mathcal{L}_w(z)$ was already complete, and yet here we have doubled the

number of potential basis functions. Therefore $L_w(z)$ and $\bar{L}_w(z)$ must be related to one another. Writing $L_w(z) = \Re_{|w|}(\mathcal{L}_w(z))$, we see that it has the same parity as Zagier's single-valued versions of the classical polylogarithms given in eq. (1.3.12). Therefore we might expect the $L_w(z)$ to form a complete basis on their own. Indeed this turns out to be the case, and the $\bar{L}_w(z)$ can be expressed as products of the functions $L_w(z)$,

$$\bar{L}_w(z) = [\text{products of lower weight } L_{w'}(z)]. \quad (1.3.20)$$

Hence we will not consider the functions $\bar{L}_w(z)$ any further and will concentrate solely on the functions $L_w(z)$.

The functions $L_w(z)$ do not automatically form simple representations of the S_3 symmetry. For the current application, we will mostly be concerned with the $\mathbb{Z}_2 \subset S_3$ subgroup generated by inversions $z \leftrightarrow 1/z$. The functions $L_w(z)$ can easily be decomposed into eigenfunctions of this \mathbb{Z}_2 , and, furthermore, these eigenfunctions form a basis for the space of all SVHPLs. The latter follows from the observation that,

$$L_w(z) - (-1)^{|w|+d_w} L_w\left(\frac{1}{z}\right) = [\text{products of lower weight}], \quad (1.3.21)$$

where $|w|$ is the weight and d_w is the depth of the word w . We will denote these eigenfunctions of $\mathbb{Z}_2 \times \mathbb{Z}_2$ by,

$$L_w^\pm(z) \equiv \frac{1}{2} \left[L_w(z) \pm L_w\left(\frac{1}{z}\right) \right], \quad (1.3.22)$$

and present most of our results in terms of this convenient basis. For low weights, appendix A.1 gives explicit representations of these basis functions in terms of HPLs. The expressions through weight six can be found in the ancillary files.

We have seen in the previous section that in the multi-Regge limit the six-point amplitude is described to all loop orders by single-valued functions of a single complex variable w satisfying certain reality and inversion properties. It turns out that the SVHPLs we just defined are particularly well-suited to describe these multi-Regge limits. This description will be the topic of the rest of this paper.

1.3.3 Explicit construction

The explicit construction of the functions $\mathcal{L}_w(z)$ is somewhat involved so we take a brief detour to describe the details. Let X^* be the set of words in the alphabet $\{x_0, x_1\}$, along with the empty word e . Define the Drinfel'd associator $Z(x_0, x_1)$ as the generating series,

$$Z(x_0, x_1) = \sum_{w \in X^*} \zeta(w)w, \quad (1.3.23)$$

where $\zeta(w) = H_w(1)$ for $w \neq x_1$ and $\zeta(x_1) = 0$. The $\zeta(w)$ are regularized by the shuffle algebra. Using the collapsed notation for w , these $\zeta(w)$ are the familiar multiple zeta values.

Next, define an alphabet $\{y_0, y_1\}$ (and a set of words Y^*) and a map $\sim : Y^* \rightarrow Y^*$ as the operation that reverses words. The alphabet $\{y_0, y_1\}$ is related to the alphabet $\{x_0, x_1\}$ by the following relations:

$$\begin{aligned} y_0 &= x_0 \\ \tilde{Z}(y_0, y_1)y_1\tilde{Z}(y_0, y_1)^{-1} &= Z(x_0, x_1)^{-1}x_1Z(x_0, x_1). \end{aligned} \quad (1.3.24)$$

The inversion operator is to be understood as a formal series expansion in the weight $|w|$. Solving eq. (1.3.24) iteratively in the weight yields a series expansion for y_1 . The first few terms are,

$$\begin{aligned} y_1 &= x_1 - \zeta_3(2x_0x_0x_1x_1 - 4x_0x_1x_0x_1 + 2x_0x_1x_1x_1 + 4x_1x_0x_1x_0 \\ &\quad - 6x_1x_0x_1x_1 - 2x_1x_1x_0x_0 + 6x_1x_1x_0x_1 - 2x_1x_1x_1x_0) + \dots \end{aligned} \quad (1.3.25)$$

Letting $\phi : Y^* \rightarrow X^*$ be the map that renames y to x , i.e. $\phi(y_0) = x_0$ and $\phi(y_1) = x_1$, define the generating functions

$$L_X(z) = \sum_{w \in X^*} H_w(z)w, \quad \tilde{L}_Y(\bar{z}) = \sum_{w \in Y^*} H_{\phi(w)}(\bar{z})\tilde{w}. \quad (1.3.26)$$

In the following, we use a condensed notation for the HPL arguments, in order to

improve the readability of explicit formulas:

$$H_w \equiv H_w(z) \quad \text{and} \quad \bar{H}_w \equiv H_w(\bar{z}). \quad (1.3.27)$$

Then we can write

$$\begin{aligned} L_X(z) = & 1 + H_0 x_0 + H_1 x_1 \\ & + H_{0,0} x_0 x_0 + H_{0,1} x_0 x_1 + H_{1,0} x_1 x_0 + H_{1,1} x_1 x_1 \\ & + H_{0,0,0} x_0 x_0 x_0 + H_{0,0,1} x_0 x_0 x_1 + H_{0,1,0} x_0 x_1 x_0 + H_{0,1,1} x_0 x_1 x_1 \\ & + H_{1,0,0} x_1 x_0 x_0 + H_{1,0,1} x_1 x_0 x_1 + H_{1,1,0} x_1 x_1 x_0 + H_{1,1,1} x_1 x_1 x_1 \\ & + \dots, \end{aligned} \quad (1.3.28)$$

and

$$\begin{aligned} \tilde{L}_Y(\bar{z}) = & 1 + \bar{H}_0 y_0 + \bar{H}_1 y_1 \\ & + \bar{H}_{0,0} y_0 y_0 + \bar{H}_{0,1} y_1 y_0 + \bar{H}_{1,0} y_0 y_1 + \bar{H}_{1,1} y_1 y_1 \\ & + \bar{H}_{0,0,0} y_0 y_0 y_0 + \bar{H}_{0,0,1} y_1 y_0 y_0 + \bar{H}_{0,1,0} y_0 y_1 y_0 + \bar{H}_{0,1,1} y_1 y_1 y_0 \\ & + \bar{H}_{1,0,0} y_0 y_0 y_1 + \bar{H}_{1,0,1} y_1 y_0 y_1 + \bar{H}_{1,1,0} y_0 y_1 y_1 + \bar{H}_{1,1,1} y_1 y_1 y_1 \\ & + \dots \\ = & 1 + \bar{H}_0 x_0 + \bar{H}_1 x_1 \\ & + \bar{H}_{0,0} x_0 x_0 + \bar{H}_{0,1} x_1 x_0 + \bar{H}_{1,0} x_0 x_1 + \bar{H}_{1,1} x_1 x_1 \\ & + \bar{H}_{0,0,0} x_0 x_0 x_0 + \bar{H}_{0,0,1} x_1 x_0 x_0 + \bar{H}_{0,1,0} x_0 x_1 x_0 + \bar{H}_{0,1,1} x_1 x_1 x_0 \\ & + \bar{H}_{1,0,0} x_0 x_0 x_1 + \bar{H}_{1,0,1} x_1 x_0 x_1 + \bar{H}_{1,1,0} x_0 x_1 x_1 + \bar{H}_{1,1,1} x_1 x_1 x_1 \\ & + \dots. \end{aligned} \quad (1.3.29)$$

In the last step of eq. (1.3.29) we used $y_0 = x_0$ and $y_1 = x_1$. Note that the latter only holds through weight three, as is clear from eq. (1.3.25). Finally, we are able to construct the SVHPLs as a generating series,

$$\mathcal{L}(z) = L_X(z) \tilde{L}_Y(\bar{z}) \equiv \sum_{w \in X^*} \mathcal{L}_w(z) w. \quad (1.3.30)$$

Indeed, taking the product of eq. (1.3.28) with eq. (1.3.29) and keeping terms through weight three, we obtain,

$$\begin{aligned}
 \sum_{w \in X^*} \mathcal{L}_w(z) w &= 1 + \mathcal{L}_0(z) x_0 + \mathcal{L}_1(z) x_1 \\
 &+ \mathcal{L}_{0,0}(z) x_0 x_0 + \mathcal{L}_{0,1}(z) x_0 x_1 + \mathcal{L}_{1,0}(z) x_1 x_0 + \mathcal{L}_{1,1}(z) x_1 x_1 \\
 &+ \mathcal{L}_{0,0,0}(z) x_0 x_0 x_0 + \mathcal{L}_{0,0,1}(z) x_0 x_0 x_1 + \mathcal{L}_{0,1,0}(z) x_0 x_1 x_0 + \mathcal{L}_{0,1,1}(z) x_0 x_1 x_1 \\
 &+ \mathcal{L}_{1,0,0}(z) x_1 x_0 x_0 + \mathcal{L}_{1,0,1}(z) x_1 x_0 x_1 + \mathcal{L}_{1,1,0}(z) x_1 x_1 x_0 + \mathcal{L}_{1,1,1}(z) x_1 x_1 x_1 \\
 &+ \dots,
 \end{aligned} \tag{1.3.31}$$

where the SVHPL's of weight one are,

$$\mathcal{L}_0(z) = H_0 + \overline{H}_0, \quad \mathcal{L}_1(z) = H_1 + \overline{H}_1, \tag{1.3.32}$$

the SVHPL's of weight two are,

$$\begin{aligned}
 \mathcal{L}_{0,0}(z) &= H_{0,0} + \overline{H}_{0,0} + H_0 \overline{H}_0, \\
 \mathcal{L}_{0,1}(z) &= H_{0,1} + \overline{H}_{1,0} + H_0 \overline{H}_1, \\
 \mathcal{L}_{1,0}(z) &= H_{1,0} + \overline{H}_{0,1} + H_1 \overline{H}_0, \\
 \mathcal{L}_{1,1}(z) &= H_{1,1} + \overline{H}_{1,1} + H_1 \overline{H}_1,
 \end{aligned} \tag{1.3.33}$$

and the SVHPL's of weight three are,

$$\begin{aligned}
 \mathcal{L}_{0,0,0}(z) &= H_{0,0,0} + \overline{H}_{0,0,0} + H_{0,0}\overline{H}_0 + H_0\overline{H}_{0,0}, \\
 \mathcal{L}_{0,0,1}(z) &= H_{0,0,1} + \overline{H}_{1,0,0} + H_{0,0}\overline{H}_1 + H_0\overline{H}_{1,0}, \\
 \mathcal{L}_{0,1,0}(z) &= H_{0,1,0} + \overline{H}_{0,1,0} + H_{0,1}\overline{H}_0 + H_0\overline{H}_{0,1}, \\
 \mathcal{L}_{0,1,1}(z) &= H_{0,1,1} + \overline{H}_{1,1,0} + H_{0,1}\overline{H}_1 + H_0\overline{H}_{1,1}, \\
 \mathcal{L}_{1,0,0}(z) &= H_{1,0,0} + \overline{H}_{0,0,1} + H_{1,0}\overline{H}_0 + H_1\overline{H}_{0,0}, \\
 \mathcal{L}_{1,0,1}(z) &= H_{1,0,1} + \overline{H}_{1,0,1} + H_{1,0}\overline{H}_1 + H_1\overline{H}_{1,0}, \\
 \mathcal{L}_{1,1,0}(z) &= H_{1,1,0} + \overline{H}_{0,1,1} + H_{1,1}\overline{H}_0 + H_1\overline{H}_{0,1}, \\
 \mathcal{L}_{1,1,1}(z) &= H_{1,1,1} + \overline{H}_{1,1,1} + H_{1,1}\overline{H}_1 + H_1\overline{H}_{1,1}.
 \end{aligned} \tag{1.3.34}$$

The y alphabet differs from the x alphabet starting at weight four. Referring to eq. (1.3.25), we expect the difference to generate factors of ζ_3 . To illustrate this effect, we list here the subset of weight-four SVHPLs with explicit ζ terms:

$$\begin{aligned}
 \mathcal{L}_{0,0,1,1}(z) &= H_{0,0,1,1} + \overline{H}_{1,1,0,0} + H_{0,0,1}\overline{H}_1 + H_0\overline{H}_{1,1,0} + H_{0,0}\overline{H}_{1,1} - 2\zeta_3 \overline{H}_1, \\
 \mathcal{L}_{0,1,0,1}(z) &= H_{0,1,0,1} + \overline{H}_{1,0,1,0} + H_{0,1,0}\overline{H}_1 + H_0\overline{H}_{1,0,1} + H_{0,1}\overline{H}_{1,0} + 4\zeta_3 \overline{H}_1, \\
 \mathcal{L}_{0,1,1,1}(z) &= H_{0,1,1,1} + \overline{H}_{1,1,1,0} + H_{0,1,1}\overline{H}_1 + H_0\overline{H}_{1,1,1} + H_{0,1}\overline{H}_{1,1} - 2\zeta_3 \overline{H}_1, \\
 \mathcal{L}_{1,0,1,0}(z) &= H_{1,0,1,0} + \overline{H}_{0,1,0,1} + H_{1,0,1}\overline{H}_0 + H_1\overline{H}_{0,1,0} + H_{1,0}\overline{H}_{0,1} - 4\zeta_3 \overline{H}_1, \\
 \mathcal{L}_{1,0,1,1}(z) &= H_{1,0,1,1} + \overline{H}_{1,1,0,1} + H_{1,0,1}\overline{H}_1 + H_1\overline{H}_{1,1,0} + H_{1,0}\overline{H}_{1,1} + 6\zeta_3 \overline{H}_1, \\
 \mathcal{L}_{1,1,0,0}(z) &= H_{1,1,0,0} + \overline{H}_{0,0,1,1} + H_{1,1,0}\overline{H}_0 + H_1\overline{H}_{0,0,1} + H_{1,1}\overline{H}_{0,0} + 2\zeta_3 \overline{H}_1, \\
 \mathcal{L}_{1,1,0,1}(z) &= H_{1,1,0,1} + \overline{H}_{1,0,1,1} + H_{1,1,0}\overline{H}_1 + H_1\overline{H}_{1,0,1} + H_{1,1}\overline{H}_{1,0} - 6\zeta_3 \overline{H}_1, \\
 \mathcal{L}_{1,1,1,0}(z) &= H_{1,1,1,0} + \overline{H}_{0,1,1,1} + H_{1,1,1}\overline{H}_0 + H_1\overline{H}_{0,1,1} + H_{1,1}\overline{H}_{0,1} + 2\zeta_3 \overline{H}_1.
 \end{aligned} \tag{1.3.35}$$

Finally, we remark that the generating series $\mathcal{L}(z)$ provides a convenient way to represent the differential equations (1.3.15). Together with the y alphabet, it also allows us to write down the differential equations in \bar{z} ,

$$\frac{\partial}{\partial z} \mathcal{L}(z) = \left(\frac{x_0}{z} + \frac{x_1}{1-z} \right) \mathcal{L}(z) \quad \text{and} \quad \frac{\partial}{\partial \bar{z}} \mathcal{L}(z) = \mathcal{L}(z) \left(\frac{y_0}{\bar{z}} + \frac{y_1}{1-\bar{z}} \right). \tag{1.3.36}$$

These equations will be particularly useful in section 1.5 when we study the multi-Regge limit of the ratio function of the six-point NMHV amplitude.

1.4 The six-point remainder function in LLA and NLLA

In section 1.2, we showed that in MRK the remainder function is fully determined by the coefficient functions $g_n^{(\ell)}(w, w^*)$ and $h_n^{(\ell)}(w, w^*)$ in the logarithmic expansion of its real and imaginary part in eq. (1.2.7). We further argued that these functions are single-valued in the complex w plane, and suggested that they can be computed explicitly by interpreting the ν -integral in eq. (1.2.9) as a contour integral and summing the residues. In this section, we describe how knowledge about the space of SVHPLs can be used to facilitate this calculation. In particular, we present results for LLA through ten loops and for NLLA through nine loops.

The main integral we consider is eq. (1.2.9), which we reproduce here for clarity, rewriting the last factor to take into account eqs. (1.2.13) and (1.2.18),

$$\begin{aligned} e^{R+i\pi\delta}|_{\text{MRK}} &= \cos \pi\omega_{ab} + i \frac{a}{2} \sum_{n=-\infty}^{\infty} (-1)^n \left(\frac{w}{w^*} \right)^{\frac{n}{2}} \int_{-\infty}^{+\infty} \frac{d\nu |w|^{2i\nu}}{\nu^2 + \frac{n^2}{4}} \Phi_{\text{Reg}}(\nu, n) \\ &\quad \times \exp \left[-\omega(\nu, n) \left(\log(1 - u_1) + i\pi + \frac{1}{2} \log \frac{|w|^2}{|1 + w|^4} \right) \right]. \end{aligned} \quad (1.4.1)$$

The integrand depends on the BFKL eigenvalue and impact factor, which are known through order a^2 and are given in eqs. (1.2.15), (1.2.16) and (1.2.17). These functions can be written as rational functions of ν and n , and polygamma functions (ψ and its derivatives) with arguments $1 \pm i\nu + |n|/2$. Recalling that the polygamma functions have poles at the non-positive integers, it is easy to see that all poles are found in the complex ν plane at values $\nu = -i(m + \frac{|n|}{2})$, $m \in \mathbb{N}$, $n \in \mathbb{Z}$. When the integral is performed by summing residues, the result will be of the form,

$$\sum_{m,n} a_{m,n} w^{m+n} w^{*m}. \quad (1.4.2)$$

Because residues of the polygamma functions are rational numbers, and because polygamma functions evaluate to Euler-Zagier sums for positive integers, the coefficients $a_{m,n}$ are combinations of

1. rational functions in m and n ,
2. Euler-Zagier sums of the form $Z_{\vec{i}}(m)$, $Z_{\vec{i}}(n)$ and $Z_{\vec{i}}(m+n)$,
3. $\log|w|$, arising from taking residues at multiple poles.

Identifying $(z, \bar{z}) \equiv (-w, -w^*)$, and comparing the double sum (1.4.2) to the formal series expansion of the HPLs around $z = 0$, eq. (1.3.9), we conclude that the double sums will evaluate to linear combinations of terms of the form $H_{w_1}(-w)H_{w_2}(-w^*)$. Moreover, as discussed above, this combination should be single-valued. Therefore, based on the discussion in section 1.3, we expect $g_n^{(\ell)}(w, w^*)$ and $h_n^{(\ell)}(w, w^*)$ to belong to the space spanned by the SVHPLs.

Furthermore, we know that $g_n^{(\ell)}(w, w^*)$ and $h_n^{(\ell)}(w, w^*)$ are invariant under the action of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ transformations of eq. (1.2.8). In terms of SVHPLs, this symmetry is just an (abelian) subgroup of the larger $\mathbb{Z}_2 \times S_3$ symmetry, where the \mathbb{Z}_2 is complex conjugation and the S_3 action is given in eq. (1.3.11). As such, we do not expect an arbitrary linear combination of SVHPLs, but only those that are eigenfunctions with eigenvalue $(+, +)$ of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry.

Putting everything together, and taking into account that scattering amplitudes in $\mathcal{N} = 4$ SYM are expected to have uniform transcendentality, we are led to conjecture that, to all loop orders, $g_n^{(\ell)}(w, w^*)$ and $h_n^{(\ell)}(w, w^*)$ should be expressible as a linear combination of SVHPLs in $(z, \bar{z}) = (-w, -w^*)$ of uniform transcendental weight, with eigenvalue $(+, +)$ under the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. Inspecting eq. (1.2.7), the weight should be $2\ell - n - 1$ for $g_n^{(\ell)}$ and $2\ell - n - 2$ for $h_n^{(\ell)}$. Our conjecture allows us to predict *a priori* the set of functions that can appear at a given loop order, and in practice this set turns out to be rather small. Knowledge of this set of functions can be used to facilitate the evaluation of eq. (1.4.1). We outline two strategies to achieve this:

1. Evaluate the double sum (1.4.2) with the summation algorithms of ref. [61]. The result is a complicated expression involving multiple polylogarithms which can be matched to a combination of SVHPLs and zeta values by means of the symbol [34–37, 147] and coproduct [62–64].
2. The double sum (1.4.2) should be equal to the formal series expansion of some linear combination of SVHPLs and zeta values. The unknown coefficients of this combination can be fixed by matching the two expressions term by term.

To see how this works, we calculate the two-loop remainder function in MRK. Expanding eq. (1.4.1) to two loops, we find,

$$\begin{aligned}
 a^2 R^{(2)} \simeq 2\pi i \left\{ a \left[-\frac{1}{2} L_1^+ + \frac{1}{4} \mathcal{I}[1] \right] \right. \\
 + a^2 \left[\log(1 - u_1) \frac{1}{4} \mathcal{I}[E_{\nu,n}] + \left(\frac{1}{2} \zeta_2 L_1^+ + \frac{1}{4} \mathcal{I}[\Phi_{\text{Reg}}^{(1)}(\nu, n)] + \frac{1}{4} L_1^+ \mathcal{I}[E_{\nu,n}] \right) \right. \\
 \left. \left. + 2\pi i \left(\frac{1}{32} [L_0^-]^2 + \frac{1}{8} [L_1^+]^2 - \frac{1}{8} L_1^+ \mathcal{I}[1] + \frac{1}{8} \mathcal{I}[E_{\nu,n}] \right) \right] \right\}, \quad (1.4.3)
 \end{aligned}$$

where we have introduced the notation,

$$\mathcal{I}[\mathcal{F}(\nu, n)] = \frac{1}{\pi} \sum_{n=-\infty}^{\infty} (-1)^n \left(\frac{w}{w^*} \right)^{\frac{n}{2}} \int_{-\infty}^{+\infty} \frac{d\nu}{\nu^2 + \frac{n^2}{4}} |w|^{2i\nu} \mathcal{F}(\nu, n). \quad (1.4.4)$$

Explicit expressions for the functions L_w^\pm for low weights are provided in appendix A.1. Equation (1.4.3) is consistent only if the term of order a vanishes. Indeed this is the case,

$$\begin{aligned}
 \mathcal{I}[1] &= \frac{1}{\pi} \sum_{n=-\infty}^{\infty} (-1)^n \left(\frac{w}{w^*} \right)^{\frac{n}{2}} \int_{-\infty}^{+\infty} \frac{d\nu}{\nu^2 + \frac{n^2}{4}} |w|^{2i\nu} \\
 &= \log |w|^2 + 2 \sum_{n=1}^{\infty} \frac{(-w)^n}{n} + 2 \sum_{n=1}^{\infty} \frac{(-w^*)^n}{n} \\
 &= \log |w|^2 - 2 \log |1 + w|^2 \\
 &= 2L_1^+.
 \end{aligned} \quad (1.4.5)$$

As previously mentioned, we only take half of the residue at $\nu = n = 0$.

Moving on to the terms of order a^2 , we refer to eq. (1.2.7) and extract from eq. (1.4.3) the expressions for the coefficient functions,

$$\begin{aligned} g_1^{(2)}(w, w^*) &= \frac{1}{4} \mathcal{I}[E_{\nu,n}] \\ g_0^{(2)}(w, w^*) &= \frac{1}{2} \zeta_2 L_1^+ + \frac{1}{4} \mathcal{I}[\Phi_{\text{Reg}}^{(1)}(\nu, n)] + \frac{1}{4} L_1^+ \mathcal{I}[E_{\nu,n}] \\ h_0^{(2)}(w, w^*) &= \frac{1}{32} [L_0^-]^2 + \frac{1}{8} [L_1^+]^2 - \frac{1}{8} L_1^+ \mathcal{I}[1] + \frac{1}{8} \mathcal{I}[E_{\nu,n}]. \end{aligned} \quad (1.4.6)$$

Note that $h_1^{(2)} = 0$, in accordance with the general expectation that $h_{l-1}^{(l)} = 0$. Proceeding onwards, we have to calculate $\mathcal{I}[E_{\nu,n}]$,

$$\begin{aligned} \mathcal{I}[E_{\nu,n}] &= \frac{1}{\pi} \sum_{n=-\infty}^{\infty} (-1)^n \left(\frac{w}{w^*} \right)^{\frac{n}{2}} \int_{-\infty}^{+\infty} \frac{d\nu}{\nu^2 + \frac{n^2}{4}} |w|^{2i\nu} \left\{ 2\gamma_E + \frac{|n|}{2(\nu^2 + \frac{n^2}{4})} \right. \\ &\quad \left. + \psi \left(i\nu + \frac{|n|}{2} \right) + \psi \left(-i\nu + \frac{|n|}{2} \right) \right\} \\ &= \sum_{m=1}^{\infty} \left\{ 2 \frac{|w|^{2m}}{m^2} - 2 \frac{(-w)^m + (-w^*)^m}{m^2} \right. \\ &\quad \left. + [\log |w|^2 + 2Z_1(m)] \frac{(-w)^m + (-w^*)^m}{m} \right\} \\ &\quad + 2 \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{(-1)^n}{m(m+n)} \{ w^{m+n} w^{*m} + w^m w^{*m+n} \}. \end{aligned} \quad (1.4.7)$$

The single sum in the first line immediately evaluates to polylogarithms,

$$\begin{aligned} &\sum_{m=1}^{\infty} \left\{ 2 \frac{|w|^{2m}}{m^2} - 2 \frac{(-w)^m + (-w^*)^m}{m^2} + [\log |w|^2 + 2Z_1(m)] \frac{(-w)^m + (-w^*)^m}{m} \right\} \\ &= \sum_{m=1}^{\infty} \left\{ 2 \frac{|w|^{2m}}{m^2} + [\log |w|^2 + 2Z_1(m-1)] \frac{(-w)^m + (-w^*)^m}{m} \right\} \\ &= \log |w|^2 [H_1(-w) + H_1(-w^*)] + 2H_{0,1}(|w|^2) + 2H_{1,1}(-w) \\ &\quad + 2H_{1,1}(-w^*). \end{aligned} \quad (1.4.8)$$

Next we transform the double sum into a nested sum by shifting the summation variables by $n = N - m$,

$$\begin{aligned}
 & \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{(-1)^n}{m(m+n)} \{w^{m+n} w^{*m} + w^m w^{*m+n}\} \\
 &= \sum_{N=1}^{\infty} \sum_{m=1}^{N-1} \left\{ \frac{(-w)^N (-w^*)^m}{N m} + \frac{(-w)^m (-w^*)^N}{N m} \right\} \\
 &= \text{Li}_{1,1}(-w, -w^*) + \text{Li}_{1,1}(-w^*, -w) \\
 &= H_1(-w) H_1(-w^*) - H_{0,1}(|w|^2),
 \end{aligned} \tag{1.4.9}$$

where the last step follows from a stuffle identity among multiple polylogarithms [65]. Putting everything together, we obtain

$$\begin{aligned}
 \mathcal{I}[E_{\nu,n}] &= \log |w|^2 [H_1(-w) + H_1(-w^*)] + 2H_{1,1}(-w) + 2H_{1,1}(-w^*) \\
 &\quad + 2H_1(-w) H_1(-w^*) \\
 &= [L_1^+]^2 - \frac{1}{4} [L_0^-]^2.
 \end{aligned} \tag{1.4.10}$$

Referring to eqs. (1.4.5) and (1.4.6), we can now write down the results,

$$\begin{aligned}
 g_1^{(2)}(w, w^*) &= \frac{1}{4} [L_1^+]^2 - \frac{1}{16} [L_0^-]^2, \\
 h_0^{(2)}(w, w^*) &= 0.
 \end{aligned} \tag{1.4.11}$$

For higher weights the nested double sums can be more complicated, but they are always of a form that can be performed using the algorithms of ref. [61]. These algorithms will in general produce complicated multiple polylogarithms that, unlike in eq. (1.4.9), cannot in general be reduced to HPLs by the simple application of stuffle identities. In this case we can use symbols [36, 37, 147] and the coproduct on multiple polylogarithms [62–64] to perform this reduction.

The above strategy becomes computationally taxing for high weights. For this reason, we also employ an alternative strategy, based on matching series expansions, which is computationally simpler. We demonstrate this method in the computation

of $g_0^{(2)}$, for which the only missing ingredient in eq. (1.4.6) is $\mathcal{I}[\Phi_{\text{Reg}}^{(1)}(\nu, n)]$, where $\Phi_{\text{Reg}}^{(1)}(\nu, n)$ is defined in eq. (1.2.17). To proceed, we write the ν -integral as a sum of residues, and truncate the resulting double sum to some finite order,

$$\begin{aligned}
 \mathcal{I}[\Phi_{\text{Reg}}^{(1)}(\nu, n)] &= \frac{1}{\pi} \sum_{n=-\infty}^{\infty} (-1)^n \left(\frac{w}{w^*}\right)^{\frac{n}{2}} \int_{-\infty}^{+\infty} \frac{d\nu |w|^{2i\nu}}{\nu^2 + \frac{n^2}{4}} \left\{ -\zeta_2 - \frac{3}{8} \frac{n^2}{(\nu^2 + \frac{n^2}{4})^2} \right. \\
 &\quad \left. - \frac{1}{2} \left(2\gamma_E + \frac{|n|}{2(\nu^2 + \frac{n^2}{4})} + \psi\left(i\nu + \frac{|n|}{2}\right) + \psi\left(-i\nu + \frac{|n|}{2}\right) \right)^2 \right\} \\
 &= -\zeta_2 \log |w|^2 - (\log |w|^2) |w|^2 - \left(1 + \frac{1}{4} \log |w|^2\right) |w|^4 + \dots \\
 &\quad + (w + w^*) \left[2\zeta_2 + \left(4 - 2 \log |w|^2 + \frac{1}{2} \log^2 |w|^2\right) \right. \\
 &\quad \quad \left. + \left(1 + \frac{1}{2} \log |w|^2\right) |w|^2 + \dots \right] \\
 &\quad + (w^2 + w^{*2}) \left[-\zeta_2 - \left(\frac{1}{2} + \frac{1}{4} \log^2 |w|^2\right) \right. \\
 &\quad \quad \left. + \left(-1 - \frac{1}{3} \log |w|^2\right) |w|^2 + \dots \right] \\
 &\quad + \dots
 \end{aligned} \tag{1.4.12}$$

Here we show on separate lines the contributions to the sum from $n = 0$, $n = \pm 1$, and $n = \pm 2$. Next, we construct an ansatz of SVHPLs whose series expansion we attempt to match to the above expression. We expect the result to be a weight-three SVHPL with parity $(+, +)$ under conjugation and inversion. Including zeta values, there are five functions satisfying these criteria, and we can write the ansatz as,

$$\mathcal{I}[\Phi_{\text{Reg}}^{(1)}(\nu, n)] = c_1 L_3^+ + c_2 [L_0^-]^2 L_1^+ + c_3 [L_1^+]^3 + c_4 \zeta_2 L_1^+ + c_5 \zeta_3. \tag{1.4.13}$$

Using the series expansions of the constituent HPLs (1.3.9), it is straightforward to

produce the series expansion of this ansatz,

$$\begin{aligned}
 \mathcal{I}[\Phi_{\text{Reg}}^{(1)}(\nu, n)] &= \left(\frac{c_1}{12} + \frac{c_2}{2} + \frac{c_3}{8} \right) \log^3 |w|^2 + \frac{1}{2} c_4 \zeta_2 \log |w|^2 + c_5 \zeta_3 \\
 &\quad + 3 c_3 (\log |w|^2) |w|^2 + \dots \\
 &\quad + (w + w^*) \left[-\zeta_2 c_4 + \left(-c_1 + \frac{1}{2} c_1 \log |w|^2 \right) \right. \\
 &\quad \quad \left. + \left(-\frac{c_1}{4} - c_2 - \frac{3c_3}{4} \right) \log^2 |w|^2 + \dots \right] \\
 &\quad + \dots
 \end{aligned} \tag{1.4.14}$$

We have only listed the terms necessary to fix the undetermined constants. In practice we generate many more terms than necessary to cross-check the result. Consistency of eqs. (1.4.12) and (1.4.14) requires,

$$c_1 = -4, \quad c_2 = \frac{3}{4}, \quad c_3 = -\frac{1}{3}, \quad c_4 = -2, \quad c_5 = 0, \tag{1.4.15}$$

which gives,

$$\mathcal{I}[\Phi_{\text{Reg}}^{(1)}(\nu, n)] = -4 L_3^+ + \frac{3}{4} [L_0^-]^2 L_1^+ - \frac{1}{3} [L_1^+]^3 - 2 \zeta_2 L_1^+. \tag{1.4.16}$$

Finally, putting everything together in eq. (1.4.6),

$$g_0^{(2)}(w, w^*) = -L_3^+ + \frac{1}{6} [L_1^+]^3 + \frac{1}{8} [L_0^-]^2 L_1^+. \tag{1.4.17}$$

This completes the two-loop calculation, and we find agreement with [10, 12]. Moving on to three loops, we can proceed in exactly the same way, and we reproduce the LLA [12] and NLLA results [14, 15] for the imaginary parts of the coefficient functions,

$$\begin{aligned}
 g_2^{(3)}(w, w^*) &= -\frac{1}{8} L_3^+ + \frac{1}{12} [L_1^+]^3, \\
 g_1^{(3)}(w, w^*) &= \frac{1}{8} L_0^- L_{2,1}^- - \frac{5}{8} L_1^+ L_3^+ + \frac{5}{48} [L_1^+]^4 + \frac{1}{16} [L_0^-]^2 [L_1^+]^2 - \frac{5}{768} [L_0^-]^4 \\
 &\quad - \frac{\pi^2}{12} [L_1^+]^2 + \frac{\pi^2}{48} [L_0^-]^2 + \frac{1}{4} \zeta_3 L_1^+.
 \end{aligned} \tag{1.4.18}$$

(The result for $g_1^{(3)}$ agrees with that in ref. [14] once the constants are fixed to $c = 0$ and $\gamma' = -9/2$ [15].) The real parts are given by,

$$\begin{aligned} h_2^{(3)}(w, w^*) &= 0, \\ h_1^{(3)}(w, w^*) &= -\frac{1}{8}L_3^+ - \frac{1}{24}[L_1^+]^3 + \frac{1}{32}[L_0^-]^2 L_1^+, \end{aligned} \quad (1.4.19)$$

in agreement with ref. [12]. Using the fact that

$$L_1^+ = \frac{1}{2} \log \frac{|w|^2}{|1+w|^4}, \quad (1.4.20)$$

it is easy to check that $h_1^{(3)}(w, w^*)$ satisfies eq. (1.2.19) for $\ell = 3$.

It is straightforward to extend these methods to higher loops. We have produced results for all functions with weight less than or equal to 10, which is equivalent to 10 loops in the LLA, and 9 loops in the NLLA. Using the C++ symbolic computation framework GiNaC [66], which allows for the efficient numerical evaluation of HPLs to high precision [67], we can evaluate these functions numerically. Figures 1.1 and 1.2 show the functions plotted on the line segment for which $w = w^*$ and $0 < w < 1$. Here we also show the analytical results through six loops. We provide a separate computer-readable text file, compatible with the *Mathematica* package HPL [68, 69], which contains all the expressions through weight 10.

Up to six loops, we find,

$$\begin{aligned} g_3^{(4)}(w, w^*) &= \frac{1}{48}[L_2^-]^2 + \frac{1}{48}[L_0^-]^2 [L_1^+]^2 + \frac{7}{2304}[L_0^-]^4 + \frac{1}{48}[L_1^+]^4 \\ &\quad - \frac{1}{16}L_0^- L_{2,1}^- - \frac{5}{48}L_1^+ L_3^+ - \frac{1}{8}L_1^+ \zeta_3, \end{aligned} \quad (1.4.21)$$

$$\begin{aligned} g_2^{(4)}(w, w^*) &= \frac{3}{64}[L_0^-]^2 [L_1^+]^3 + \frac{1}{128}L_1^+ [L_0^-]^4 - \frac{3}{32}L_3^+ [L_0^-]^2 + \frac{1}{8}\zeta_3 [L_0^-]^2 \\ &\quad - \frac{1}{8}\zeta_3 [L_1^+]^2 + \frac{3}{80}[L_1^+]^5 - \frac{\pi^2}{24}[L_1^+]^3 - \frac{1}{16}L_0^- L_{2,1}^- L_1^+ \\ &\quad + \frac{13}{16}L_5^+ + \frac{3}{8}L_{3,1,1}^+ + \frac{1}{4}L_{2,2,1}^+ - \frac{5}{16}L_3^+ [L_1^+]^2 + \frac{\pi^2}{16}L_3^+, \end{aligned} \quad (1.4.22)$$

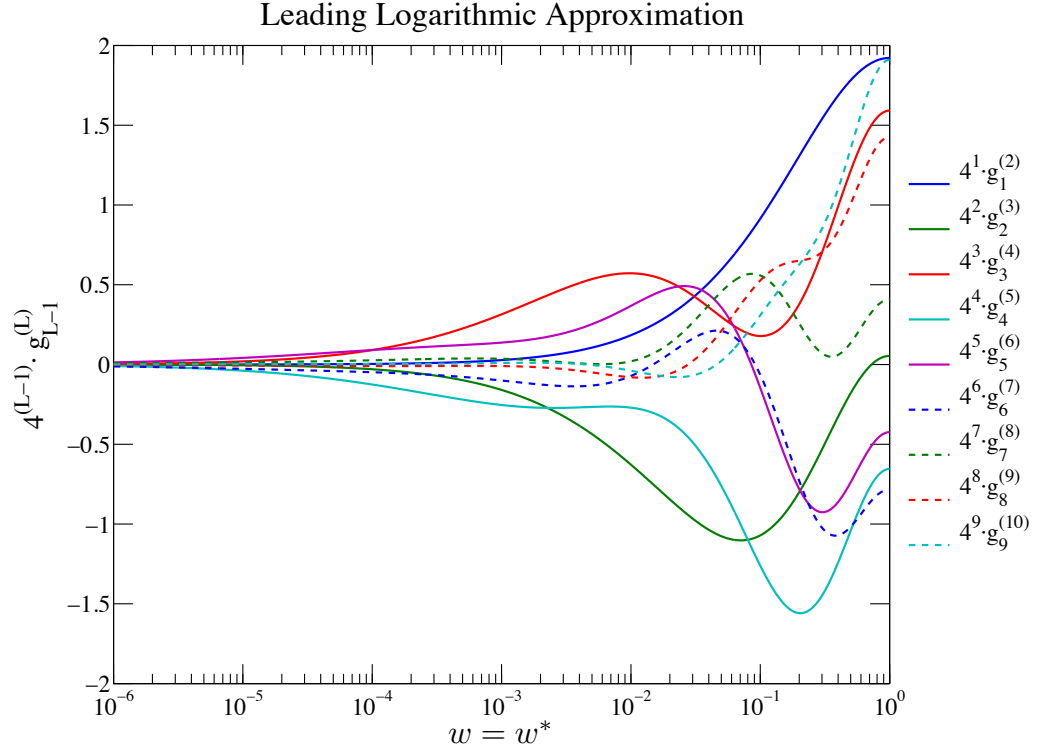


Figure 1.1: Imaginary parts $g_{\ell-1}^{(\ell)}$ of the MHV remainder function in MRK and LLA through 10 loops, on the line segment with $w = w^*$ running from 0 to 1. The functions have been rescaled by powers of 4 so that they are all roughly the same size.

$$\begin{aligned}
 g_4^{(5)}(w, w^*) = & \frac{1}{96} [L_0^-]^2 [L_1^+]^3 + \frac{17}{9216} L_1^+ [L_0^-]^4 - \frac{5}{384} L_3^+ [L_0^-]^2 \quad (1.4.23) \\
 & - \frac{1}{12} [L_1^+]^2 \zeta_3 + \frac{1}{240} [L_1^+]^5 - \frac{1}{24} L_0^- L_{2,1}^- L_1^+ + \frac{43}{384} L_5^+ \\
 & + \frac{1}{8} L_{3,1,1}^+ + \frac{1}{12} L_{2,2,1}^+ - \frac{1}{24} L_3^+ [L_1^+]^2 + \frac{1}{24} [L_0^-]^2 \zeta_3,
 \end{aligned}$$

$$\begin{aligned}
 g_3^{(5)}(w, w^*) = & -\frac{1}{384} [L_2^-]^2 [L_0^-]^2 + \frac{5}{64} [L_2^-]^2 [L_1^+]^2 - \frac{\pi^2}{72} [L_2^-]^2 \quad (1.4.24) \\
 & + \frac{1}{384} [L_0^-]^4 [L_1^+]^2 - \frac{7}{48} \zeta_3^2 + \frac{5}{144} [L_0^-]^2 [L_1^+]^4 \\
 & - \frac{31}{1152} L_{2,1}^- [L_0^-]^3 - \frac{11}{384} L_1^+ L_3^+ [L_0^-]^2 - \frac{7}{48} L_1^+ [L_0^-]^2 \zeta_3 \\
 & + \frac{31}{69120} [L_0^-]^6 + \frac{7}{48} [L_{2,1}^-]^2 - \frac{31}{192} L_0^- L_{2,1}^- [L_1^+]^2
 \end{aligned}$$

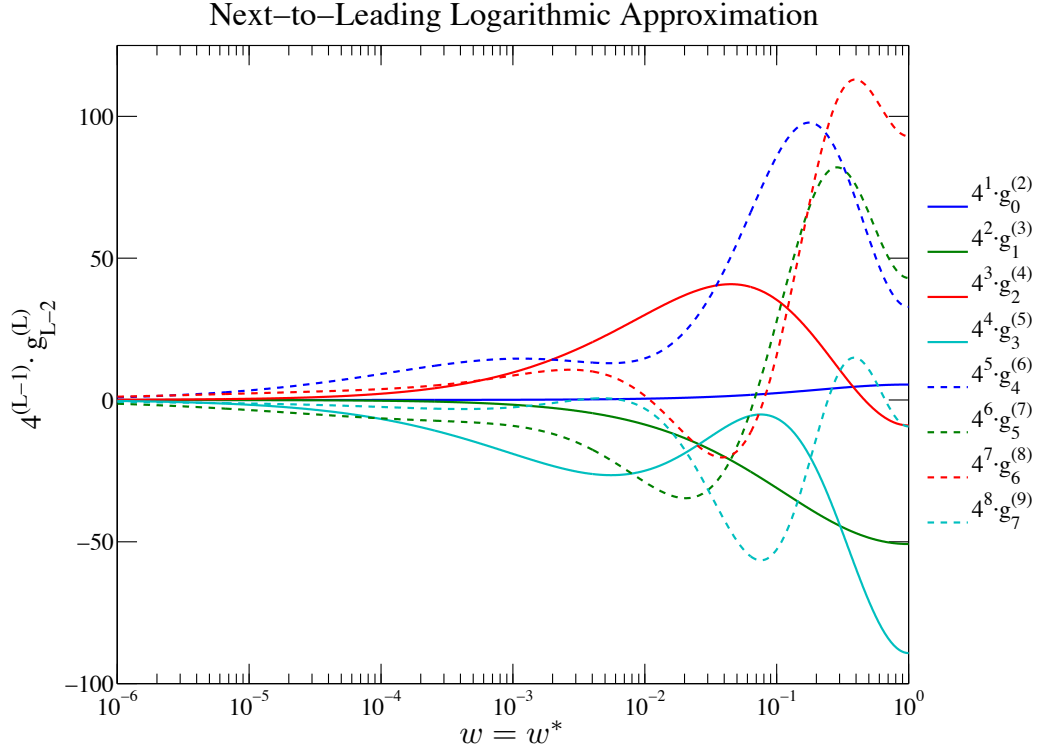


Figure 1.2: Imaginary parts $g_{\ell-2}^{(\ell)}$ of the MHV remainder function in MRK and NLLA through 9 loops.

$$\begin{aligned}
 & -\frac{65}{576} L_3^+ [L_1^+]^3 - \frac{13}{96} [L_1^+]^3 \zeta_3 + \frac{7}{720} [L_1^+]^6 - \frac{\pi^2}{72} [L_1^+]^4 \\
 & + \frac{5}{96} L_4^- L_2^- - \frac{7}{24} L_2^- L_{2,1,1}^- + \frac{1}{192} L_0^- L_{4,1}^- + \frac{1}{16} L_0^- L_{3,2}^- \\
 & + \frac{\pi^2}{24} L_0^- L_{2,1}^- + \frac{9}{16} L_0^- L_{2,1,1,1}^- - \frac{5}{32} L_3^+ \zeta_3 + \frac{33}{64} L_5^+ L_1^+ \\
 & + \frac{1}{48} [L_3^+]^2 + \frac{5\pi^2}{72} L_1^+ L_3^+ - \frac{7}{48} L_1^+ L_{3,1,1}^+ + \frac{25}{32} L_1^+ \zeta_5 \\
 & - \frac{\pi^2}{72} [L_0^-]^2 [L_1^+]^2 - \frac{7\pi^2}{3456} [L_0^-]^4 + \frac{\pi^2}{12} L_1^+ \zeta_3, \\
 g_5^{(6)}(w, w^*) = & \frac{103}{15360} [L_2^-]^2 [L_0^-]^2 - \frac{1}{64} [L_2^-]^2 [L_1^+]^2 + \frac{1}{576} [L_0^-]^2 [L_1^+]^4 \\
 & + \frac{1}{720} [L_0^-]^4 [L_1^+]^2 + \frac{29}{9216} L_{2,1}^- [L_0^-]^3 - \frac{77}{5120} L_1^+ L_3^+ [L_0^-]^2 \\
 & + \frac{29}{512} L_1^+ [L_0^-]^2 \zeta_3 + \frac{73}{1382400} [L_0^-]^6 - \frac{1}{48} [L_{2,1}^-]^2
 \end{aligned} \tag{1.4.25}$$

$$\begin{aligned}
 & -\frac{1}{192} L_0^- L_{2,1}^- [L_1^+]^2 - \frac{7}{576} L_3^+ [L_1^+]^3 + \frac{1}{1440} [L_1^+]^6 \\
 & + \frac{43}{3840} [L_3^+]^2 - \frac{29}{960} L_4^- L_2^- + \frac{1}{24} L_2^- L_{2,1,1}^- - \frac{25}{768} L_0^- L_{4,1}^- \\
 & - \frac{3}{128} L_0^- L_{3,2}^- - \frac{1}{16} L_0^- L_{2,1,1,1}^- + \frac{301}{3840} L_5^+ L_1^+ + \frac{7}{48} L_1^+ L_{3,1,1}^+ \\
 & + \frac{1}{12} L_1^+ L_{2,2,1}^+ - \frac{1}{32} [L_1^+]^3 \zeta_3 - \frac{3}{128} L_1^+ \zeta_5 + \frac{3}{128} L_3^+ \zeta_3 + \frac{1}{48} \zeta_3^2,
 \end{aligned}$$

$$\begin{aligned}
 g_4^{(6)}(w, w^*) = & \frac{5}{1536} L_1^+ [L_2^-]^2 [L_0^-]^2 + \frac{1}{48} [L_2^-]^2 [L_1^+]^3 - \frac{101}{3072} L_3^+ [L_0^-]^2 [L_1^+]^2 \quad (1.4.26) \\
 & + \frac{89}{1536} [L_0^-]^2 [L_1^+]^2 \zeta_3 + \frac{59}{5760} [L_0^-]^2 [L_1^+]^5 - \frac{1}{128} L_{2,2,1}^+ [L_0^-]^2 \\
 & - \frac{317}{9216} L_{2,1}^- L_1^+ [L_0^-]^3 - \frac{43}{768} L_5^+ [L_0^-]^2 + \frac{77}{221184} L_1^+ [L_0^-]^6 \\
 & + \frac{65}{9216} L_3^+ [L_0^-]^4 + \frac{25\pi^2}{2304} L_3^+ [L_0^-]^2 + \frac{85}{18432} [L_0^-]^4 [L_1^+]^3 \\
 & - \frac{1}{24} L_1^+ [L_{2,1}^-]^2 - \frac{3}{64} L_0^- L_{2,1}^- [L_1^+]^3 + \frac{205}{768} L_5^+ [L_1^+]^2 \\
 & - \frac{17}{576} L_3^+ [L_1^+]^4 - \frac{1}{48} L_{3,1,1}^+ [L_1^+]^2 + \frac{1}{24} L_{2,2,1}^+ [L_1^+]^2 \\
 & + \frac{5\pi^2}{72} [L_1^+]^2 \zeta_3 + \frac{1}{504} [L_1^+]^7 - \frac{\pi^2}{288} [L_1^+]^5 + \frac{7}{192} L_1^+ [L_3^+]^2 \\
 & - \frac{5}{192} L_4^- L_2^- L_1^+ + \frac{11}{192} L_2^- L_0^- L_{3,1}^+ - \frac{1}{6} L_2^- L_{2,1,1}^- L_1^+ \\
 & - \frac{13}{384} L_0^- L_{3,2}^- L_1^+ + \frac{5\pi^2}{144} L_0^- L_{2,1}^- L_1^+ + \frac{23}{384} L_0^- L_{2,1}^- L_3^+ \\
 & + \frac{3}{16} L_0^- L_{2,1,1,1}^- L_1^+ - \frac{215\pi^2}{2304} L_5^+ + \frac{1}{16} L_7^+ - \frac{5}{768} L_0^- L_{4,1}^- L_1^+ \\
 & - \frac{151}{128} L_{5,1,1}^+ - \frac{3}{32} L_{4,1,2}^+ - \frac{27}{64} L_{4,2,1}^+ - \frac{5\pi^2}{48} L_{3,1,1}^+ - \frac{7}{64} L_{3,3,1}^+ \\
 & + \frac{13}{4} L_{3,1,1,1,1}^+ + \frac{1}{2} L_{2,1,2,1,1}^+ + \frac{3}{2} L_{2,2,1,1,1}^+ - \frac{7}{96} [L_1^+]^4 \zeta_3 \\
 & - \frac{1}{48} [L_2^-]^2 \zeta_3 - \frac{5\pi^2}{576} [L_0^-]^2 [L_1^+]^3 - \frac{85\pi^2}{55296} L_1^+ [L_0^-]^4 + \frac{1}{768} [L_0^-]^4 \zeta_3 \\
 & - \frac{17}{192} [L_0^-]^2 \zeta_5 - \frac{5\pi^2}{144} [L_0^-]^2 \zeta_3 + \frac{5\pi^2}{144} L_3^+ [L_1^+]^2 + \frac{65}{128} [L_1^+]^2 \zeta_5 \\
 & - \frac{21}{64} L_0^- L_{2,1}^- \zeta_3 - \frac{29}{384} L_1^+ L_3^+ \zeta_3 - \frac{19}{192} L_1^+ \zeta_3^2 - \frac{5\pi^2}{72} L_{2,2,1}^+.
 \end{aligned}$$

We present only the imaginary parts, as the real parts are determined by eq. (1.2.19). However, as a cross-check of our result, we computed the $h_n^{(\ell)}$ explicitly and checked that eq. (1.2.19) is satisfied. Furthermore, we checked that in the collinear limit $w \rightarrow 0$ our results agree with the all-loop prediction for the six-point MHV amplitude in the double-leading-logarithmic (DLL) and next-to-double-leading-logarithmic (NDLL) approximations of ref. [70],

$$\begin{aligned} e^{R_{\text{DLLA}}} &= i\pi a (w + w^*) \left[1 - I_0 \left(2\sqrt{a \log |w| \log(1 - u_1)} \right) \right], \\ \text{Re} \left(e^{R_{\text{NDLLA}}} \right) &= 1 + \pi^2 a^{3/2} (w + w^*) \sqrt{\log |w|} \frac{I_1 \left(2\sqrt{a \log |w| \log(1 - u_1)} \right)}{\sqrt{\log(1 - u_1)}} \\ &\quad - \pi^2 a^2 (w + w^*) \log |w| I_0 \left(2\sqrt{a \log |w| \log(1 - u_1)} \right), \end{aligned} \quad (1.4.27)$$

where $I_0(z)$ and $I_1(z)$ denote modified Bessel functions.

Let us conclude this section with an observation: All the results for the six-point remainder function that we computed only involve ordinary ζ values of depth one (ζ_k for some k), despite the fact that multiple ζ values are expected to appear starting from weight eight. In addition, the LLA results only involve odd ζ values – even ζ values never appear.

1.5 The six-point NMHV amplitude in MRK

So far we have only discussed the multi-Regge limit of the six-point amplitude in an MHV helicity configuration. In this section we extend the discussion to the second independent helicity configuration for six points, the NMHV configuration. We will see that the SVHPLs provide the natural function space for describing this case as well.

The NMHV case was recently analyzed in the LLA [18]. It was shown that the two-loop expression agrees with the limit of the analytic formula for the NMHV amplitude for general kinematics [71], and the three-loop result was also obtained. Here we will extend these results to 10 loops.

Due to helicity conservation along the high-energy line, the only difference between

the MHV and NMHV configurations is a flip in helicity of one of the lower energy external gluons (labeled by 4 and 5). Instead of the MHV helicity configuration $(++-+-)$, we consider $(++--+-)$. The tree amplitudes for MHV and NMHV become identical in MRK [18]. In this limit, we can define the NMHV remainder function R_{NMHV} in the same way as in the MHV case (1.1.1),

$$A_6^{\text{NMHV}}|_{\text{MRK}} = A_6^{\text{BDS}} \times \exp(R_{\text{NMHV}}). \quad (1.5.1)$$

Recall the LLA version⁴ of eq. (1.2.9):

$$R_{\text{MHV}}^{\text{LLA}} = i \frac{a}{2} \sum_{n=-\infty}^{\infty} (-1)^n \int_{-\infty}^{+\infty} \frac{d\nu w^{i\nu+n/2} w^{*i\nu-n/2}}{(i\nu + \frac{n}{2})(-i\nu + \frac{n}{2})} \left[(1 - u_1)^{a E_{\nu,n}} - 1 \right]. \quad (1.5.2)$$

At LLA, the effect of changing the impact factor for emitting gluon 4 with positive helicity to the one for a negative-helicity emission is simply to perform the replacement

$$\frac{1}{-i\nu + \frac{n}{2}} \rightarrow -\frac{1}{i\nu + \frac{n}{2}} \quad (1.5.3)$$

in eq. (1.5.2), obtaining [18]

$$R_{\text{NMHV}}^{\text{LLA}} \simeq -\frac{ia}{2} \sum_{n=-\infty}^{\infty} (-1)^n \int_{-\infty}^{+\infty} \frac{d\nu w^{i\nu+n/2} w^{*i\nu-n/2}}{(i\nu + \frac{n}{2})^2} \left[(1 - u_1)^{a E_{\nu,n}} - 1 \right]. \quad (1.5.4)$$

The NMHV ratio function is normally defined in terms of the ratio of NMHV to MHV superamplitudes \mathcal{A} ,

$$\mathcal{P}_{\text{NMHV}} = \frac{\mathcal{A}_{\text{NMHV}}}{\mathcal{A}_{\text{MHV}}}. \quad (1.5.5)$$

However, in MRK, because the tree amplitudes become identical, it suffices to consider the ordinary ratio, which in LLA becomes

$$\mathcal{P}_{\text{NMHV}}^{\text{LLA}} = \frac{A_{\text{NMHV}}^{\text{LLA}}}{A_{\text{MHV}}^{\text{LLA}}} = \exp(R_{\text{NMHV}}^{\text{LLA}} - R_{\text{MHV}}^{\text{LLA}}). \quad (1.5.6)$$

⁴The distinction between R and $\exp(R)$ is irrelevant at LLA, because the LLA has one fewer logarithm than the loop order, so the square of an LL term has two fewer logarithms and is NLL.

Thus eq. (1.5.4), together with eq. (1.5.2), is sufficient to generate both the remainder function and the ratio function in LLA.

Comparing eq. (1.5.4) to eq. (1.2.9), we see that in MRK the MHV and NMHV remainder functions are related by

$$R_{\text{NMHV}}^{\text{LLA}} = \int dw \frac{w^*}{w} \frac{\partial}{\partial w^*} R_{\text{MHV}}^{\text{LLA}}. \quad (1.5.7)$$

It is convenient to write this equation slightly differently. First, define a sequence of single-valued functions $f^{(l)}(w, w^*)$ in analogy with eq. (1.2.7)⁵

$$R_{\text{NMHV}}^{\text{LLA}} = 2\pi i \sum_{l=2}^{\infty} a^l \log^{l-1}(1 - u_1) \left[\frac{1}{1 + w^*} f^{(l)}(w, w^*) + \frac{w^*}{1 + w^*} f^{(l)}\left(\frac{1}{w}, \frac{1}{w^*}\right) \right]. \quad (1.5.8)$$

Then eq. (1.5.7) can be used to relate $f^{(l)}(w, w^*)$ to $g_{l-1}^{(l)}(w, w^*)$,

$$\int dw \frac{w^*}{w} \frac{\partial}{\partial w^*} g_{l-1}^{(l)}(w, w^*) = \frac{1}{1 + w^*} f^{(l)}(w, w^*) + \frac{w^*}{1 + w^*} f^{(l)}\left(\frac{1}{w}, \frac{1}{w^*}\right). \quad (1.5.9)$$

In section 1.4 we computed the MHV remainder function in the LLA in the multi-Regge limit up to ten loops. Using these results and eq. (1.5.9), we can immediately obtain NMHV expressions through ten loops as well. Indeed, $g_{l-1}^{(l)}(w, w^*)$ is a sum of SVHPLs, so the differentiation $\frac{\partial}{\partial w^*}$ can be performed with the aid of eq. (1.3.36). The result is again a sum of SVHPLs with rational coefficients $1/(1 + w^*)$ and $w^*/(1 + w^*)$. As such, the differential equations (1.3.36) also uniquely determine the result of the w -integral as a sum of SVHPLs, up to an undetermined function $F(w^*)$. This function can be at most a constant in order to preserve the single-valuedness condition. It turns out that to respect the vanishing of the remainder function in the collinear limit, $F(w^*)$ must actually be zero.

To see how this works, consider the two loop case. From eq. (1.4.11),

$$g_1^{(2)}(w, w^*) = \frac{1}{4} [L_1^+]^2 - \frac{1}{16} [L_0^-]^2 = \frac{1}{2} \mathcal{L}_{1,1} + \frac{1}{4} \mathcal{L}_{0,1} + \frac{1}{4} \mathcal{L}_{1,0}. \quad (1.5.10)$$

⁵Ref. [18] defines a similar set of functions, f_l , which are related to ours by $f_2 = -\frac{1}{4}f^{(2)}$, $f_3 = \frac{1}{8}f^{(3)}$, etc.

Recalling that $(w, w^*) = (-z, -\bar{z})$, first use the second eq. (1.3.36) to take the w^* derivative, which clips off the last index in the SVHPL, with a different prefactor depending on whether it is a ‘0’ or a ‘1’ (and with corrections due to the y alphabet at higher weights):

$$\begin{aligned} w^* \frac{\partial}{\partial w^*} g_1^{(2)}(w, w^*) &= -\frac{1}{2} \left(\frac{w^*}{1+w^*} \right) \mathcal{L}_1 - \frac{1}{4} \left(\frac{w^*}{1+w^*} \right) \mathcal{L}_0 + \frac{1}{4} \mathcal{L}_1 \\ &= \frac{w^*}{1+w^*} \left[-\frac{1}{4} \mathcal{L}_1 - \frac{1}{4} \mathcal{L}_0 \right] + \frac{1}{1+w^*} \left[\frac{1}{4} \mathcal{L}_1 \right]. \end{aligned} \quad (1.5.11)$$

Next, use the first eq. (1.3.36) to perform the w -integration. In practice, this amounts to prepending a ‘0’ to the weight vector of each SVHPL,

$$\begin{aligned} \int dw \frac{w^*}{w} \frac{\partial}{\partial w^*} g_1^{(2)} &= \frac{w^*}{1+w^*} \left[-\frac{1}{4} \mathcal{L}_{0,1} - \frac{1}{4} \mathcal{L}_{0,0} \right] + \frac{1}{1+w^*} \left[\frac{1}{4} \mathcal{L}_{0,1} \right] \\ &= \frac{1}{1+w^*} f^{(2)}(w, w^*) + \frac{w^*}{1+w^*} f^{(2)}\left(\frac{1}{w}, \frac{1}{w^*}\right), \end{aligned} \quad (1.5.12)$$

where

$$\begin{aligned} f^{(2)}(w, w^*) &= \frac{1}{4} \mathcal{L}_{0,1} \\ &= \frac{1}{4} L_2 + \frac{1}{8} L_0 L_1 \\ &= -\frac{1}{4} \left(\log |w|^2 \log(1+w^*) - \text{Li}_2(-w) + \text{Li}_2(-w^*) \right). \end{aligned} \quad (1.5.13)$$

This result agrees with the one presented in ref. [18]. Furthermore, we can check that the inversion property implicit in eq. (1.5.12) is satisfied,

$$\begin{aligned} f^{(2)}\left(\frac{1}{w}, \frac{1}{w^*}\right) &= -\frac{1}{4} \left[-\log |w|^2 \log \left(1 + \frac{1}{w^*} \right) - \text{Li}_2 \left(-\frac{1}{w} \right) + \text{Li}_2 \left(-\frac{1}{w^*} \right) \right] \\ &= -\frac{1}{4} \left[\frac{1}{2} \log^2 |w|^2 - \log |w|^2 \log(1+w^*) + \text{Li}_2(-w) - \text{Li}_2(-w^*) \right] \\ &= -\frac{1}{4} \mathcal{L}_{0,1} - \frac{1}{4} \mathcal{L}_{0,0}. \end{aligned} \quad (1.5.14)$$

Moving on to three loops, we start with the MHV LLA term,

$$\begin{aligned}
 g_2^{(3)}(w, w^*) &= -\frac{1}{8}L_3^+ + \frac{1}{12}[L_1^+]^3 \\
 &= \frac{1}{16}\mathcal{L}_{0,0,1} + \frac{1}{8}\mathcal{L}_{0,1,0} + \frac{1}{4}\mathcal{L}_{0,1,1} + \frac{1}{16}\mathcal{L}_{1,0,0} + \frac{1}{4}\mathcal{L}_{1,0,1} + \frac{1}{4}\mathcal{L}_{1,1,0} \\
 &\quad + \frac{1}{2}\mathcal{L}_{1,1,1}.
 \end{aligned} \tag{1.5.15}$$

As before, we can take derivatives and integrate using eq. (1.3.36),

$$\begin{aligned}
 \int dw \frac{w^*}{w} \frac{\partial}{\partial w^*} g_2^{(3)} &= \frac{w^*}{1+w^*} \left[-\frac{1}{16}\mathcal{L}_{0,0,0} - \frac{1}{8}\mathcal{L}_{0,0,1} - \frac{3}{16}\mathcal{L}_{0,1,0} - \frac{1}{4}\mathcal{L}_{0,1,1} \right] \\
 &\quad + \frac{1}{1+w^*} \left[\frac{1}{8}\mathcal{L}_{0,0,1} + \frac{1}{16}\mathcal{L}_{0,1,0} + \frac{1}{4}\mathcal{L}_{0,1,1} \right],
 \end{aligned} \tag{1.5.16}$$

and we find,

$$\begin{aligned}
 f^{(3)}(w, w^*) &= \frac{1}{8}\mathcal{L}_{0,0,1} + \frac{1}{16}\mathcal{L}_{0,1,0} + \frac{1}{4}\mathcal{L}_{0,1,1} \\
 &= \frac{1}{4}L_{2,1} + \frac{1}{8}L_1L_2 + \frac{1}{16}L_0L_2 + \frac{1}{32}L_0^2L_1 \\
 &= \frac{1}{8} \left[-2\text{Li}_3(1+w) - 2\text{Li}_3(1+w^*) - \frac{1}{2}\log^2|w|^2\log(1+w^*) \right. \\
 &\quad \left. + \log(-w)\left(\log^2(1+w^*) - \log^2(1+w)\right) \right. \\
 &\quad \left. + \frac{1}{2}\log|w|^2\left(\text{Li}_2(-w) - \text{Li}_2(-w^*)\right) \right. \\
 &\quad \left. - 2\log|1+w|^2\text{Li}_2(-w) + 2\zeta_2\log|1+w|^2 + 4\zeta_3 \right].
 \end{aligned} \tag{1.5.17}$$

The last form agrees with the one given in ref. [18], up to the sign of the second line, which we find must be +1 for the function to be single-valued.

Continuing on to higher loops, we find,

$$\begin{aligned}
 f^{(4)}(w, w^*) &= -\frac{1}{8}L_1\zeta_3 + \frac{1}{4}L_{2,1,1} - \frac{1}{8}L_{3,1} + \frac{1}{32}L_2^2 - \frac{1}{32}L_4 + \frac{1}{8}L_1L_{2,1} \\
 &\quad - \frac{1}{96}L_0L_1^3 + \frac{1}{96}L_0^2L_2 - \frac{1}{192}L_0L_3 + \frac{1}{256}L_0^3L_1 + \frac{3}{128}L_0^2L_1^2 \\
 &\quad + \frac{1}{16}L_0L_1L_2 - \frac{1}{16}L_1L_3,
 \end{aligned} \tag{1.5.18}$$

$$\begin{aligned}
f^{(5)}(w, w^*) = & -\frac{1}{96} L_2 \zeta_3 - \frac{1}{24} L_0 L_1 \zeta_3 + \frac{1}{4} L_{2,1,1,1} - \frac{1}{8} L_{2,2,1} + \frac{1}{32} L_{4,1} \quad (1.5.19) \\
& + \frac{1}{8} L_1 L_{2,1,1} + \frac{1}{16} L_0 L_{2,1,1} - \frac{1}{16} L_1 L_{3,1} + \frac{1}{32} L_1 L_2^2 - \frac{1}{64} L_1 L_4 \\
& - \frac{1}{96} L_1^3 L_2 + \frac{1}{192} L_0 L_2^2 - \frac{1}{256} L_0 L_4 - \frac{1}{384} L_0^2 L_1^3 + \frac{1}{1152} L_0^3 L_2 \\
& + \frac{5}{768} L_0^3 L_1^2 + \frac{5}{18432} L_0^4 L_1 - \frac{7}{192} L_0 L_{3,1} + \frac{1}{16} L_0 L_1 L_{2,1} \\
& + \frac{1}{64} L_0 L_1^2 L_2 + \frac{11}{768} L_0^2 L_1 L_2 - \frac{3}{8} L_{3,1,1} + \frac{1}{48} L_{3,2} - \frac{1}{96} L_0^2 L_{2,1} \\
& - \frac{1}{1536} L_0^2 L_3 - \frac{1}{48} L_0 L_1 L_3,
\end{aligned}$$

$$\begin{aligned}
f^{(6)}(w, w^*) = & \frac{1}{4} L_{2,1,1,1,1} - \frac{1}{8} L_{3,1,1,1} + \frac{1}{12} L_{3,2,1} - \frac{1}{32} L_{2,1}^2 + \frac{1}{48} L_{5,1} + \frac{1}{288} L_2^3 \quad (1.5.20) \\
& + \frac{1}{768} L_6 - \frac{1}{768} L_{4,2} + \frac{7}{32} L_{4,1,1} + \frac{1}{8} L_1 L_{2,1,1,1} - \frac{1}{16} L_1 L_{3,1,1} \\
& + \frac{1}{24} L_1 L_{3,2} + \frac{1}{32} L_3 L_{2,1} - \frac{1}{32} L_2 L_{3,1} + \frac{1}{96} L_0^2 L_{2,1,1} \\
& - \frac{1}{128} L_1^2 L_2^2 - \frac{1}{192} L_0 L_{3,1,1} - \frac{1}{192} L_1 \zeta_5 + \frac{1}{192} L_1^3 L_3 \\
& - \frac{1}{512} L_0 L_{3,2} - \frac{1}{768} L_0 L_{4,1} + \frac{1}{960} L_0 L_1^5 - \frac{1}{2560} L_0^2 L_4 \\
& - \frac{1}{18432} L_0^3 L_3 + \frac{1}{73728} L_0^5 L_1 + \frac{5}{96} L_{2,1} \zeta_3 + \frac{5}{384} L_1 L_5 \\
& + \frac{5}{4096} L_0^4 L_1^2 + \frac{7}{64} L_1 L_{4,1} + \frac{7}{1536} L_0^3 L_1^3 - \frac{11}{1536} L_0^2 L_{3,1} \\
& + \frac{11}{184320} L_0^4 L_2 - \frac{19}{9216} L_0^3 L_{2,1} + \frac{1}{16} L_0 L_1 L_{2,1,1} - \frac{1}{24} L_1 L_2 \zeta_3 \\
& - \frac{1}{32} L_0 L_1 L_{3,1} + \frac{1}{32} L_0 L_1^2 L_{2,1} - \frac{1}{48} L_0 L_{2,1} L_2 - \frac{1}{48} L_1 L_3 L_2 \\
& + \frac{1}{96} L_0^2 L_1^2 L_2 - \frac{1}{192} L_0 L_1^3 L_2 + \frac{1}{384} L_0 L_1 L_2^2 - \frac{3}{256} L_0^2 L_1 L_{2,1} \\
& - \frac{3}{512} L_0^2 L_1 \zeta_3 - \frac{5}{96} L_0 L_1^2 \zeta_3 - \frac{5}{768} L_0 L_2 \zeta_3 - \frac{11}{1536} L_0 L_1 L_4 \\
& - \frac{11}{2048} L_0^2 L_1 L_3 - \frac{19}{768} L_0 L_1^2 L_3 + \frac{49}{18432} L_0^3 L_1 L_2 \\
& + \frac{1}{384} L_3^2 + \frac{1}{16} L_2 L_{2,1,1} - \frac{1}{96} L_1^3 L_{2,1} + \frac{1}{96} L_1^3 \zeta_3 + \frac{1}{384} L_3 \zeta_3 \\
& - \frac{1}{256} L_0^2 L_1^4 + \frac{1}{7680} L_0 L_5 + \frac{5}{2048} L_0^2 L_2^2 - \frac{11}{1536} L_2 L_4.
\end{aligned}$$

The remaining expressions through 10 loops can be found in computer-readable format in a separate file attached to this article.

1.6 Single-valued HPLs and Fourier-Mellin transforms

1.6.1 The multi-Regge limit in (ν, n) space

So far we have only used the machinery of SVHPLs in order to obtain compact analytic expressions for the six-point MHV amplitude in the LL and NLL approximation. However, this was only possible because we knew *a priori* the BFKL eigenvalues and the impact factor to the desired order in perturbation theory. Going beyond NLLA requires higher-order corrections to the BFKL eigenvalues and the impact factor which, by the same logic, can be computed if the corresponding amplitude is known. In other words, if we are given the functions $g_n^{(\ell)}(w, w^*)$ up to some loop order, we can use them to extract the corresponding impact factors and BFKL eigenvalues by transforming the expression from (w, w^*) space back to (ν, n) space. The impact factors and BFKL eigenvalues obtained in this way can then be used to compute the six-point amplitude to any loop order for a given logarithmic accuracy.

In ref. [14] the three-loop six point amplitude was computed up to next-to-next-to-leading logarithmic accuracy (NNLLA),

$$\begin{aligned}
 g_0^{(3)}(w, w^*) &= \frac{27}{8} L_5^+ + \frac{3}{4} L_{3,1,1}^+ - \frac{1}{2} L_3^+ [L_1^+]^2 - \frac{15}{32} L_3^+ [L_0^-]^2 - \frac{1}{8} L_1^+ L_{2,1}^- L_0^- \\
 &\quad + \frac{3}{32} [L_0^-]^2 [L_1^+]^3 + \frac{19}{384} L_1^+ [L_0^-]^4 + \frac{3}{8} [L_1^+]^2 \zeta_3 - \frac{5}{32} [L_0^-]^2 \zeta_3 \\
 &\quad - \frac{\pi^2}{384} L_1^+ [L_0^-]^2 - \frac{\pi^2}{6} \gamma'' \left\{ L_3^+ - \frac{1}{6} [L_1^+]^3 - \frac{1}{8} [L_0^-]^2 L_1^+ \right\} \\
 &\quad + \frac{1}{4} d_1 \zeta_3 \left\{ [L_1^+]^2 - \frac{1}{4} [L_0^-]^2 \right\} - \frac{\pi^2}{3} d_2 L_1^+ \left\{ [L_1^+]^2 - \frac{1}{4} [L_0^-]^2 \right\} \\
 &\quad + \frac{\pi^2}{96} [L_1^+]^3 + \frac{1}{30} [L_1^+]^5 - \frac{3}{4} \zeta_5, \\
 h_0^{(3)}(w, w^*) &= \frac{3}{16} L_1^+ L_3^+ + \frac{1}{16} L_{2,1}^- L_0^- - \frac{1}{32} [L_1^+]^4 - \frac{1}{32} [L_0^-]^2 [L_1^+]^2 \\
 &\quad - \frac{5}{1536} [L_0^-]^4 + \frac{1}{8} L_1^+ \zeta_3,
 \end{aligned} \tag{1.6.1}$$

where d_1 , d_2 and γ'' are some undetermined rational numbers. (To obtain eq. (1.6.1) from ref. [14] one also needs the value for another constant, $\gamma' = -9/2$, or equivalently $\gamma''' = 0$, which was obtained in ref. [15] using the MRK limit at NLLA.)

These functions can be used to extract the NNLLA correction to the impact factor⁶. Indeed, the NNLL impact factor has already been expressed [15] as an integral over the complex w plane,

$$\Phi_{\text{Reg}}^{(2)}(\nu, n) = (-1)^n \left(\nu^2 + \frac{n^2}{4} \right) \int \frac{d^2 w}{\pi} \rho(w, w^*) |w|^{-2i\nu-2} \left(\frac{w^*}{w} \right)^{\frac{n}{2}}, \tag{1.6.2}$$

where the kernel $\rho(w, w^*)$ is related to the three-loop amplitude in MRK,

$$\begin{aligned}
 \rho(w, w^*) &= 2 g_0^{(3)}(w, w^*) + \log \frac{|1+w|^2}{|w|} \left(\zeta_2 \log^2 \frac{|1+w|^2}{|w|} - \frac{11}{2} \zeta_4 \right) \\
 &\quad + 2 \log \frac{|1+w|^2}{|w|} g_1^{(3)}(w, w^*) + 2 \left(\log^2 \frac{|1+w|^2}{|w|} + \pi^2 \right) g_2^{(3)}(w, w^*).
 \end{aligned} \tag{1.6.3}$$

⁶In principle we should expect the amplitude to NNLLA to depend on both the NNLL impact factor and BFKL eigenvalue. The NNLL BFKL eigenvalue however only enters at four loops, see section 1.7.2.

However, no analytic expression for $\Phi_{\text{Reg}}^{(2)}(\nu, n)$ is yet known. Indeed, an explicit evaluation of the integral (1.6.2) would require a detailed study of the integrand's branch structure, a task which, if feasible in this case, does not seem particularly amenable to generalization.

Here we propose an alternative to evaluating the integral explicitly. The basic idea is to write down an ansatz for the function in (ν, n) space, and then perform the inverse transform to fix the unknown coefficients. The inverse transform is easily performed using the methods outlined in section 1.4, so we are left only with the task of writing down a suitable ansatz. To be precise, consider the inverse Fourier-Mellin transform defined in eq. (1.4.4). Our goal is to find a set of linearly independent functions $\{\mathcal{F}_i\}$ defined in (ν, n) space such that their transforms $\{\mathcal{I}[\mathcal{F}_i]\}$:

1. are combinations of HPLs of uniform weight,
2. are single-valued in the complex w plane,
3. have a definite parity under $\mathbb{Z}_2 \times \mathbb{Z}_2$ transformations in (w, w^*) space,
4. span the whole space of SVHPLs.

Through weight six, we find empirically that this problem has a unique solution, the construction of which we present in the remainder of this section. In particular, we will be led to extend the action of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry and the notion of uniform transcendentality to (ν, n) space.

1.6.2 Symmetries in (ν, n) space

Let us start by analyzing the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry in (ν, n) space. It is easy to see from eq. (1.4.4) that

$$\begin{aligned} \mathcal{I}[\mathcal{F}(\nu, n)](w^*, w) &= \mathcal{I}[\mathcal{F}(\nu, -n)](w, w^*), \\ \mathcal{I}[\mathcal{F}(\nu, n)]\left(\frac{1}{w}, \frac{1}{w^*}\right) &= \mathcal{I}[\mathcal{F}(-\nu, -n)](w, w^*). \end{aligned} \tag{1.6.4}$$

In other words, the $\mathbb{Z}_2 \times \mathbb{Z}_2$ of conjugation and inversion acts on the (ν, n) space via $[n \leftrightarrow -n]$ and $[\nu \leftrightarrow -\nu, n \leftrightarrow -n]$, respectively. Hence, in order that the functions

$(w \leftrightarrow w^*, w \leftrightarrow 1/w)$	$(\nu \leftrightarrow -\nu, n \leftrightarrow -n)$	$\mathcal{F}(\nu, n)$
$(+, +)$	$[+, +]$	$1/2 [f(\nu, n) + f(-\nu, n)]$
$(+, -)$	$[-, +]$	$1/2 [f(\nu, n) - f(-\nu, n)]$
$(-, +)$	$[-, -]$	$1/2 \operatorname{sgn}(n) [f(\nu, n) - f(-\nu, n)]$
$(-, -)$	$[+, -]$	$1/2 \operatorname{sgn}(n) [f(\nu, n) + f(-\nu, n)]$

Table 1.2: Decomposition of functions in (ν, n) space into eigenfunctions of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ action. Note the use of brackets rather than parentheses to denote the parity under (ν, n) transformations.

in (w, w^*) space have definite parity under conjugation and inversion, $\mathcal{F}(\nu, n)$ should have definite parity under $n \leftrightarrow -n$ and $\nu \leftrightarrow -\nu$. Our experience shows that the n - and ν -symmetries manifest themselves differently: the ν -symmetry appears as an explicit symmetrization or anti-symmetrization, whereas the n -symmetry requires the introduction of an overall factor of $\operatorname{sgn}(n)$. For example, suppose the target function in (w, w^*) space is odd under conjugation, and even under inversion. This implies that the function in (ν, n) space must be odd under $n \leftrightarrow -n$ and odd under $\nu \leftrightarrow -\nu$. Such a function will decompose as follows,

$$\mathcal{F}(\nu, n) = \frac{1}{2} \operatorname{sgn}(n) [f(\nu, |n|) - f(-\nu, |n|)] , \quad (1.6.5)$$

for some suitable function f . See Table 1.2 for the typical decomposition in all four cases. Furthermore, in the cases we have studied so far, the constituents $f(\nu, |n|)$ can always be expressed as sums of products of single-variable functions with arguments $\pm i\nu + |n|/2$,

$$f(\nu, |n|) = \sum_j c_j \prod_k f_{j,k}(\delta_k i\nu + |n|/2), \quad (1.6.6)$$

where c_j are constants, $\delta_k \in \{+1, -1\}$, and the $f_{j,k}(z)$ are single-variable functions that we now describe.

1.6.3 General construction

The functional form of $\mathcal{F}_i(\nu, n)$ can be further restricted by demanding that the integral (1.4.4) evaluate to a combination of HPLs. To see how, consider closing the

ν -contour in the lower half plane and summing residues at poles with $\text{Im}(\nu) < 0$. A necessary condition for the result to yield HPLs is that the residues evaluate exclusively to rational functions and generalized harmonic numbers, e.g., the Euler-Zagier sums defined in eq. (1.3.10). This condition will clearly be satisfied if the $f_{j,k}(z)$ are purely rational functions of z . Less obviously, it is also satisfied by polygamma functions. Indeed, the polygamma functions evaluate to ordinary (depth one) harmonic numbers at integer values,

$$\psi(1+n) = -\gamma_E + Z_1(n) \quad \text{and} \quad \psi^{(k)}(1+n) = (-1)^{k+1} k! (\zeta_{k+1} - Z_{k+1}(n)), \quad (1.6.7)$$

where $\psi^{(1)} = \psi'$, $\psi^{(2)} = \psi''$, etc. Referring to eq. (1.3.9), we see that all HPLs through weight three can be constructed using ordinary harmonic numbers⁷.

We therefore expect the $f_{j,k}(z)$ to be rational functions or polygamma functions through weight three. Starting at weight four, however, ordinary harmonic numbers are insufficient to cover all possible HPLs. Indeed, at weight four, the HPL

$$H_{1,2,1}(z) = \sum_{k=1}^{\infty} \frac{z^k}{k} Z_{2,1}(k-1) \quad (1.6.8)$$

requires a depth-two sum⁸, $Z_{2,1}(k-1)$. A meromorphic function that generates $Z_{2,1}(k-1)$ was presented in ref. [54]. It can be written as a Mellin transform,

$$F_4(N) = \mathbf{M} \left[\left(\frac{\text{Li}_2(x)}{1-x} \right)_+ \right] (N), \quad N \in \mathbb{C}, \quad (1.6.9)$$

where the Mellin transform \mathbf{M} is defined by

$$\mathbf{M}[(f(x))_+](N) \equiv \int_0^1 dx (x^N - 1) f(x). \quad (1.6.10)$$

⁷Harmonic numbers of depth greater than one do appear at weight three; however, after applying the stuffle algebra relations for Euler-Zagier sums, they all can be rewritten in terms of ordinary harmonic numbers of depth one, namely $Z_{1,1}(k-1) = \frac{1}{2} Z_1(k-1)^2 - \frac{1}{2} Z_2(k-1)$.

⁸Another depth-two sum appears in $H_{1,1,2}(x) = \sum_{k=1}^{\infty} \frac{x^k}{k} Z_{1,2}(k-1)$ but the two are related by a stuffle identity, $Z_{2,1}(k-1) + Z_{1,2}(k-1) = Z_2(k-1) Z_1(k-1) - Z_3(k-1)$.

If N is a positive integer, then $F_4(N)$ evaluates to harmonic numbers of depth two,

$$F_4(N) = Z_{2,1}(N) + Z_3(N) - \zeta_2 Z_1(N), \quad N \in \mathbb{N}. \quad (1.6.11)$$

Going to higher weight, new harmonic sums will be necessary to construct the full space of HPLs, and, correspondingly, new meromorphic functions will be necessary to give rise to those sums. The analysis of refs. [53–55] uncovers precisely the functions we need⁹. They are summarized in appendix A.2. Through weight five, three new functions are necessary: F_4 , F_{6a} and F_7 .

There is one final special case that deserves attention. Unlike the other SVHPLs, the pure logarithmic functions $[L_0^-]^k$ diverge as $|w| \rightarrow 0$. These functions have special behavior in (ν, n) space as well, requiring a Kronecker delta function:

$$\mathcal{I}[\delta_{n,0}/(i\nu)^k] = \frac{1}{\pi} \sum_{n=-\infty}^{\infty} (-1)^n \left(\frac{w}{w^*}\right)^{\frac{n}{2}} \int_{-\infty}^{+\infty} \frac{d\nu}{\nu^2 + \frac{n^2}{4}} |w|^{2i\nu} \frac{\delta_{n,0}}{(i\nu)^k} = \frac{[L_0^-]^{k+1}}{(k+1)!}. \quad (1.6.12)$$

Altogether, we find that the following functions of $z = \pm i\nu + |n|/2$ are sufficient to construct all the remaining SVHPLs through weight five:

$$f_{j,k}(z) \in \left\{ 1, \frac{1}{z}, \psi(1+z), \psi'(1+z), \psi''(1+z), \psi'''(1+z), F_4(z), F_{6a}(z), F_7(z) \right\}. \quad (1.6.13)$$

However, as we will see, not all combinations of elements in the list (1.6.13) lead to functions of (w, w^*) that are both single-valued and of definite transcendental weight. Instead we will construct a smaller set of *building blocks* that do have this property.

1.6.4 Examples

Let us see how to use the elements in the list (1.6.13) to construct SVHPLs. The simplest case is $f(\nu, |n|) = 1$. Referring to Table 1.2, only two of the four sectors yield non-zero choices for \mathcal{F} . One of these, $\mathcal{F} = \text{sgn}(n)$, produces something proportional

⁹Actually, in refs. [53–55] a more general class of functions is defined. It involves generic HPLs that are singular at $x = -1$ as well as at $x = 0$ and 1 . As we never encounter these HPLs in our present context, we do not discuss these functions any further.

to $H_1 - \overline{H}_1$, which is not single-valued. This leaves $\mathcal{F} = 1$, which should produce a function in the $(+, +)$ sector. Closing the ν -contour in the lower half plane, and summing up the residues at $\nu = -i|n|/2$, we obtain the integral of eq. (1.4.5),

$$\mathcal{I}[1] = 2L_1^+, \quad (1.6.14)$$

indeed a function in the $(+, +)$ sector. Including the special case L_0^- from eq. (1.6.12), this completes the analysis at weight one.

The next simplest element is $1/z$, yielding $f(\nu, |n|) = 1/(i\nu + |n|/2)$. It generates two single-valued functions, one in the $(+, -)$ sector and one in the $(-, -)$ sector (using the (w, w^*) labeling in the first column of Table 1.2). Symmetrizing as indicated in Table 1.2, the two functions in (ν, n) space are $\mathcal{F} = -V$ and $\mathcal{F} = N/2$, with the useful shorthands

$$\begin{aligned} V &\equiv -\frac{1}{2} \left[\frac{1}{i\nu + \frac{|n|}{2}} - \frac{1}{-i\nu + \frac{|n|}{2}} \right] = \frac{i\nu}{\nu^2 + \frac{|n|^2}{4}}, \\ N &\equiv \text{sgn}(n) \left[\frac{1}{i\nu + \frac{|n|}{2}} + \frac{1}{-i\nu + \frac{|n|}{2}} \right] = \frac{n}{\nu^2 + \frac{|n|^2}{4}}. \end{aligned} \quad (1.6.15)$$

The transforms of these functions yield two of the four SVHPLs of weight two.

$$\begin{aligned} \mathcal{I}[V] &= -L_0^- L_1^+, \\ \mathcal{I}[N] &= 4L_2^-. \end{aligned} \quad (1.6.16)$$

A third weight-two function is the pure logarithmic function $[L_0^-]^2$, a special case already considered. To find the fourth weight-two function, we turn to the next element in the list (1.6.13), $\psi(1+z)$. On its own, it does not generate any single-valued functions; however, a particular linear combination of $\{1, 1/z, \psi(1+z)\}$ indeed produces such a function. Specifically, $f(\nu, |n|) = 2\psi(1 + i\nu + |n|/2) + 2\gamma_E - 1/(i\nu + |n|/2)$ generates the last weight-two SVHPL, which transforms in the $(+, +)$ sector.

The function in (ν, n) space is actually the leading-order BFKL eigenvalue, $E_{\nu, n}$,

$$\mathcal{F} = \psi \left(1 + i\nu + \frac{|n|}{2} \right) + \psi \left(1 - i\nu + \frac{|n|}{2} \right) + 2\gamma_E - \frac{\text{sgn}(n)N}{2} = E_{\nu, n}, \quad (1.6.17)$$

and its transform is the last SVHPL of weight two,

$$\mathcal{I}[E_{\nu, n}] = [L_1^+]^2 - \frac{1}{4} [L_0^-]^2. \quad (1.6.18)$$

The next element in the list (1.6.13) is $\psi'(1+z)$. Like $\psi(1+z)$, $\psi'(1+z)$ does not by itself generate any single-valued functions; however, there is a particular linear combination that does, and it is given by $f(\nu, |n|) = 2\psi'(1+i\nu+|n|/2) + 1/(i\nu+|n|/2)^2$. Notice that, for the first time, the product in eq. (1.6.6) extends over more than one term (in this case, $f_{1,1} = f_{1,2} = 1/(i\nu+|n|/2)$, but in general the $f_{j,k}$ will be different). The function in (ν, n) space is,

$$\mathcal{F} = \psi' \left(1 + i\nu + \frac{|n|}{2} \right) - \psi' \left(1 - i\nu + \frac{|n|}{2} \right) - \text{sgn}(n)NV = D_\nu E_{\nu, n}, \quad (1.6.19)$$

where $D_\nu \equiv -i\partial_\nu \equiv -i\partial/\partial\nu$. The main observation is that the basis in eq. (1.6.13) can be modified to consistently generate single-valued functions: $1/z$ is replaced by V and N , ψ is replaced by $E_{\nu, n}$, and $\psi^{(k)}$ is replaced by $D_\nu^k E_{\nu, n}$.

Furthermore, as mentioned previously, the basis at weight four requires a new function $F_4(z)$ that is outside the class of polygamma functions. Like the polygamma functions, $F_4(z)$ does not by itself generate a single-valued function; it too requires additional terms. We denote the resulting basis element by \tilde{F}_4 . It is related to the function $F_4(z)$ in eq. (1.6.9) by,

$$\begin{aligned} \tilde{F}_4 = \text{sgn}(n) \left\{ F_4 \left(i\nu + \frac{|n|}{2} \right) + F_4 \left(-i\nu + \frac{|n|}{2} \right) - \frac{1}{4} D_\nu^2 E_{\nu, n} - \frac{1}{8} N^2 E_{\nu, n} \right. \\ \left. - \frac{1}{2} V^2 E_{\nu, n} + \frac{1}{2} (\psi_- + V) D_\nu E_{\nu, n} + \zeta_2 E_{\nu, n} - 4\zeta_3 \right\} \\ + N \left\{ \frac{1}{2} V \psi_- + \frac{1}{2} \zeta_2 \right\}, \end{aligned} \quad (1.6.20)$$

where

$$\psi_- \equiv \psi\left(1 + i\nu + \frac{|n|}{2}\right) - \psi\left(1 - i\nu + \frac{|n|}{2}\right). \quad (1.6.21)$$

Appendix A.2 contains further details about the functions in (ν, n) space, including the basis through weight five and expressions for the building blocks \tilde{F}_{6a} and \tilde{F}_7 generated by the functions $F_{6a}(z)$ and $F_7(z)$.

Finally, we describe a heuristic method for assembling the basis in (ν, n) space. The idea is to start with the building blocks,

$$\{1, N, V, E_{\nu, n}, \tilde{F}_4, \tilde{F}_{6a}, \tilde{F}_7\}, \quad (1.6.22)$$

and piece them together with multiplication and ν -differentiation. These two operations do not always produce independent functions. For example,

$$D_\nu N = 2NV \quad \text{and} \quad D_\nu V = \frac{1}{4}N^2 + V^2. \quad (1.6.23)$$

The building blocks have definite parity under $\nu \leftrightarrow -\nu$ and $n \leftrightarrow -n$ which helps determine which combinations appear in which sector. Additionally, we observe that they can be assigned a transcendental weight, which further assists in the classification. The weight in (w, w^*) space is found by calculating the total weight of the constituent building blocks in (ν, n) space, and then adding one (to account for the increase in weight due to the integral transform itself). The relevant properties of the basic building blocks are summarized in Table 1.3.

As an example, let us consider the function $ND_\nu E_{\nu, n}$. Referring to Table 1.3, the transcendental weight is $1 + 1 + 1 = 3$ in (ν, n) space, or $3 + 1 = 4$ in (w, w^*) space. Under $[\nu \leftrightarrow -\nu, n \leftrightarrow -n]$, N has parity $[+, -]$, D_ν has parity $[-, +]$, and $E_{\nu, n}$ has parity $[+, +]$, so $ND_\nu E_{\nu, n}$ has parity $[-, -]$. We therefore expect this function to transform into a weight four function of (w, w^*) , with parity $(-, +)$ under $(w \leftrightarrow w^*, w \leftrightarrow 1/w)$ (see Table 1.2). Indeed this turns out to be the case. A complete basis through weight three is presented in Table 1.4.

	weight	$(\nu \leftrightarrow -\nu, n \leftrightarrow -n)$		weight	$(\nu \leftrightarrow -\nu, n \leftrightarrow -n)$
1	0	$[+, +]$	$E_{\nu,n}$	1	$[+, +]$
D_ν	1	$[-, +]$	\tilde{F}_4	3	$[+, -]$
V	1	$[-, +]$	\tilde{F}_{6a}	4	$[-, -]$
N	1	$[+, -]$	\tilde{F}_7	4	$[-, +]$

 Table 1.3: Properties of the building blocks for the basis in (ν, n) space.

weight	$\mathbb{Z}_2 \times \mathbb{Z}_2$	(w, w^*) basis	(ν, n) basis	dimension
1	$(+, +)$	L_1^+	1	1
	$(+, -)$	L_0^-	$\delta_{n,0}$	1
	$(-, +)$	$-$	$-$	0
	$(-, -)$	$-$	$-$	0
2	$(+, +)$	$[L_1^+]^2, [L_0^-]^2$	$\delta_{n,0}/(i\nu), E_{\nu,n}$	2
	$(+, -)$	$L_0^- L_1^+$	V	1
	$(-, +)$	$-$	$-$	0
	$(-, -)$	L_2^-	N	1
3	$(+, +)$	$[L_1^+]^3, [L_0^-]^2 L_1^+, L_3^+$	$V^2, N^2, E_{\nu,n}^2$	3
	$(+, -)$	$[L_0^-]^3, L_0^- [L_1^+]^2, L_{2,1}^-$	$\delta_{n,0}/(i\nu)^2, V E_{\nu,n}, D_\nu E_{\nu,n}$	3
	$(-, +)$	$L_0^- L_2^-$	VN	1
	$(-, -)$	$L_1^+ L_2^-$	$N E_{\nu,n}$	1

 Table 1.4: Basis of SVHPLs in (w, w^*) and (ν, n) space through weight three. Note that at each weight we can also add the product of zeta values with lower-weight entries.

1.7 Applications in (ν, n) space: the BFKL eigenvalues and impact factor

1.7.1 The impact factor at NNLLA

In this section we report results for $g_1^{(4)}$ and $g_0^{(4)}$ and discuss how to transform these functions to (ν, n) space using the basis constructed in the previous section. We then give our results for the new data for the MRK logarithmic expansion: $\Phi_{\text{Reg}}^{(2)}, \Phi_{\text{Reg}}^{(3)}$,

and $E_{\nu,n}^{(2)}$.

Before discussing the case of the higher-order corrections to the BFKL eigenvalue and the impact factor, let us review how the known results for $E_{\nu,n}$, $E_{\nu,n}^{(1)}$ and $\Phi_{\text{Reg}}^{(1)}$ fit into the framework for (ν, n) space that we have developed in the previous section. First, we have already seen in section 1.6 that the LL BFKL eigenvalue is one of our basis elements of weight one in (ν, n) space (see Table 1.3). Next, we know that the first time the NLL impact factor $\Phi_{\text{Reg}}^{(1)}$ appears is in the NLLA of the two-loop amplitude, $g_0^{(2)}(w, w^*)$, which is a pure single-valued function of weight three. Following our analysis from the previous section, it should then be possible to express $\Phi_{\text{Reg}}^{(1)}$ as a pure function of weight two in (ν, n) space with the correct symmetries. Indeed, we can easily recast eq. (1.2.17) in terms of the basis elements shown in Table 1.3,

$$\Phi_{\text{Reg}}^{(1)}(\nu, n) = -\frac{1}{2}E_{\nu,n}^2 - \frac{3}{8}N^2 - \zeta_2. \quad (1.7.1)$$

Similarly, the NLL BFKL eigenvalue can be written as a linear combination of weight three of the basis elements in Table 1.3,

$$E_{\nu,n}^{(1)} = -\frac{1}{4}D_\nu^2 E_{\nu,n} + \frac{1}{2}V D_\nu E_{\nu,n} - \zeta_2 E_{\nu,n} - 3\zeta_3. \quad (1.7.2)$$

This completes the data for the MRK logarithmic expansion that can be extracted through two loops.

Now we proceed to three loops. By expanding eq. (1.4.1) to order a^3 , we obtain the following relation for the NNLLA correction to the impact factor, $\Phi_{\text{Reg}}^{(2)}(\nu, n)$,

$$\begin{aligned} \mathcal{I} \left[\Phi_{\text{Reg}}^{(2)}(\nu, n) \right] &= 4g_2^{(3)}(w, w^*) \{ [L_1^+]^2 + \pi^2 \} - 4g_1^{(3)}(w, w^*) L_1^+ + 4g_0^{(3)}(w, w^*) \\ &\quad - 4\pi^2 g_1^{(2)}(w, w^*) L_1^+ + \frac{\pi^2}{180} L_1^+ \{ -45 [L_0^-]^2 + 120 [L_1^+]^2 + 22 \pi^2 \}. \end{aligned} \quad (1.7.3)$$

This expression is exactly $2\rho(w, w^*)$, where ρ was given in eq. (1.6.3) and in ref. [15]. (The factor of two just has to do with our normalization of the Fourier-Mellin transform.)

To invert eq. (1.7.3) and obtain $\Phi_{\text{Reg}}^{(2)}(\nu, n)$, we begin by observing that the right-hand side is a pure function of weight five in (w, w^*) space. Moreover, it is an eigenfunction with eigenvalue $(+, +)$ under the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. Following the analysis of section 1.6, and using the results at the end of appendix A.2, we are led to make the following ansatz,

$$\begin{aligned} \Phi_{\text{Reg}}^{(2)}(\nu, n) = & \alpha_1 E_{\nu,n}^4 + \alpha_2 N^2 E_{\nu,n}^2 + \alpha_3 N^4 + \alpha_4 V^2 E_{\nu,n}^2 + \alpha_5 N^2 V^2 + \alpha_6 V^4 \\ & + \alpha_7 E_{\nu,n} V D_\nu E_{\nu,n} + \alpha_8 [D_\nu E_{\nu,n}]^2 + \alpha_9 E_{\nu,n} D_\nu^2 E_{\nu,n} + \alpha_{10} \tilde{F}_4 N \\ & + \alpha_{11} \zeta_2 E_{\nu,n}^2 + \alpha_{12} \zeta_2 N^2 + \alpha_{13} \zeta_2 V^2 + \alpha_{14} \zeta_3 E_{\nu,n} \\ & + \alpha_{15} \zeta_3 [\delta_{n,0}/(i\nu)] + \alpha_{16} \zeta_4. \end{aligned} \quad (1.7.4)$$

The α_i are rational numbers that can be determined by computing the integral transform to (w, w^*) space of eq. (1.7.4) (see appendix A.2) and then matching the result to the right-hand side of eq. (1.7.3). We find

$$\begin{aligned} \Phi_{\text{Reg}}^{(2)}(\nu, n) = & \frac{1}{2} \left[\Phi_{\text{Reg}}^{(1)}(\nu, n) \right]^2 - E_{\nu,n}^{(1)} E_{\nu,n} + \frac{1}{8} [D_\nu E_{\nu,n}]^2 + \frac{5\pi^2}{16} E_{\nu,n}^2 \\ & - \frac{1}{2} \zeta_3 E_{\nu,n} + \frac{5}{64} N^4 + \frac{5}{16} N^2 V^2 - \frac{5\pi^2}{64} N^2 - \frac{\pi^2}{4} V^2 + \frac{17\pi^4}{360} \\ & + d_1 \zeta_3 E_{\nu,n} - d_2 \frac{\pi^2}{6} [12 E_{\nu,n}^2 + N^2] + \gamma'' \frac{\pi^2}{6} \left[E_{\nu,n}^2 - \frac{1}{4} N^2 \right]. \end{aligned} \quad (1.7.5)$$

Here d_1 , d_2 and γ'' are the (not yet determined) rational numbers that appear in eq. (1.6.1). We emphasize that the expression for $\Phi_{\text{Reg}}^{(2)}(\nu, n)$ does not involve the basis element $N \tilde{F}_4$ (see eq. (A.2.52)). That is, $\Phi_{\text{Reg}}^{(2)}(\nu, n)$ can be written purely in terms of ψ functions (and their derivatives).

To determine the six-point remainder function in MRK to all loop orders in the NNLL approximation, we must apply some additional information beyond $\Phi_{\text{Reg}}^{(2)}(\nu, n)$. In particular, at four loops and higher, the second-order correction to the BFKL eigenvalue, $E_{\nu,n}^{(2)}$, is necessary. In the next section, we will show how to use information from the symbol of the four-loop remainder function to determine $E_{\nu,n}^{(2)}$. We will also derive the next correction to the impact factor, $\Phi_{\text{Reg}}^{(3)}(\nu, n)$, which enters the N³LL approximation.

1.7.2 The four-loop remainder function in the multi-Regge limit

In order to compute the next term in the perturbative expansion of the BFKL eigenvalue and the impact factor, we need the analytic expressions for the four-loop six-point remainder function in the multi-Regge limit. In an independent work, the symbol of the four-loop six-point remainder function has been heavily constrained [56]. In ref. [56] the symbol of $R_6^{(4)}$ is written in the form

$$\mathcal{S}(R_6^{(4)}) = \sum_{i=1}^{113} \alpha_i S_i, \quad (1.7.6)$$

where α_i are undetermined rational numbers. The S_i denote integrable tensors of weight eight satisfying the first- and final-entry conditions mentioned in the introduction, such that:

0. All entries in the symbol are drawn from the set $\{u_i, 1 - u_i, y_i\}_{i=1,2,3}$, where the y_i 's are defined in eq. (1.1.4).
1. The symbol is integrable.
2. The tensor is totally symmetric in u_1, u_2, u_3 . Note that under a permutation $u_i \rightarrow u_{\sigma(i)}$, $\sigma \in S_3$, the y_i variables transform as $y_i \rightarrow 1/y_{\sigma(i)}$.
3. The tensor is invariant under the transformation $y_i \rightarrow 1/y_i$.
4. The tensor vanishes in all simple collinear limits.
5. The tensor is in agreement with the prediction coming from the collinear OPE of ref. [38]. We implement this condition on the leading singularity exactly as was done at three loops [14].

In section 1.4, we presented analytic expressions for the four-loop remainder function in the LLA and NLLA of MRK. We can use these results to obtain further constraints on the free coefficients α_i appearing in eq. (1.7.6). In order to achieve this, we first

have to understand how to write the symbol (1.7.6) in MRK. In the following we give very brief account of this procedure.

To begin, recall that the remainder function is non-zero in MRK only after performing the analytic continuation (1.2.6), $u_1 \rightarrow e^{-2\pi i} |u_1|$. The function can then be expanded as in eq. (1.2.7),

$$R_6^{(4)}|_{\text{MRK}} = 2\pi i \sum_{n=0}^3 \log^n(1 - u_1) [g_n^{(4)}(w, w^*) + 2\pi i h_n^{(4)}(w, w^*)] . \quad (1.7.7)$$

The symbols of the imaginary and real parts can be extracted by taking single and double discontinuities,

$$\begin{aligned} 2\pi i \sum_{n=0}^3 \mathcal{S} [\log^n(1 - u_1) g_n^{(4)}(w, w^*)] &= \mathcal{S}(\Delta_{u_1} R_6^{(4)})|_{\text{MRK}} \\ &= -2\pi i \sum_{i=1}^{113} \alpha_i \Delta_{u_1}(S_i)|_{\text{MRK}} \\ (2\pi i)^2 \sum_{n=0}^3 \mathcal{S} [\log^n(1 - u_1) h_n^{(4)}(w, w^*)] &= \mathcal{S}(\Delta_{u_1}^2 R_6^{(4)})|_{\text{MRK}} \\ &= (-2\pi i)^2 \sum_{i=1}^{113} \alpha_i \Delta_{u_1}^2(S_i)|_{\text{MRK}} , \end{aligned} \quad (1.7.8)$$

where the discontinuity operator Δ acts on symbols via,

$$\Delta_{u_1}(a_1 \otimes a_2 \otimes \dots \otimes a_n) = \begin{cases} a_2 \otimes \dots \otimes a_n , & \text{if } a_1 = u_1 , \\ 0 , & \text{otherwise.} \end{cases} \quad (1.7.9)$$

$$\Delta_{u_1}^2(a_1 \otimes a_2 \otimes \dots \otimes a_n) = \begin{cases} \frac{1}{2} (a_3 \otimes \dots \otimes a_n) , & \text{if } a_1 = a_2 = u_1 , \\ 0 , & \text{otherwise.} \end{cases} \quad (1.7.10)$$

As indicated in eq. (1.7.8), we need to evaluate the symbols S_i in MRK, which we do by taking the multi-Regge limit of each entry of the symbol. This can be achieved by replacing u_2 and u_3 by the variables x and y , defined in eq. (1.2.3) (which we then write in terms of w and w^* using eq. (1.2.4)), while the y_i 's are replaced by their

limits in MRK [14],

$$y_1 \rightarrow 1, \quad y_2 \rightarrow \frac{1+w^*}{1+w}, \quad y_3 \rightarrow \frac{w^*(1+w)}{w(1+w^*)}. \quad (1.7.11)$$

Finally, we drop all terms in $\Delta_{u_1}^k(S_i)$, $k = 1, 2$, that have an entry corresponding to u_1 , y_1 , $1 - u_2$ or $1 - u_3$, since these quantities approach unity in MRK. In the end, the resulting tensors have entries drawn from the set $\{1 - u_1, w, w^*, 1 + w, 1 + w^*\}$. The $1 - u_1$ entries come from factors of $\log(1 - u_1)$ and can be shuffled out, so that we can write eq. (1.7.8) as,

$$\begin{aligned} \sum_{n=0}^3 \mathcal{S}[\log^n(1 - u_1)] \mathbb{I} \mathcal{S}[g_n^{(4)}(w, w^*)] &= \sum_{i=1}^{113} \sum_{n=0}^7 \alpha_i \mathcal{S}[\log^n(1 - u_1)] \mathbb{I} G_{i,n} \\ \sum_{n=0}^3 \mathcal{S}[\log^n(1 - u_1)] \mathbb{I} \mathcal{S}[h_n^{(4)}(w, w^*)] &= \sum_{i=1}^{113} \sum_{n=0}^6 \alpha_i \mathcal{S}[\log^n(1 - u_1)] \mathbb{I} H_{i,n}, \end{aligned} \quad (1.7.12)$$

for some suitable tensors $G_{i,n}$ of weight $(7 - n)$ and $H_{i,n}$ of weight $(6 - n)$. The sums on the right-hand side of eq. (1.7.12) turn out to extend past $n = 3$. Because the sums on the left-hand side do not, we immediately obtain homogeneous constraints on the α_i for the cases $n = 4, 5, 6, 7$. Furthermore, since the quantities on the left-hand side of eq. (1.7.12) are known for $n = 3$ and $n = 2$, we can use this information to further constrain the α_i . Finally, there is a consistency condition which relates the real and imaginary parts,

$$\begin{aligned} h_1^{(4)}(w, w^*) &= g_2^{(4)}(w, w^*) + \frac{\pi^2}{12} g_1^{(2)}(w, w^*) L_1^+ - \frac{1}{2} g_1^{(3)}(w, w^*) L_1^+ \\ &\quad - g_1^{(2)}(w, w^*) g_0^{(2)}(w, w^*), \\ h_0^{(4)}(w, w^*) &= \frac{1}{2} g_1^{(4)}(w, w^*) + \pi^2 g_3^{(4)}(w, w^*) - \pi^2 g_2^{(3)}(w, w^*) L_1^+ \\ &\quad - \frac{1}{2} g_0^{(3)}(w, w^*) L_1^+ + \frac{\pi^2}{2} g_1^{(2)}(w, w^*) [L_1^+]^2 + \frac{\pi^2}{12} g_0^{(2)}(w, w^*) L_1^+ \\ &\quad + \frac{\pi^2}{64} [L_0^-]^2 [L_1^+]^2 - \frac{\pi^2}{1536} [L_0^-]^4 + \frac{3}{640} \pi^4 [L_0^-]^2 - \frac{5}{96} \pi^2 [L_1^+]^4 \\ &\quad - \frac{3}{160} \pi^4 [L_1^+]^2 - \frac{1}{2} [g_0^{(2)}(w, w^*)]^2. \end{aligned} \quad (1.7.13)$$

In total, these constraints allow us to fix all of the coefficients α_i that survive in the multi-Regge limit, except for a single parameter which we will refer to as a_0 .

The results of the above analysis are expressions for the symbols of the functions $g_1^{(4)}$ and $g_0^{(4)}$. We would like to use this information to calculate new terms in the perturbative expansions of the BFKL eigenvalue $\omega(\nu, n)$ and the MHV impact factor $\Phi_{\text{Reg}}(\nu, n)$. For this purpose, we actually need the functions $g_1^{(4)}$ and $g_0^{(4)}$, and not just their symbols. Thankfully, using our knowledge of the space of SVHPLs, it is easy to integrate these symbols. We can constrain the beyond-the-symbol ambiguities by demanding that the function vanish in the collinear limit $(w, w^*) \rightarrow 0$, and that it be invariant under conjugation and inversion of the w variables. Putting everything together, we find the following expressions for $g_1^{(4)}$ and $g_0^{(4)}$,

$$\begin{aligned}
 g_1^{(4)}(w, w^*) = & \frac{3}{128} [L_2^-]^2 [L_0^-]^2 - \frac{3}{32} [L_2^-]^2 [L_1^+]^2 + \frac{19}{384} [L_0^-]^2 [L_1^+]^4 \\
 & + \frac{73}{1536} [L_0^-]^4 [L_1^+]^2 - \frac{17}{48} L_3^+ [L_1^+]^3 + \frac{1}{4} L_0^- L_{4,1}^- - \frac{3}{4} L_0^- L_{2,1,1,1}^- \\
 & + \frac{1}{96} L_{2,1}^- [L_0^-]^3 - \frac{29}{64} L_1^+ L_3^+ [L_0^-]^2 - \frac{11}{30720} [L_0^-]^6 - \frac{1}{8} [L_{2,1}^-]^2 \\
 & + \frac{23}{12} [L_1^+]^3 \zeta_3 + \frac{11}{480} [L_1^+]^6 + \frac{5}{32} [L_3^+]^2 - \frac{1}{4} L_4^- L_2^- + \frac{1}{4} L_2^- L_{2,1,1}^- \\
 & + \frac{19}{8} L_5^+ L_1^+ + \frac{5}{4} L_1^+ L_{3,1,1}^+ + \frac{1}{2} L_1^+ L_{2,2,1}^+ - \frac{3}{2} L_1^+ \zeta_5 + \frac{1}{8} \zeta_3^2 \\
 & + a_0 \left\{ \frac{1027}{2} [L_2^-]^2 [L_0^-]^2 + \frac{417}{8} [L_0^-]^2 [L_1^+]^4 + \frac{431}{24} [L_0^-]^4 [L_1^+]^2 \right. \\
 & + \frac{3155}{48} L_{2,1}^- [L_0^-]^3 - \frac{709}{4} L_3^+ [L_1^+]^3 + \frac{2223}{2} L_5^+ L_1^+ \\
 & - \frac{1581}{16} L_1^+ L_3^+ [L_0^-]^2 + \frac{9823}{1152} [L_0^-]^6 - \frac{871}{4} L_0^- L_{2,1}^- [L_1^+]^2 \\
 & - 157 [L_2^-]^2 [L_1^+]^2 - 256 [L_{2,1}^-]^2 + 1593 [L_1^+]^3 \zeta_3 \\
 & + 681 [L_3^+]^2 - 1606 L_4^- L_2^- + 512 L_2^- L_{2,1,1}^- - 3371 L_0^- L_{4,1}^- \\
 & - 1730 L_0^- L_{3,2}^- - 299 L_0^- L_{2,1,1,1}^- + 2127 L_1^+ L_{3,1,1}^+ \\
 & \left. + 744 L_1^+ L_{2,2,1}^+ + 5489 L_1^+ \zeta_5 + 256 \zeta_3^2 \right\} \\
 & + a_1 \pi^2 g_1^{(3)}(w, w^*) + a_2 \pi^2 g_3^{(4)}(w, w^*)
 \end{aligned} \tag{1.7.14}$$

$$\begin{aligned}
 & + a_3 \pi^2 [g_1^{(2)}(w, w^*)]^2 + a_4 \pi^2 h_2^{(4)}(w, w^*) + a_5 \pi^2 h_0^{(3)}(w, w^*) \\
 & + a_6 \pi^4 g_1^{(2)}(w, w^*) + a_7 \zeta_3 g_0^{(2)}(w, w^*) + a_8 \zeta_3 g_2^{(3)}(w, w^*), \\
 g_0^{(4)}(w, w^*) = & \frac{5}{64} L_1^+ [L_2^-]^2 [L_0^-]^2 - \frac{1}{16} [L_2^-]^2 [L_1^+]^3 - \frac{21}{64} L_3^+ [L_0^-]^2 [L_1^+]^2 \\
 & + \frac{7}{144} [L_0^-]^4 [L_1^+]^3 + \frac{1007}{46080} L_1^+ [L_0^-]^6 + \frac{1}{4} L_2^- L_{2,1,1}^- L_1^+ - \frac{125}{8} L_7^+ \\
 & + \frac{9}{320} [L_0^-]^2 [L_1^+]^5 - \frac{7}{192} L_{2,1}^- L_1^+ [L_0^-]^3 + \frac{129}{64} L_5^+ [L_0^-]^2 \\
 & - \frac{5}{24} L_3^+ [L_0^-]^4 + \frac{3}{32} L_{3,1,1}^+ [L_0^-]^2 - \frac{1}{16} L_{2,2,1}^+ [L_0^-]^2 + \frac{7}{16} [L_0^-]^2 \zeta_5 \\
 & - \frac{1}{16} L_0^- L_{2,1}^- [L_1^+]^3 + \frac{25}{16} L_5^+ [L_1^+]^2 - \frac{7}{48} L_3^+ [L_1^+]^4 \\
 & + \frac{25}{12} [L_1^+]^4 \zeta_3 + \frac{1}{210} [L_1^+]^7 - \frac{1}{4} L_4^- L_2^- L_1^+ - \frac{5}{16} L_2^- L_0^- L_{3,1}^+ \\
 & + \frac{1}{4} L_0^- L_{4,1}^- L_1^+ - \frac{1}{8} L_0^- L_{2,1}^- L_3^+ - \frac{1}{4} L_0^- L_{2,1,1,1}^- L_1^+ + \frac{3}{2} L_1^+ \zeta_3^2 \\
 & + \frac{1}{2} L_{4,1,2}^+ + \frac{11}{4} L_{4,2,1}^+ + \frac{3}{4} L_{3,3,1}^+ - \frac{1}{2} L_{2,1,2,1,1}^+ - \frac{3}{2} L_{2,2,1,1,1}^+ \\
 & + \frac{7}{8} L_{3,1,1}^+ [L_1^+]^2 + \frac{25}{4} \zeta_7 + 5 L_{5,1,1}^+ - 4 L_{3,1,1,1,1}^+ + \frac{1}{4} L_{2,2,1}^+ [L_1^+]^2 \quad (1.7.15) \\
 & + a_0 \left\{ - \frac{1309}{4} L_1^+ [L_2^-]^2 [L_0^-]^2 + 1911 L_3^+ [L_2^-]^2 + 63 L_{3,1,1}^+ [L_1^+]^2 \right. \\
 & - \frac{8535}{4} L_3^+ [L_0^-]^2 [L_1^+]^2 + \frac{235}{4} [L_0^-]^2 [L_1^+]^5 + \frac{4617}{16} [L_0^-]^4 [L_1^+]^3 \\
 & - \frac{32027}{24} L_{2,1}^- L_1^+ [L_0^-]^3 - \frac{11415}{8} L_5^+ [L_0^-]^2 - \frac{310}{9} L_1^+ [L_0^-]^6 \\
 & + \frac{15225}{64} L_3^+ [L_0^-]^4 + \frac{24279}{4} L_{3,1,1}^+ [L_0^-]^2 - \frac{823}{2} L_0^- L_{2,1}^- [L_1^+]^3 \\
 & + \frac{2235}{2} L_5^+ [L_1^+]^2 - \frac{365}{4} L_3^+ [L_1^+]^4 + 205 [L_2^-]^2 [L_1^+]^3 \\
 & + 2130 L_{2,2,1}^+ [L_0^-]^2 - 2623 [L_0^-]^2 \zeta_5 + 992 L_1^+ [L_{2,1}^-]^2 \\
 & - 288 L_{2,2,1}^+ [L_1^+]^2 + 2396 [L_1^+]^4 \zeta_3 + 1830 L_1^+ [L_3^+]^2 \\
 & + 1344 L_2^- L_0^- L_{3,1}^+ - 520 L_2^- L_{2,1,1}^- L_1^+ + 11839 L_0^- L_{4,1}^- L_1^+ \\
 & + 4330 L_0^- L_{3,2}^- L_1^+ + 3780 L_0^- L_{2,1}^- L_3^+ + 562 L_0^- L_{2,1,1,1}^- L_1^+ \\
 & + 2256 L_7^+ - 164778 L_{5,1,1}^+ - 33216 L_{4,1,2}^+ - 89088 L_{4,2,1}^+ \\
 & \left. - 33912 L_{3,3,1}^+ - 12048 L_{3,2,2}^+ - 17820 L_{3,1,1,1,1}^+ - 2928 L_{2,1,2,1,1}^+ \right\}
 \end{aligned}$$

$$\begin{aligned}
 & \left. - 1612 L_4^- L_2^- L_1^+ - 8784 L_{2,2,1,1,1}^+ + 3556 L_1^+ \zeta_3^2 - 23796 \zeta_7 \right\} \\
 & + b_1 \zeta_2 [L_2^-]^2 L_1^+ + b_2 \zeta_2 [L_0^-]^2 L_1^+ g_1^{(2)}(w, w^*) \\
 & + b_3 \zeta_2 g_1^{(2)}(w, w^*) g_2^{(3)}(w, w^*) + b_4 \zeta_2 g_0^{(2)}(w, w^*) g_1^{(2)}(w, w^*) \\
 & + b_5 \zeta_2 h_1^{(4)}(w, w^*) + b_6 \zeta_2 h_3^{(5)}(w, w^*) + b_7 \zeta_2 g_0^{(3)}(w, w^*) \\
 & + b_8 \zeta_2 g_2^{(4)}(w, w^*) + b_9 \zeta_2 g_4^{(5)}(w, w^*) + b_{10} \zeta_3 h_2^{(4)}(w, w^*) \\
 & + b_{11} \zeta_3 h_0^{(3)}(w, w^*) + b_{12} \zeta_3 [g_1^{(2)}(w, w^*)]^2 + b_{13} \zeta_3 g_3^{(4)}(w, w^*) \\
 & + b_{14} \zeta_3 g_1^{(3)}(w, w^*) + b_{15} \zeta_4 g_2^{(3)}(w, w^*) + b_{16} \zeta_4 g_0^{(2)}(w, w^*) \\
 & + b_{17} \zeta_3 \zeta_2 g_1^{(2)}(w, w^*) + b_{18} \zeta_5 g_1^{(2)}(w, w^*) .
 \end{aligned}$$

In these expressions, a_i for $i = 0, \dots, 8$, and b_j for $j = 1, \dots, 18$, denote undetermined rational numbers. The one symbol-level parameter, a_0 , enters both $g_1^{(4)}$ and $g_0^{(4)}$. We observe that a_0 enters these formulae in a complicated way, and that there is no nonzero value of a_0 that simplifies the associated large rational numbers. We therefore suspect that $a_0 = 0$, although we currently have no proof. The remaining parameters account for beyond-the-symbol ambiguities. We will see in the next section that one of these parameters, b_1 , is not independent of the others.

1.7.3 Analytic results for the NNLL correction to the BFKL eigenvalue and the N³LL correction to the impact factor

Having at our disposal analytic expressions for the four-loop remainder function at NNLLA and N³LLA, we use these results to extract the BFKL eigenvalue and the impact factors to the same accuracy in perturbation theory. We proceed as in section 1.7.1, i.e., we use our knowledge of the space of SVHPLs and the corresponding functions in (ν, n) space to find a function whose inverse Fourier-Mellin transform reproduces the four-loop results we have derived.

Let us start with the computation of the BFKL eigenvalue at NNLLA. Expanding

eq. (1.4.1) to order a^4 , we can extract the following relation,

$$\begin{aligned}
 \mathcal{I} [E_{\nu,n}^{(2)}] &= 12 \{ [L_1^+]^2 + \pi^2 \} g_3^{(4)}(w, w^*) - 8 L_1^+ g_2^{(4)}(w, w^*) + 4 g_1^{(4)}(w, w^*) \\
 &\quad - 8 L_1^+ \pi^2 g_2^{(3)}(w, w^*) + 2 \pi^2 g_1^{(2)}(w, w^*) [L_1^+]^2 \\
 &\quad - \mathcal{I} [E_{\nu,n}^{(1)} \Phi_{\text{Reg}}^{(1)}(\nu, n)] - \mathcal{I} [E_{\nu,n} \Phi_{\text{Reg}}^{(2)}(\nu, n)] .
 \end{aligned} \tag{1.7.16}$$

The right-hand side of eq. (1.7.16) is completely known, up to some rational numbers mostly parameterizing our ignorance of beyond-the-symbol terms in the three- and four-loop coefficient functions at NNLLA. It can be written exclusively in terms of SVHPLs of weight six with eigenvalue $(+, +)$ under $\mathbb{Z}_2 \times \mathbb{Z}_2$ transformations. The results of section 1.6 then allow us to write down an ansatz for the NNLLA correction to the BFKL eigenvalue, similar to the ansatz (1.7.4) we made for the NNLLA correction to the impact factor, but at higher weight. More precisely, we assume that we can write $E_{\nu,n}^{(2)} = \sum_i \alpha_i P_i$, where α_i denote rational numbers and P_i runs through all possible monomials of weight five with the correct symmetry properties that we can construct out of the building blocks given in eq. (1.6.22), i.e.,

$$P_i \in \left\{ E_{\nu,n}^5, \zeta_2 V D_\nu E_{\nu,n}, E_{\nu,n} N \tilde{F}_4, \zeta_5, \dots \right\} . \tag{1.7.17}$$

The rational coefficients α_i can then be fixed by inserting our ansatz into eq. (1.7.16) and performing the inverse Fourier-Mellin transform to (w, w^*) space. We find that there is a unique solution for the α_i , and the result for the NNLLA correction to the

BFKL eigenvalue then takes the form,

$$\begin{aligned}
 E_{\nu,n}^{(2)} = & -E_{\nu,n}^{(1)} \Phi_{\text{Reg}}^{(1)}(\nu, n) - E_{\nu,n} \Phi_{\text{Reg}}^{(2)}(\nu, n) + \frac{3}{8} D_\nu^2 E_{\nu,n} E_{\nu,n}^2 + \frac{3}{32} N^2 D_\nu^2 E_{\nu,n} \\
 & + \frac{1}{8} V^2 D_\nu^2 E_{\nu,n} - \frac{1}{8} V D_\nu^3 E_{\nu,n} + \frac{1}{8} E_{\nu,n} [D_\nu E_{\nu,n}]^2 + \frac{5}{16} E_{\nu,n} N^2 V^2 \\
 & + \frac{1}{48} D_\nu^4 E_{\nu,n} + \frac{\pi^2}{12} D_\nu^2 E_{\nu,n} - \frac{3}{4} D_\nu E_{\nu,n} V E_{\nu,n}^2 - \frac{5}{16} D_\nu E_{\nu,n} N^2 V \\
 & - \frac{\pi^2}{4} D_\nu E_{\nu,n} V + \frac{3}{16} N^2 E_{\nu,n}^3 + \frac{61}{4} E_{\nu,n}^2 \zeta_3 + \frac{1}{8} E_{\nu,n}^5 + \frac{5\pi^2}{6} E_{\nu,n}^3 \\
 & + \frac{19}{128} E_{\nu,n} N^4 + \frac{3\pi^2}{16} E_{\nu,n} N^2 + \frac{\pi^2}{4} E_{\nu,n} V^2 + \frac{35}{16} N^2 \zeta_3 + \frac{1}{2} V^2 \zeta_3 \\
 & + \frac{11\pi^2}{6} \zeta_3 + 10 \zeta_5 + a_0 \mathcal{E}_5 + \sum_{i=1}^5 a_i \zeta_2 \mathcal{E}_{3,i} + a_6 \zeta_4 \mathcal{E}_2 + \sum_{i=7}^8 a_i \zeta_3 \mathcal{E}_{1,i},
 \end{aligned} \tag{1.7.18}$$

where the quantities $\mathcal{E}_{3,i}$, \mathcal{E}_2 , and $\mathcal{E}_{1,i}$ capture the beyond-the-symbol ambiguities in $g_1^{(4)}$, and \mathcal{E}_5 corresponds to the one symbol-level ambiguity. They are given by,

$$\begin{aligned}
 \mathcal{E}_5 = & \frac{124}{3} N^2 D_\nu^2 E_{\nu,n} + \frac{1210}{3} V^2 D_\nu^2 E_{\nu,n} - \frac{35}{3} V D_\nu^3 E_{\nu,n} \\
 & + \frac{124}{3} N^2 E_{\nu,n}^3 - \frac{140}{3} V^2 E_{\nu,n}^3 - \frac{31}{2} E_{\nu,n} N^4 + \frac{10903}{12} N^2 \zeta_3 \\
 & + \frac{13960}{3} V^2 \zeta_3 + 248 E_{\nu,n} [D_\nu E_{\nu,n}]^2 - \frac{151}{2} D_\nu E_{\nu,n} N^2 V \\
 & - 62 D_\nu^2 E_{\nu,n} E_{\nu,n}^2 + 70 D_\nu E_{\nu,n} V E_{\nu,n}^2 - 760 D_\nu E_{\nu,n} V^3 \\
 & - \frac{31}{6} D_\nu^4 E_{\nu,n} + 7431 E_{\nu,n}^2 \zeta_3 - 97 E_{\nu,n} N^2 V^2 + 16072 \zeta_5,
 \end{aligned} \tag{1.7.19}$$

$$\mathcal{E}_{3,1} = -\frac{3}{4} E_{\nu,n} N^2 - D_\nu^2 E_{\nu,n} + 5 E_{\nu,n}^3 + 6 E_{\nu,n} V^2 - 2 E_{\nu,n} \pi^2 + 8 \zeta_3, \tag{1.7.20}$$

$$\mathcal{E}_{3,2} = E_{\nu,n}^3, \tag{1.7.21}$$

$$\mathcal{E}_{3,3} = \frac{3}{4} E_{\nu,n} N^2 - 3 D_\nu E_{\nu,n} V + 3 E_{\nu,n}^3 + 12 \zeta_3, \tag{1.7.22}$$

$$\begin{aligned}
 \mathcal{E}_{3,4} = & -\frac{1}{8} D_\nu^2 E_{\nu,n} + \frac{9}{4} D_\nu E_{\nu,n} V - \frac{3}{4} E_{\nu,n} N^2 - \frac{3}{2} E_{\nu,n} V^2 - \frac{25}{2} \zeta_3 \\
 & - 2 E_{\nu,n}^3,
 \end{aligned} \tag{1.7.23}$$

$$\mathcal{E}_{3,5} = \frac{3}{8} E_{\nu,n} N^2 - \frac{3}{2} E_{\nu,n}^3, \tag{1.7.24}$$

$$\mathcal{E}_2 = 90 E_{\nu,n}, \tag{1.7.25}$$

$$\mathcal{E}_{1,7} = E_{\nu,n}^2 - \frac{1}{4} N^2, \quad (1.7.26)$$

$$\mathcal{E}_{1,8} = \frac{1}{2} E_{\nu,n}^2. \quad (1.7.27)$$

We observe that the most complicated piece is \mathcal{E}_5 . It would be absent if our conjecture that $a_0 = 0$ is correct. Some further comments are in order about eq. (1.7.18):

1. In ref. [15] it was argued, based on earlier work [72–75], that the BFKL eigenvalue should vanish as $(\nu, n) \rightarrow 0$ to all orders in perturbation theory, i.e., $\omega(0, 0) = 0$. While this statement depends on how one approaches the limit, the most natural way seems to be to set the discrete variable n to 0 before taking the limit $\nu \rightarrow 0$. Indeed in this limit $E_{\nu,n}$ and $E_{\nu,n}^{(1)}$ vanish. However, we find that $E_{\nu,n}^{(2)}$ does not vanish in this limit, but rather it approaches a constant,

$$\lim_{\nu \rightarrow 0} E_{\nu,0}^{(2)} = -\frac{1}{2} \pi^2 \zeta_3. \quad (1.7.28)$$

We stress that the limit is independent of any of the undetermined constants that parameterize the beyond-the-symbol terms in the three- and four-loop coefficients. While we have confidence in our result for $E_{\nu,n}^{(2)}$ given our assumptions (such as the vanishing of $g_n^{(\ell)}$ and $h_n^{(\ell)}$ as $w \rightarrow 0$), we have so far no explanation for this observation.

2. While the (ν, n) -space basis constructed in section 1.6 involves the new functions \tilde{F}_4 , \tilde{F}_{6a} and \tilde{F}_7 , we find that $E_{\nu,n}^{(2)}$ is free of these functions and can be expressed entirely in terms of ψ functions and rational functions of ν and n . Moreover, the ψ functions arise only in the form of the LLA BFKL eigenvalue and its derivative with respect to ν . We are therefore led to conjecture that, to all loop orders, the BFKL eigenvalue and the impact factor can be expressed as linear combinations of uniform weight of monomials that are even in both ν and n and are constructed exclusively out of multiple ζ values¹⁰ and the quantities N , V , $E_{\nu,n}$ and D_ν defined in section 1.6.

¹⁰Note that we can not exclude the appearance of multiple ζ values at higher weights, as multiple ζ values are reducible to ordinary ζ values until weight eight.

We now move on and extract the impact factor at N³LLA from the four-loop amplitude at the same logarithmic accuracy. Equation (1.4.1) at order a^4 yields the following relation for the impact factor at N³LLA,

$$\begin{aligned}
 \mathcal{I} \left[\Phi_{\text{Reg}}^{(3)}(\nu, n) \right] = & -4 \left\{ [L_1^+]^3 + 3 L_1^+ \pi^2 \right\} g_3^{(4)}(w, w^*) \\
 & + 4 \left\{ [L_1^+]^2 + \pi^2 \right\} g_2^{(4)}(w, w^*) - 4 L_1^+ g_1^{(4)}(w, w^*) \\
 & + 4 g_0^{(4)}(w, w^*) + 8 \pi^2 g_2^{(3)}(w, w^*) [L_1^+]^2 - 4 L_1^+ \pi^2 g_1^{(3)}(w, w^*) \\
 & - 2 \pi^2 \left\{ [L_1^+]^3 - \frac{\pi^2}{3} L_1^+ \right\} g_1^{(2)}(w, w^*) + 2 \pi^2 g_0^{(2)}(w, w^*) [L_1^+]^2 \\
 & + \frac{\pi^4}{8} L_1^+ [L_0^-]^2 - \frac{\pi^4}{3} [L_1^+]^3 - \frac{73\pi^6}{1260} L_1^+ - 2 L_1^+ \zeta_3^2.
 \end{aligned} \tag{1.7.29}$$

In order to determine $\Phi_{\text{Reg}}^{(3)}(\nu, n)$, we proceed in the same way as we did for $E_{\nu,n}^{(2)}$, i.e., we write down an ansatz for $\Phi_{\text{Reg}}^{(3)}(\nu, n)$ that has the correct transcendentality and symmetry properties and fix the free coefficients by requiring the inverse Fourier-Mellin transform of the ansatz to match the right-hand side of eq. (1.7.29). Building upon our conjecture that the impact factor can be expressed purely in terms of ψ functions and rational functions of ν and n , we construct a restricted ansatz¹¹ that is a linear combination just of monomials of ζ values and N , V , D_ν and $E_{\nu,n}$. Just like in the case of $E_{\nu,n}^{(2)}$, we find that there is a unique solution for the coefficients in the ansatz, thus giving further support to our conjecture. Furthermore, we are forced along the way to fix one of the beyond-the-symbol parameters appearing in $g_0^{(4)}$,

$$\begin{aligned}
 b_1 = & -\frac{15}{8} a_1 - \frac{3}{16} a_2 - \frac{3}{32} a_4 + \frac{9}{16} a_5 + \frac{1}{64} b_3 + \frac{1}{8} b_4 - \frac{3}{16} b_5 - \frac{1}{32} b_6 \\
 & + \frac{1}{4} b_7 + \frac{3}{32} b_8 + \frac{3}{16}.
 \end{aligned} \tag{1.7.30}$$

The final result for the impact factor at N³LLA then takes the form,

$$\Phi_{\text{Reg}}^{(3)}(\nu, n) = \frac{1}{3} \left[\Phi_{\text{Reg}}^{(1)}(\nu, n) \right]^3 - E_{\nu,n}^{(2)} E_{\nu,n} - \Phi_{\text{Reg}}^{(2)}(\nu, n) E_{\nu,n}^2 - \frac{1}{24} [D_\nu^2 E_{\nu,n}]^2 \tag{1.7.31}$$

¹¹We have constructed the full basis of functions in (ν, n) space through weight six and the explicit map to (w, w^*) functions of weight seven. It is therefore not necessary for us to restrict our ansatz in this way. It is, however, sufficient, and computationally simpler to do so.

$$\begin{aligned}
 & -\frac{3}{64} N^2 [D_\nu E_{\nu,n}]^2 + \frac{1}{4} D_\nu E_{\nu,n} V D_\nu^2 E_{\nu,n} - \frac{1}{24} D_\nu E_{\nu,n} D_\nu^3 E_{\nu,n} \\
 & -\frac{3}{32} E_{\nu,n} N^2 D_\nu^2 E_{\nu,n} + \frac{3}{16} D_\nu E_{\nu,n} E_{\nu,n} N^2 V - \frac{1}{4} D_\nu E_{\nu,n} V E_{\nu,n}^3 \\
 & -\frac{37\pi^2}{96} E_{\nu,n} D_\nu^2 E_{\nu,n} - \frac{1}{24} D_\nu^2 E_{\nu,n} \zeta_3 + \frac{161}{12} E_{\nu,n}^3 - \frac{3}{16} N^2 V^4 \\
 & + \frac{11\pi^2}{24} D_\nu E_{\nu,n} E_{\nu,n} V + \frac{9}{4} D_\nu E_{\nu,n} V \zeta_3 + \frac{1}{16} [D_\nu E_{\nu,n}]^2 E_{\nu,n}^2 \\
 & -\frac{1}{8} V^2 [D_\nu E_{\nu,n}]^2 + \frac{3\pi^2}{32} [D_\nu E_{\nu,n}]^2 + \frac{37}{256} N^4 E_{\nu,n}^2 + \frac{5}{32} N^2 V^2 E_{\nu,n}^2 \\
 & + \frac{1}{8} D_\nu^2 E_{\nu,n} E_{\nu,n}^3 - \frac{21\pi^2}{32} V^2 E_{\nu,n}^2 \zeta_3 + \frac{7}{48} E_{\nu,n}^6 + \frac{\pi^2}{3} E_{\nu,n}^4 - \frac{\pi^4}{72} E_{\nu,n}^2 \\
 & + \frac{7}{16} E_{\nu,n} N^2 \zeta_3 - \frac{13\pi^2}{2} E_{\nu,n} \zeta_3 - \frac{45}{1024} N^6 - \frac{41}{128} N^4 V^2 + \frac{5\pi^2}{512} N^4 \\
 & -\frac{5\pi^2}{128} N^2 V^2 + \frac{\pi^4}{24} N^2 + \frac{\pi^4}{8} V^2 + \frac{5}{2} \zeta_3^2 - \frac{311\pi^6}{11340} + 3 E_{\nu,n} V^2 \zeta_3 \\
 & -\frac{23\pi^2}{128} N^2 E_{\nu,n}^2 + 10 E_{\nu,n} \zeta_5 + \frac{15}{64} N^2 E_{\nu,n}^4 + a_0 \mathcal{P}_6 + \sum_{i=1}^5 a_i \zeta_2 \mathcal{P}_{a,4,i} \\
 & + a_6 \zeta_4 \mathcal{P}_{a,2} + \sum_{i=7}^8 a_i \zeta_3 \mathcal{P}_{a,3,i} + \sum_{i=2}^9 b_i \zeta_2 \mathcal{P}_{b,4,i} + \sum_{i=10}^{14} b_i \zeta_3 \mathcal{P}_{b,3,i} \\
 & + \sum_{i=15}^{16} b_i \zeta_4 \mathcal{P}_{b,2,i} + b_{17} \zeta_2 \zeta_3 \mathcal{P}_{b,1,1} + b_{18} \zeta_5 \mathcal{P}_{b,1,2},
 \end{aligned}$$

where $\mathcal{P}_{i,j,\dots}$ parametrize the beyond-the-symbol terms in the four-loop coefficient functions, and \mathcal{P}_6 parameterizes the one symbol-level ambiguity,

$$\begin{aligned}
 \mathcal{P}_6 = & \frac{105}{2} [D_\nu^2 E_{\nu,n}]^2 - \frac{152}{3} E_{\nu,n} N^2 D_\nu^2 E_{\nu,n} - \frac{2690}{3} E_{\nu,n} V^2 D_\nu^2 E_{\nu,n} \quad (1.7.32) \\
 & + \frac{595}{3} E_{\nu,n} V D_\nu^3 E_{\nu,n} - \frac{7}{6} E_{\nu,n} D_\nu^4 E_{\nu,n} + \frac{103}{16} N^4 E_{\nu,n}^2 \\
 & + \frac{13777}{3} E_{\nu,n} V^2 \zeta_3 + 16 D_\nu^2 E_{\nu,n} E_{\nu,n}^3 + 6548 E_{\nu,n} \zeta_5 \\
 & - \frac{10455}{2} D_\nu^2 E_{\nu,n} \zeta_3 + \frac{249}{8} N^2 [D_\nu E_{\nu,n}]^2 + \frac{2655}{2} V^2 [D_\nu E_{\nu,n}]^2 \\
 & + \frac{317}{4} N^2 V^2 E_{\nu,n}^2 + \frac{197}{24} N^2 E_{\nu,n}^4 + \frac{515}{6} V^2 E_{\nu,n}^4 + \frac{61793}{6} E_{\nu,n} N^2 \zeta_3 \\
 & + \frac{111}{128} N^6 + \frac{345}{32} N^4 V^2 - 385 D_\nu E_{\nu,n} V D_\nu^2 E_{\nu,n} - 30 D_\nu E_{\nu,n} D_\nu^3 E_{\nu,n}
 \end{aligned}$$

$$\begin{aligned}
 & -420 D_\nu E_{\nu,n} V E_{\nu,n}^3 + 7 D_\nu E_{\nu,n} E_{\nu,n} N^2 V - 760 D_\nu E_{\nu,n} E_{\nu,n} V^3 \\
 & -22606 D_\nu E_{\nu,n} V \zeta_3 - 34 [D_\nu E_{\nu,n}]^2 E_{\nu,n}^2 + 1140 V^4 E_{\nu,n}^2 \\
 & + 15231 E_{\nu,n}^3 \zeta_3 + 46992 \zeta_3^2, \\
 \mathcal{P}_{a,4,1} = & \frac{5}{8} E_{\nu,n} D_\nu^2 E_{\nu,n} - \frac{3}{2} D_\nu E_{\nu,n} E_{\nu,n} V + \frac{33}{8} [D_\nu E_{\nu,n}]^2 \\
 & - \frac{129}{8} V^2 E_{\nu,n}^2 - \frac{5}{4} E_{\nu,n}^4 + \frac{3}{128} N^4 + \frac{171}{32} N^2 V^2 + \frac{\pi^2}{4} N^2 \\
 & - \frac{183}{32} N^2 E_{\nu,n}^2 + \pi^2 E_{\nu,n}^2 - 68 E_{\nu,n} \zeta_3,
 \end{aligned} \tag{1.7.33}$$

$$\begin{aligned}
 \mathcal{P}_{a,4,2} = & -\frac{3}{16} E_{\nu,n} D_\nu^2 E_{\nu,n} + \frac{3}{4} D_\nu E_{\nu,n} E_{\nu,n} V + \frac{7}{16} [D_\nu E_{\nu,n}]^2 \\
 & - \frac{51}{64} N^2 E_{\nu,n}^2 - \frac{33}{16} V^2 E_{\nu,n}^2 - \frac{1}{4} E_{\nu,n}^4 - \frac{7}{256} N^4 + \frac{19}{64} N^2 V^2 \\
 & - 12 E_{\nu,n} \zeta_3,
 \end{aligned} \tag{1.7.34}$$

$$\begin{aligned}
 \mathcal{P}_{a,4,3} = & -\frac{3}{2} E_{\nu,n} D_\nu^2 E_{\nu,n} + \frac{9}{4} [D_\nu E_{\nu,n}]^2 - \frac{3}{2} N^2 E_{\nu,n}^2 - \frac{9}{2} V^2 E_{\nu,n}^2 \\
 & - \frac{3}{4} E_{\nu,n}^4 - \frac{9}{64} N^4 + \frac{9}{8} N^2 V^2 + 6 D_\nu E_{\nu,n} E_{\nu,n} V - 48 E_{\nu,n} \zeta_3,
 \end{aligned} \tag{1.7.35}$$

$$\begin{aligned}
 \mathcal{P}_{a,4,4} = & \frac{49}{32} E_{\nu,n} D_\nu^2 E_{\nu,n} - \frac{27}{8} D_\nu E_{\nu,n} E_{\nu,n} V - \frac{45}{32} [D_\nu E_{\nu,n}]^2 \\
 & + \frac{117}{128} N^2 E_{\nu,n}^2 + \frac{111}{32} V^2 E_{\nu,n}^2 + \frac{1}{2} E_{\nu,n}^4 + \frac{73}{2} E_{\nu,n} \zeta_3 + \frac{69}{512} N^4 \\
 & - \frac{21}{128} N^2 V^2,
 \end{aligned} \tag{1.7.36}$$

$$\begin{aligned}
 \mathcal{P}_{a,4,5} = & -\frac{3}{16} E_{\nu,n} D_\nu^2 E_{\nu,n} - \frac{3}{4} D_\nu E_{\nu,n} E_{\nu,n} V - \frac{15}{16} [D_\nu E_{\nu,n}]^2 \\
 & + \frac{105}{64} N^2 E_{\nu,n}^2 + \frac{63}{16} V^2 E_{\nu,n}^2 + \frac{3}{8} E_{\nu,n}^4 + \frac{3}{256} N^4 - \frac{69}{64} N^2 V^2 \\
 & + 18 E_{\nu,n} \zeta_3,
 \end{aligned} \tag{1.7.37}$$

$$\mathcal{P}_{a,2} = -\frac{45}{4} N^2 - 45 E_{\nu,n}^2, \tag{1.7.38}$$

$$\mathcal{P}_{a,3,7} = \frac{1}{6} D_\nu^2 E_{\nu,n} - \frac{1}{3} E_{\nu,n}^3 - \frac{4}{3} \zeta_3 - E_{\nu,n} V^2, \tag{1.7.39}$$

$$\begin{aligned}
 \mathcal{P}_{a,3,8} = & -\frac{1}{24} D_\nu^2 E_{\nu,n} + \frac{1}{4} D_\nu E_{\nu,n} V - \frac{1}{6} E_{\nu,n}^3 - \frac{1}{8} E_{\nu,n} N^2 - \frac{1}{2} E_{\nu,n} V^2 \\
 & - \frac{13}{6} \zeta_3,
 \end{aligned} \tag{1.7.40}$$

$$\mathcal{P}_{b,4,2} = \frac{3}{4} N^2 E_{\nu,n}^2 + \frac{3}{16} N^4 + \frac{21}{4} N^2 V^2 + 3 E_{\nu,n} D_\nu^2 E_{\nu,n} \tag{1.7.41}$$

$$\begin{aligned}
 & +12 D_\nu E_{\nu,n} E_{\nu,n} V + 3 [D_\nu E_{\nu,n}]^2 + 9 V^2 E_{\nu,n}^2, \\
 \mathcal{P}_{b,4,3} = & \frac{7}{192} E_{\nu,n} D_\nu^2 E_{\nu,n} - \frac{7}{16} D_\nu E_{\nu,n} E_{\nu,n} V - \frac{9}{64} [D_\nu E_{\nu,n}]^2 \\
 & + \frac{33}{256} N^2 E_{\nu,n}^2 + \frac{19}{64} V^2 E_{\nu,n}^2 + \frac{5}{24} E_{\nu,n}^4 + \frac{37}{12} E_{\nu,n} \zeta_3 + \frac{9}{1024} N^4 \\
 & - \frac{1}{256} N^2 V^2,
 \end{aligned} \tag{1.7.42}$$

$$\begin{aligned}
 \mathcal{P}_{b,4,4} = & -\frac{5}{24} E_{\nu,n} D_\nu^2 E_{\nu,n} - \frac{1}{2} D_\nu E_{\nu,n} E_{\nu,n} V - \frac{3}{8} [D_\nu E_{\nu,n}]^2 \\
 & + \frac{9}{32} N^2 E_{\nu,n}^2 + \frac{7}{8} V^2 E_{\nu,n}^2 + \frac{5}{12} E_{\nu,n}^4 + \frac{14}{3} E_{\nu,n} \zeta_3 + \frac{3}{128} N^4 \\
 & + \frac{11}{32} N^2 V^2,
 \end{aligned} \tag{1.7.43}$$

$$\begin{aligned}
 \mathcal{P}_{b,4,5} = & \frac{3}{16} E_{\nu,n} D_\nu^2 E_{\nu,n} + \frac{1}{2} D_\nu E_{\nu,n} E_{\nu,n} V + \frac{1}{2} [D_\nu E_{\nu,n}]^2 - \frac{31}{64} N^2 E_{\nu,n}^2 \\
 & - \frac{27}{16} V^2 E_{\nu,n}^2 - \frac{9}{16} E_{\nu,n}^4 + \frac{\pi^2}{8} E_{\nu,n}^2 - \frac{1}{128} N^4 - \frac{3}{64} N^2 V^2 \\
 & + \frac{\pi^2}{32} N^2 - 8 E_{\nu,n} \zeta_3,
 \end{aligned} \tag{1.7.44}$$

$$\begin{aligned}
 \mathcal{P}_{b,4,6} = & -\frac{5}{96} E_{\nu,n} D_\nu^2 E_{\nu,n} + \frac{1}{2} D_\nu E_{\nu,n} E_{\nu,n} V + \frac{17}{96} [D_\nu E_{\nu,n}]^2 \\
 & - \frac{25}{128} N^2 E_{\nu,n}^2 - \frac{15}{32} V^2 E_{\nu,n}^2 - \frac{11}{48} E_{\nu,n}^4 - \frac{49}{12} E_{\nu,n} \zeta_3 - \frac{17}{1536} N^4 \\
 & + \frac{11}{384} N^2 V^2,
 \end{aligned} \tag{1.7.45}$$

$$\begin{aligned}
 \mathcal{P}_{b,4,7} = & \Phi_{\text{Reg}}^{(2)}(\nu, n) - \frac{2}{3} E_{\nu,n} D_\nu^2 E_{\nu,n} - \frac{3}{8} [D_\nu E_{\nu,n}]^2 + \frac{1}{4} N^2 E_{\nu,n}^2 \\
 & + \frac{7}{4} V^2 E_{\nu,n}^2 - \frac{\pi^2}{2} E_{\nu,n}^2 + \frac{1}{3} E_{\nu,n} \zeta_3 - \frac{5}{128} N^4 - \frac{7}{8} N^2 V^2 \\
 & + \frac{\pi^2}{48} N^2 + \frac{\pi^2}{4} V^2 - \frac{11\pi^4}{180} + \frac{5}{24} E_{\nu,n}^4 + D_\nu E_{\nu,n} E_{\nu,n} V,
 \end{aligned} \tag{1.7.46}$$

$$\begin{aligned}
 \mathcal{P}_{b,4,8} = & -\frac{5}{32} E_{\nu,n} D_\nu^2 E_{\nu,n} + \frac{1}{8} D_\nu E_{\nu,n} E_{\nu,n} V - \frac{7}{32} [D_\nu E_{\nu,n}]^2 \\
 & + \frac{27}{128} N^2 E_{\nu,n}^2 + \frac{33}{32} V^2 E_{\nu,n}^2 + \frac{3}{8} E_{\nu,n}^4 - \frac{\pi^2}{4} E_{\nu,n}^2 + \frac{7}{512} N^4 \\
 & - \frac{19}{128} N^2 V^2 + 3 E_{\nu,n} \zeta_3,
 \end{aligned} \tag{1.7.47}$$

$$\mathcal{P}_{b,4,9} = \frac{1}{24} E_{\nu,n}^4, \tag{1.7.48}$$

$$\mathcal{P}_{b,3,10} = -\frac{1}{48} D_\nu^2 E_{\nu,n} + \frac{3}{8} D_\nu E_{\nu,n} V - \frac{1}{3} E_{\nu,n}^3 - \frac{1}{8} E_{\nu,n} N^2 - \frac{1}{4} E_{\nu,n} V^2 \tag{1.7.49}$$

$$\begin{aligned} & -\frac{25}{12}\zeta_3, \\ \mathcal{P}_{b,3,11} &= \frac{1}{16}E_{\nu,n}N^2 - \frac{1}{4}E_{\nu,n}^3, \end{aligned} \quad (1.7.50)$$

$$\mathcal{P}_{b,3,12} = -\frac{1}{2}D_\nu E_{\nu,n}V + \frac{1}{2}E_{\nu,n}^3 + \frac{1}{8}E_{\nu,n}N^2 + 2\zeta_3, \quad (1.7.51)$$

$$\mathcal{P}_{b,3,13} = \frac{1}{6}E_{\nu,n}^3, \quad (1.7.52)$$

$$\mathcal{P}_{b,3,14} = -\frac{1}{6}D_\nu^2 E_{\nu,n} + \frac{5}{6}E_{\nu,n}^3 - \frac{1}{8}E_{\nu,n}N^2 - \frac{\pi^2}{3}E_{\nu,n} + \frac{4}{3}\zeta_3 + E_{\nu,n}V^2, \quad (1.7.53)$$

$$\mathcal{P}_{b,2,15} = \frac{1}{2}E_{\nu,n}^2, \quad (1.7.54)$$

$$\mathcal{P}_{b,2,16} = E_{\nu,n}^2 - \frac{1}{4}N^2, \quad (1.7.55)$$

$$\mathcal{P}_{b,1,1} = E_{\nu,n}, \quad (1.7.56)$$

$$\mathcal{P}_{b,1,2} = E_{\nu,n}. \quad (1.7.57)$$

Again, the undetermined function at symbol level, \mathcal{P}_6 , is the most complicated term, but it would be absent if $a_0 = 0$.

Finally, we remark that the $\nu \rightarrow 0$ behavior of $\Phi_{\text{Reg}}^{(\ell)}(\nu, n)$ is nonvanishing, and even singular for $\ell = 2$ and 3. Taking the limit after setting $n = 0$, as in the case of $E_{\nu,n}^{(2)}$, we find that the constant term is given in terms of the cusp anomalous dimension,

$$\lim_{\nu \rightarrow 0} \Phi_{\text{Reg}}^{(1)}(\nu, 0) \sim \frac{\gamma_K^{(2)}}{4} + \mathcal{O}(\nu^4), \quad (1.7.58)$$

$$\lim_{\nu \rightarrow 0} \Phi_{\text{Reg}}^{(2)}(\nu, 0) \sim \frac{\pi^2}{4\nu^2} + \frac{\gamma_K^{(3)}}{4} + \mathcal{O}(\nu^2), \quad (1.7.59)$$

$$\lim_{\nu \rightarrow 0} \Phi_{\text{Reg}}^{(3)}(\nu, 0) \sim -\frac{\pi^4}{8\nu^2} + \frac{\gamma_K^{(4)}}{4} + \mathcal{O}(\nu^2). \quad (1.7.60)$$

This fact is presumably related to the appearance of $\gamma_K(a)$ in the factors ω_{ab} and δ , which carry logarithmic dependence on $|w|$ as $w \rightarrow 0$. It may play a role in understanding the failure of $E_{\nu,0}^{(2)}$ to vanish as $\nu \rightarrow 0$ in eq. (1.7.28).

1.8 Conclusions and Outlook

In this article we exposed the structure of the multi-Regge limit of six-gluon scattering in planar $\mathcal{N} = 4$ super-Yang-Mills theory in terms of the single-valued harmonic polylogarithms introduced by Brown. Given the finite basis of such functions, it is extremely simple to determine any quantity that is defined by a power series expansion around the origin of the (w, w^*) plane. Two examples which we could evaluate with no ambiguity are the LL and NLL terms in the multi-Regge limit of the MHV amplitude. We could carry this exercise out through transcendental weight 10, and we presented the analytic formulae explicitly through six loops in section 1.4. The NMHV amplitudes also fit into the same mathematical framework, as we saw in section 1.5: An integro-differential operator that generates the NMHV LLA terms from the MHV LLA ones [18] has a very natural action on the SVHPLs, making it simple to generate NMHV LLA results to high order as well. A clear avenue for future investigation utilizing the SVHPLs is the NMHV six-point amplitude at next-to-leading-logarithm and beyond.

A second thrust of this article was to understand the Fourier-Mellin transform from (w, w^*) to (ν, n) variables. In practice, we constructed this map in the reverse direction: We built an ansatz out of various elements: harmonic sums and specific rational combinations of ν and n . We then implemented the inverse Fourier-Mellin transform as a truncated sum, or power series around the origin of the (w, w^*) plane, and matched to the basis of SVHPLs. We thereby identified specific combinations of the elements as building blocks from which to generate the full set of SVHPL Fourier-Mellin transforms. We have executed this procedure completely through weight six in the (ν, n) space, corresponding to weight seven in the (w, w^*) space. In generalizing the procedure to yet higher weight, we expect the procedure to be much the same. Beginning with a linear combination of weight $(p - 2)$ HPLs in a single variable x , perform a Mellin transformation to produce weight $(p - 1)$ harmonic sums such as ψ , F_4 , F_{6a} , etc. For suitable combinations of these elements, the inverse Fourier-Mellin transform will generate weight p SVHPLs in the complex conjugate pair (w, w^*) . The step of determining which combinations of elements correspond to the SVHPLs was

carried out empirically in this paper. It would be interesting to investigate further the mathematical properties of these building blocks.

Using our understanding of the Fourier-Mellin transform, we could explicitly evaluate the NNLL MHV impact factor $\Phi_{\text{Reg}}^{(2)}(\nu, n)$ which derives from a knowledge of the three-loop remainder function in the MRK limit [14, 15]. We then went on to four loops, using a computation of the four-loop symbol [56] in conjunction with additional constraints from the multi-Regge limit to determine the MRK symbol up to one free parameter a_0 (which we suspect is zero). We matched this symbol to the symbols of the SVHPLs in order to determine the complete four-loop remainder function in MRK, up to a number of beyond-the-symbol constants. This data, in particular $g_1^{(4)}$ and $g_0^{(4)}$, then led to the NNLL BFKL eigenvalue $E_{\nu, n}^{(2)}$ and N³LL impact factor $\Phi_{\text{Reg}}^{(3)}(\nu, n)$. These quantities also contain the various beyond-the-symbol constants. Clearly the higher-loop NNLL MRK terms can be determined just as we did at LL and NLL, using the master formula (1.2.9) and the SVHPL basis. However, it would also be worthwhile to understand what constraint can fix a_0 , and the host of beyond-the-symbol constants, since they will afflict all of these terms. This task may require backing away somewhat from the multi-Regge limit, or utilizing coproduct information in some way.

We also remind the reader that we found that the NNLL BFKL eigenvalue $E_{\nu, n}^{(2)}$ does not vanish as $\nu \rightarrow 0$, taking the limit after setting $n = 0$. This behavior is in contrast to what happens in the LL and NLL case. It also goes against the expectations in ref. [15], and thus calls for further study.

Although the structure of QCD amplitudes in the multi-Regge limit is more complicated than those of planar $\mathcal{N} = 4$ super-Yang-Mills theory, one can still hope that the understanding of the Fourier-Mellin (ν, n) space that we have developed here may prove useful in the QCD context.

Finally, we remark that the SVHPLs are very likely to be applicable to another current problem in $\mathcal{N} = 4$ super-Yang-Mills theory, namely the determination of correlation functions for four off-shell operators. Conformal invariance implies that these quantities depend on two separate cross ratios. The natural arguments of the polylogarithms that appear at low loop order, after a change of variables from the

original cross ratios, are again a complex pair (w, w^*) (or (z, \bar{z})). The same single-valued conditions apply here as well. For example, the one-loop off-shell box integral that enters the correlation function is proportional to $L_2^-(z, \bar{z})/(z - \bar{z})$. We expect that the SVHPL framework will allow great progress to be made in this arena, just as it has to the study of the multi-Regge limit.

Chapter 2

The six-point remainder function to all loop orders in the multi-Regge limit

2.1 Introduction

In recent years, considerable progress has been made in the study of relativistic scattering amplitudes in gauge theory and gravity. A growing set of computational tools, including unitarity [76], BCFW recursion [77–80], BCJ duality [81, 82], and symbol-ology [34–37, 147], has facilitated many impressive perturbative calculations at weak coupling. The AdS/CFT correspondence has provided access to the new, previously inaccessible frontier of strong coupling [21]. The theory that has reaped the most benefit from these advances is, arguably, maximally supersymmetric $\mathcal{N} = 4$ Yang-Mills theory, specifically in the planar limit of a large number of colors. Indeed, $\mathcal{N} = 4$ super-Yang-Mills theory provides an excellent laboratory for the AdS/CFT correspondence, as well as for the structure of gauge theory amplitudes in general.

One of the reasons for the relative simplicity of $\mathcal{N} = 4$ super-Yang-Mills theory is its high degree of symmetry. The extended supersymmetry puts strong constraints on the form of scattering amplitudes, and it guarantees a conformal symmetry in position space. Recently, an additional conformal symmetry was found in the planar

theory [3, 21–26]. It acts on a set of dual variables, x_i , which are related to the external momenta k_i^μ by $k_i = x_i - x_{i+1}$. At tree level, this dual conformal symmetry can be extended to a dual super-conformal symmetry [27] and even combined with the original conformal symmetry into an infinite-dimensional Yangian symmetry [41]. At loop level, the dual conformal symmetry is broken by infrared divergences. According to the Wilson-loop/amplitude duality [21, 24, 25], these infrared divergences can be understood as ultraviolet divergences of particular polygonal Wilson loops. In this context, the breaking of dual conformal symmetry is governed by an anomalous Ward identity [3, 26, 83]. For maximally-helicity violating (MHV) amplitudes, a solution to the Ward identity may be written as,

$$A_n^{\text{MHV}} = A_n^{\text{BDS}} \times \exp(R_n), \quad (2.1.1)$$

where A_n^{BDS} is an all-loop, all-multiplicity ansatz proposed by Bern, Dixon, and Smirnov [32], and R_n is a dual-conformally invariant function referred to as the *remainder function* [1, 2, 2].

Dual conformal invariance provides a strong constraint on the form of R_n . For example, it is impossible to construct a non-trivial dual-conformally invariant function with fewer than six external momenta. As a result, $R_4 = R_5 = 0$, and, consequently, the four- and five-point scattering amplitudes are equal to the BDS ansatz. At six points, there are three independent invariant cross ratios built from distances x_{ij}^2 in the dual space,

$$u_1 = \frac{x_{13}^2 x_{46}^2}{x_{14}^2 x_{36}^2} = \frac{s_{12} s_{45}}{s_{123} s_{345}}, \quad u_2 = \frac{x_{24}^2 x_{15}^2}{x_{25}^2 x_{14}^2} = \frac{s_{23} s_{56}}{s_{234} s_{456}}, \quad u_3 = \frac{x_{35}^2 x_{26}^2}{x_{36}^2 x_{25}^2} = \frac{s_{34} s_{61}}{s_{345} s_{561}} \quad (2.1.2)$$

Dual conformal invariance restricts R_6 to be a function of these variables only, i.e. $R_6 = R_6(u_1, u_2, u_3)$. This function is not arbitrary since, among other conditions, it must be totally symmetric under permutations of the u_i and vanish in the collinear limit [1, 2].

In the absence of an explicit computation, it remained a possibility that $R_6 = 0$, despite the fact that all known symmetries allow for a non-zero function $R_6(u_1, u_2, u_3)$.

However, a series of calculations have since been performed and they showed definitively that $R_6 \neq 0$. The first evidence of a non-vanishing R_6 came from an analysis of the multi-Regge limits of $2 \rightarrow 4$ gluon scattering amplitudes at two loops [5]. Numerical evidence was soon found at specific kinematic points $[1, 2, 2]$, and an explicit calculation for general kinematics followed shortly thereafter [6, 7, 7]. Interestingly, the two-loop calculation for general kinematics was actually performed in a quasi-multi-Regge limit; the full kinematic dependence could then be inferred because this type of Regge limit does not modify the analytic dependence of the remainder function on the u_i .

Even beyond the two-loop remainder function, the limit of multi-Regge kinematics (MRK) has received considerable attention in the context of $\mathcal{N} = 4$ super-Yang Mills theory [5, 8–20]. One reason for this is that multi-leg scattering amplitudes become considerably simpler in MRK while still maintaining a non-trivial analytic structure. Taking the multi-Regge limit at six points, for example, essentially reduces the amplitude to a function of just two variables, w and w^* , which are complex conjugates of each other. This latter point has proved particularly important in describing the relevant function space in this limit. In fact, it has been argued recently [19] that the function space is spanned by the set of single-valued harmonic polylogarithms (SVHPLs) introduced by Brown [47]. These functions will play a prominent role in the remainder of this article.

The MRK limit of $2 \rightarrow 4$ scattering is characterized by the condition that the outgoing particles are widely separated in rapidity while having comparable transverse momenta. In terms of the cross ratios u_i , the limit is approached by sending one of the u_i , say u_1 , to unity, while letting the other two cross ratios vanish at the same rate that $u_1 \rightarrow 1$, i.e. $u_2 = x(1 - u_1)$ and $u_3 = y(1 - u_1)$ for two fixed variables x and y . Actually, this prescription produces the Euclidean version of the MRK limit in which the six-point remainder function vanishes [84–86]. To reach the Minkowski version, which is relevant for $2 \rightarrow 4$ scattering, u_1 must be analytically continued around the origin, $u_1 \rightarrow e^{-2\pi i}|u_1|$, before taking the limit. The remainder function may then be expanded around $u_1 = 1$ and the coefficients of this expansion are functions of only two variables, x and y . The variables w and w^* mentioned previously are related to

x and y by [12, 13],

$$x \equiv \frac{1}{(1+w)(1+w^*)}, \quad y \equiv \frac{w w^*}{(1+w)(1+w^*)}. \quad (2.1.3)$$

Neglecting terms that vanish like powers of $1 - u_1$, the expansion of the remainder function may be written as¹,

$$R_6^{\text{MHV}}|_{\text{MRK}} = 2\pi i \sum_{\ell=2}^{\infty} \sum_{n=0}^{\ell-1} a^\ell \log^n(1 - u_1) [g_n^{(\ell)}(w, w^*) + 2\pi i h_n^{(\ell)}(w, w^*)], \quad (2.1.4)$$

where the coupling constant for planar $\mathcal{N} = 4$ super-Yang-Mills theory is $a = g^2 N_c / (8\pi^2)$. This expansion is organized hierarchically into the leading-logarithmic approximation (LLA) with $n = \ell - 1$, the next-to-leading-logarithmic approximation (NLLA) with $n = \ell - 2$, and in general the $N^k\text{LL}$ terms with $n = \ell - k - 1$. In this article, we study the leading-logarithmic approximation, for which we may rewrite eq. (2.1.4) as,

$$R_6^{\text{MHV}}|_{\text{LLA}} = \frac{2\pi i}{\log(1 - u_1)} \sum_{\ell=2}^{\infty} \eta^\ell g_{\ell-1}^{(\ell)}(w, w^*), \quad (2.1.5)$$

where we have identified $\eta = a \log(1 - u_1)$ as the relevant expansion parameter. In LLA, the real part of R_6 vanishes, so $h_{\ell-1}^{(\ell)}(w, w^*)$ is absent in eq. (2.1.5). Expressions for $g_{\ell-1}^{(\ell)}(w, w^*)$ have been given in the literature for two, three [12], and recently up to ten [19] loops.

An all-orders integral-sum representation for $R_6^{\text{MHV}}|_{\text{LLA}}$ was presented in ref. [12] and was generalized to the NMHV helicity configuration in ref. [18]. (The MHV case was extended to NLLA in ref. [15].) The formula may be understood as an inverse Fourier-Mellin transform from a space of moments labeled by (ν, n) to the space of kinematic variables (w, w^*) . In the moment space, $R_6|_{\text{LLA}}(\nu, n)$ assumes a simple factorized form and may be written succinctly to all loop orders in terms of polygamma functions. This structure is obscured in (w, w^*) space, as the inverse Fourier-Mellin transform generates complicated combinations of polylogarithmic functions. Nevertheless, these complicated expressions should bear the mark of their simple ancestry.

¹We follow the conventions of ref. [14].

In this article, we expose this inherited structure by presenting an explicit all-orders formula for $R_6|_{\text{LLA}}$ directly in (w, w^*) space.

We do not present a proof of this formula, but we do test its validity using several non-trivial consistency checks. For example, our result agrees with the integral formula mentioned above through at least 14 loops. In ref. [18], Lipatov, Prygarin, and Schnitzer give a simple differential equation linking the MHV and NMHV helicity configurations,

$$w^* \frac{\partial}{\partial w^*} R_6^{\text{MHV}}|_{\text{LLA}} = w \frac{\partial}{\partial w} R_6^{\text{NMHV}}|_{\text{LLA}}, \quad (2.1.6)$$

which is also obeyed by our formula. In the near-collinear limit, we find agreement with the all-orders double-leading-logarithmic approximation of Bartels, Lipatov, and Prygarin [70].

This article is organized as follows. In section 1.2, we review the aspects of multi-Regge kinematics relevant to six-particle scattering and recall the integral formulas for $R_6|_{\text{LLA}}$ in the MHV and NMHV helicity configurations. The construction and properties of single-valued harmonic polylogarithms are reviewed in section 1.3. An all-orders expression for $R_6|_{\text{LLA}}$ is presented in terms of these functions in section 2.4. After verifying several consistency conditions of this formula, we examine its near-collinear limit in section 2.5. Section 2.6 offers some concluding remarks and prospects for future work.

2.2 The six-point remainder function in multi-Regge kinematics

We consider the six-gluon scattering process $g_3 g_6 \rightarrow g_1 g_5 g_4 g_2$ where the momenta are taken to be outgoing and the gluons are labeled cyclically in the clockwise direction. The limit of multi-Regge kinematics is defined by the condition that the produced gluons are strongly ordered in rapidity while having comparable transverse momenta,

$$y_1 \gg y_5 \gg y_4 \gg y_2, \quad |p_{1\perp}| \simeq |p_{5\perp}| \simeq |p_{4\perp}| \simeq |p_{2\perp}|. \quad (2.2.1)$$

In the Euclidean region, this limit is equivalent to the hierarchy of scales,

$$s_{12} \gg s_{345}, s_{456} \gg s_{34}, s_{45}, s_{56} \gg s_{23}, s_{61}, s_{234}, \quad (2.2.2)$$

which leads to the limiting behavior of the cross ratios (2.1.2),

$$1 - u_1, u_2, u_3 \sim 0, \quad (2.2.3)$$

subject to the constraint that the following ratios are held fixed,

$$x \equiv \frac{u_2}{1 - u_1} = \mathcal{O}(1) \quad \text{and} \quad y \equiv \frac{u_3}{1 - u_1} = \mathcal{O}(1). \quad (2.2.4)$$

Unitarity restricts the branch cuts of physical quantities like the remainder function $R_6(u_1, u_2, u_3)$ to appear in physical channels. In terms of the cross ratios u_i , this requirement implies that all branch points occur when a cross ratio vanishes or approaches infinity. If we re-express the two real variables x and y by a single complex variable w ,

$$x \equiv \frac{1}{(1 + w)(1 + w^*)} \quad \text{and} \quad y \equiv \frac{w w^*}{(1 + w)(1 + w^*)}, \quad (2.2.5)$$

then the equivalent statement in MRK is that any function of (w, w^*) must be *single-valued* in the complex w plane.

In the Euclidean region, the remainder function actually vanishes in the multi-Regge limit. To obtain a non-vanishing result, we must consider a physical region in which one of the cross ratios acquires a phase [5]. One such region corresponds to the $2 \rightarrow 4$ scattering process described above. It can be reached by flipping the signs of s_{12} and s_{45} , or, in terms of the cross ratios, by rotating u_1 around the origin,

$$u_1 \rightarrow e^{-2\pi i} |u_1|. \quad (2.2.6)$$

In the course of this analytic continuation, we pick up the discontinuity across a Mandelstam cut [5, 10]. The six-point remainder function can then be expanded in

the form given in eq. (2.1.4),

$$R_6^{\text{MHV}}|_{\text{MRK}} = 2\pi i \sum_{\ell=2}^{\infty} \sum_{n=0}^{\ell-1} a^\ell \log^n(1-u_1) \left[g_n^{(\ell)}(w, w^*) + 2\pi i h_n^{(\ell)}(w, w^*) \right]. \quad (2.2.7)$$

The large logarithms $\log(1-u_1)$ organize this expansion into the leading-logarithmic approximation (LLA) with $n = \ell - 1$, the next-to-leading-logarithmic approximation (NLLA) with $n = \ell - 2$, and in general the $N^k\text{LL}$ terms with $n = \ell - k - 1$.

In refs. [12, 15] an all-loop integral formula for $R_6^{\text{MHV}}|_{\text{MRK}}$ was presented for LLA and NLLA²,

$$\begin{aligned} e^{R+i\pi\delta}|_{\text{MRK}} &= \cos \pi\omega_{ab} \\ &+ i \frac{a}{2} \sum_{n=-\infty}^{\infty} (-1)^n \left(\frac{w}{w^*} \right)^{\frac{n}{2}} \int_{-\infty}^{+\infty} \frac{d\nu}{\nu^2 + \frac{n^2}{4}} |w|^{2i\nu} \Phi_{\text{Reg}}(\nu, n) \left(-\frac{1}{\sqrt{u_2 u_3}} \right)^{\omega(\nu, n)}. \end{aligned} \quad (2.2.8)$$

Here, $\omega(\nu, n)$ is the BFKL eigenvalue and $\Phi_{\text{Reg}}(\nu, n)$ is the regularized impact factor. They may be expanded perturbatively,

$$\begin{aligned} \omega(\nu, n) &= -a \left(E_{\nu, n} + a E_{\nu, n}^{(1)} + a^2 E_{\nu, n}^{(2)} + \mathcal{O}(a^3) \right), \\ \Phi_{\text{Reg}}(\nu, n) &= 1 + a \Phi_{\text{Reg}}^{(1)}(\nu, n) + a^2 \Phi_{\text{Reg}}^{(2)}(\nu, n) + a^3 \Phi_{\text{Reg}}^{(3)}(\nu, n) + \mathcal{O}(a^4). \end{aligned} \quad (2.2.9)$$

The leading-order eigenvalue, $E_{\nu, n}$, was given in ref. [8] and may be written in terms of the digamma function $\psi(z) = \frac{d}{dz} \log \Gamma(z)$,

$$E_{\nu, n} = -\frac{1}{2} \frac{|n|}{\nu^2 + \frac{n^2}{4}} + \psi \left(1 + i\nu + \frac{|n|}{2} \right) + \psi \left(1 - i\nu + \frac{|n|}{2} \right) - 2\psi(1). \quad (2.2.10)$$

In this article, we will only need the leading-order terms, but, remarkably, the higher-order corrections listed in (2.2.9) may also be expressed in terms of the ψ function and its derivatives [15, 19].

²There is a difference in conventions regarding the definition of the remainder function. What we call R is called $\log(R)$ in refs. [12, 15]. Apart from the zeroth order term, this distinction has no effect on LLA terms. The first place it makes a difference is at four loops in NLLA, in the real part.

Returning to (2.2.8), the remaining functions are,

$$\begin{aligned}\omega_{ab} &= \frac{1}{8} \gamma_K(a) \log \frac{u_3}{u_2} = \frac{1}{8} \gamma_K(a) \log |w|^2, \\ \delta &= \frac{1}{8} \gamma_K(a) \log(xy) = \frac{1}{8} \gamma_K(a) \log \frac{|w|^2}{|1+w|^4},\end{aligned}\tag{2.2.11}$$

and the cusp anomalous dimension, which is known to all orders in perturbation theory [57],

$$\gamma_K(a) = \sum_{\ell=1}^{\infty} \gamma_K^{(\ell)} a^\ell = 4a - 4\zeta_2 a^2 + 22\zeta_4 a^3 - \left(\frac{219}{2}\zeta_6 + 4\zeta_3^2\right) a^4 + \dots \tag{2.2.12}$$

In addition, there is an ambiguity regarding the Riemann sheet of the exponential factor on the right-hand side of (2.2.8). We resolve this ambiguity with the identification,

$$\left(-\frac{1}{\sqrt{u_2 u_3}}\right)^{\omega(\nu, n)} \rightarrow e^{-i\pi\omega(\nu, n)} \left(\frac{1}{1-u_1} \frac{|1+w|^2}{|w|}\right)^{\omega(\nu, n)}.\tag{2.2.13}$$

The $i\pi$ factor in the right-hand side of eq. (2.2.13) generates the real parts $h_n^{(\ell)}$ in eq. (2.2.7). For example, at LLA and NLLA, the following relations [19] are satisfied³,

$$\begin{aligned}h_{\ell-1}^{(\ell)}(w, w^*) &= 0, \\ h_{\ell-2}^{(\ell)}(w, w^*) &= \frac{\ell-1}{2} g_{\ell-1}^{(\ell)}(w, w^*) + \frac{1}{16} \gamma_K^{(1)} g_{\ell-2}^{(\ell-1)}(w, w^*) \log \frac{|1+w|^4}{|w|^2} \\ &\quad - \frac{1}{2} \sum_{k=2}^{\ell-2} g_{k-1}^{(k)} g_{\ell-k-1}^{(\ell-k)}, \quad \ell > 2,\end{aligned}\tag{2.2.14}$$

where $\gamma_K^{(1)} = 4$ from eq. (2.2.12). Making use of eq. (2.1.5), we present an alternate

³Note that the sum over k in the formula for $h_{\ell-2}^{(\ell)}$ would not have been present if we had used the convention for R in refs. [12, 15].

form of these identities which will be useful later,

$$\begin{aligned} \text{Re} (R_6^{\text{MHV}}|_{\text{NLLA}}) &= \frac{2\pi i}{\log(1-u_1)} \left(\frac{1}{2} \eta^2 \frac{\partial}{\partial \eta} \frac{1}{\eta} + \frac{\gamma_K^{(1)}}{16} \eta \log \frac{|1+w|^4}{|w|^2} \right) R_6^{\text{MHV}}|_{\text{LLA}} \\ &+ \frac{2\pi^2}{\log^2(1-u_1)} \eta^2 g_1^{(2)}(w, w^*) - \frac{1}{2} (R_6^{\text{MHV}}|_{\text{LLA}})^2. \end{aligned} \quad (2.2.15)$$

The term proportional to $g_1^{(2)}(w, w^*)$ addresses the special case of $\ell = 2$ in eq. (2.2.14).

In what follows, we will focus on the leading-logarithmic approximation of (2.2.8), which takes the form,

$$R_6^{\text{MHV}}|_{\text{LLA}} = i \frac{a}{2} \sum_{n=-\infty}^{\infty} (-1)^n \int_{-\infty}^{+\infty} \frac{d\nu w^{i\nu+n/2} w^{*i\nu-n/2}}{(i\nu + \frac{n}{2})(-i\nu + \frac{n}{2})} \left[(1-u_1)^{a E_{\nu,n}} - 1 \right]. \quad (2.2.16)$$

The ν -integral may be evaluated by closing the contour and summing residues⁴. To perform the resulting double sums, one may apply the summation algorithms of ref. [61], although this approach is computationally challenging for high loop orders. Alternatively, an ansatz for the result may be expanded around $|w| = 0$ and matched term-by-term to the truncated double sum. The latter method requires knowledge of the complete set of functions that might arise in this context. In ref. [19], it was argued that the single-valued harmonic polylogarithms (SVHPLs) completely characterize this function space, and, using these functions, eq. (2.2.16) was evaluated through ten loops.

So far we have only discussed the MHV helicity configuration. We now turn to the only other independent helicity configuration at six points, the NMHV configuration. In MRK, the MHV and NMHV tree amplitudes are equal [18, 87]. It is natural, therefore, to define an NMHV remainder function, analogous to eq. (2.1.1),

$$A_6^{\text{NMHV}}|_{\text{MRK}} = A_6^{\text{BDS}} \times \exp(R_{\text{NMHV}}). \quad (2.2.17)$$

⁴For the special case of $n = 0$, our prescription is to take half the residue at $\nu = 0$.

In ref. [18], it was argued that the effect of changing the helicity of one of the positive-helicity gluons⁵ was equivalent to changing the impact factor for that gluon by means of the following replacement,

$$\frac{1}{-i\nu + \frac{n}{2}} \rightarrow -\frac{1}{i\nu + \frac{n}{2}}. \quad (2.2.18)$$

Referring to eq. (2.2.16), this replacement leads to an integral formula for $R_6^{\text{NMHV}}|_{\text{LLA}}$,

$$R_6^{\text{NMHV}}|_{\text{LLA}} = -\frac{ia}{2} \sum_{n=-\infty}^{\infty} (-1)^n \int_{-\infty}^{+\infty} \frac{d\nu w^{i\nu+n/2} w^{*i\nu-n/2}}{(i\nu + \frac{n}{2})^2} \left[(1-u_1)^{a_{E\nu,n}} - 1 \right]. \quad (2.2.19)$$

Following refs. [18] and [19], we can extract a simple rational prefactor and write eq. (2.2.19) in a manifestly inversion-symmetric form,

$$R_6^{\text{NMHV}}|_{\text{LLA}} = \frac{2\pi i}{\log(1-u_1)} \sum_{\ell=2}^{\infty} \frac{\eta^\ell}{1+w^*} f^{(\ell)}(w, w^*) + \left\{ (w, w^*) \leftrightarrow \left(\frac{1}{w}, \frac{1}{w^*} \right) \right\}, \quad (2.2.20)$$

for some single-valued functions $f^{(\ell)}(w, w^*)$. It is possible to obtain expressions for $f^{(\ell)}(w, w^*)$ directly from eq. (2.2.19) by means of the truncated series approach outlined above, for example. A simpler method is to make use of the following differential equation, which may be deduced by comparing the two expressions (2.2.16) and (2.2.19),

$$w^* \frac{\partial}{\partial w^*} R_6^{\text{MHV}}|_{\text{LLA}} = w \frac{\partial}{\partial w} R_6^{\text{NMHV}}|_{\text{LLA}}. \quad (2.2.21)$$

In principle, solving this equation requires the difficult step of fixing the constants of integration in such a way that single-valuedness is preserved. As discussed in ref. [19], this step becomes trivial when working in the space of SVHPLs, which are the subject of the next section.

⁵Up to power-suppressed terms, helicity must be conserved along high-energy lines, so the helicity flip must occur on one of the lower-energy legs, 4 or 5.

2.3 Review of single-valued harmonic polylogarithms

Harmonic polylogarithms (HPLs) [48] are a class of generalized polylogarithmic functions that finds frequent application in multi-loop calculations. The HPLs are functions of a single complex variable, z , which will be related to the kinematic variable w by $z = -w$. We will continue to use z throughout this section in order to make contact with the existing mathematical literature. In general, the HPLs have branch cuts that originate at $z = -1$, $z = 0$, or $z = 1$. In the present application, we will consider the restricted class of HPLs⁶ whose branch points are either $z = 0$ or $z = 1$. To construct them, consider the set X^* of all words w formed from the letters x_0 and x_1 , together with e , the empty word⁷. Then, for each $w \in X^*$, define a function $H_w(z)$ which obeys the differential equations,

$$\frac{\partial}{\partial z} H_{x_0 w}(z) = \frac{H_w(z)}{z} \quad \text{and} \quad \frac{\partial}{\partial z} H_{x_1 w}(z) = \frac{H_w(z)}{1-z}, \quad (2.3.1)$$

subject to the following conditions,

$$H_e(z) = 1, \quad H_{x_0^n}(z) = \frac{1}{n!} \log^n z, \quad \text{and} \quad \lim_{z \rightarrow 0} H_{w \neq x_0^n}(z) = 0. \quad (2.3.2)$$

There is a unique family of solutions to these equations, and it defines the HPLs. For $w \neq x_0^n$, they can be written as iterated integrals,

$$H_{x_0 w}(z) = \int_0^z dz' \frac{H_w(z')}{z'} \quad \text{and} \quad H_{x_1 w} = \int_0^z dz' \frac{H_w(z')}{1-z'}. \quad (2.3.3)$$

⁶In the mathematical literature, these functions are sometimes referred to as *multiple polylogarithms in one variable*. With a small abuse of notation, we will continue to use the term “HPL” to refer to this restricted set of functions.

⁷Context should distinguish the word w from the kinematic variable with the same name.

The structure of the iterated integrals endows the HPLs with an important property: they form a *shuffle algebra*. The shuffle relations can be written as,

$$H_{w_1}(z) H_{w_2}(z) = \sum_{w \in w_1 \sqcup w_2} H_w(z), \quad (2.3.4)$$

where $w_1 \sqcup w_2$ is the set of mergers of the sequences w_1 and w_2 that preserve their relative ordering. The shuffle algebra may be used to remove all zeros from the right of an index vector in favor of some explicit logarithms. For example, it is easy to obtain the following formula for HPLs with a single x_1 ,

$$H_{x_0^n x_1 x_0^m} = \sum_{j=0}^m \frac{(-1)^j}{(m-j)!} \binom{n+j}{j} H_{x_0}^{m-j} H_{x_0^{n+j} x_1}. \quad (2.3.5)$$

After removing all right-most zeros, the Taylor expansions around $z = 0$ are particularly simple and involve only a special class of harmonic numbers [48],

$$H_{m_1, \dots, m_k}(z) = \sum_{l=1}^{\infty} \frac{z^l}{l^{m_1}} Z_{m_2, \dots, m_k}(l-1), \quad m_i > 0, \quad (2.3.6)$$

where $Z_{m_1, \dots, m_k}(n)$ are Euler-Zagier sums [50, 51], defined recursively by

$$Z(n) = 1 \quad \text{and} \quad Z_{m_1, \dots, m_k}(n) = \sum_{l=1}^n \frac{1}{l^{m_1}} Z_{m_2, \dots, m_k}(l-1). \quad (2.3.7)$$

Note that the indexing of the weight vectors m_1, \dots, m_k in eqs. (2.3.6) and (2.3.7) is in the collapsed notation in which a subscript m denotes $m-1$ zeros followed by a single 1.

The HPLs are multi-valued functions; nevertheless, it is possible to build specific combinations such that the branch cuts cancel and the result is single-valued. An algorithm that explicitly constructs these combinations was presented in ref. [47] and reviewed in ref. [19]. Here we provide a very brief description.

The SVHPLs $\mathcal{L}_w(z)$ are generated by the series,

$$\mathcal{L}(z) = L_X(z)\tilde{L}_Y(\bar{z}) \equiv \sum_{w \in X^*} \mathcal{L}_w(z)w, \quad (2.3.8)$$

where,

$$L_X(z) = \sum_{w \in X^*} H_w(z)w, \quad \tilde{L}_Y(\bar{z}) = \sum_{w \in Y^*} H_{\phi(w)}(\bar{z})\tilde{w}. \quad (2.3.9)$$

Here $\sim : X^* \rightarrow X^*$ is the operation that reverses words, $\phi : Y^* \rightarrow X^*$ is the map that renames y to x , and Y^* is the set of words in $\{y_0, y_1\}$, which are defined by the relations,

$$\begin{aligned} y_0 &= x_0 \\ \tilde{Z}(y_0, y_1)y_1\tilde{Z}(y_0, y_1)^{-1} &= Z(x_0, x_1)^{-1}x_1Z(x_0, x_1), \end{aligned} \quad (2.3.10)$$

where $Z(x_0, x_1)$ is a generating function of multiple zeta values,

$$Z(x_0, x_1) = \sum_{w \in X^*} \zeta(w)w. \quad (2.3.11)$$

The $\zeta(w)$ are regularized by the shuffle algebra and obey $\zeta(w \neq x_1) = H_w(1)$ and $\zeta(x_1) = 0$.

Alternatively, one may formally define these functions as solutions to simple differential equations, i.e. the $\mathcal{L}_w(z)$ are the unique single-valued linear combinations of functions $H_{w_1}(z)H_{w_2}(\bar{z})$ that obey the differential equations [47],

$$\frac{\partial}{\partial z} \mathcal{L}_{x_0 w}(z) = \frac{\mathcal{L}_w(z)}{z} \quad \text{and} \quad \frac{\partial}{\partial z} \mathcal{L}_{x_1 w}(z) = \frac{\mathcal{L}_w(z)}{1-z}, \quad (2.3.12)$$

subject to the conditions,

$$\mathcal{L}_e(z) = 1, \quad \mathcal{L}_{x_0^n}(z) = \frac{1}{n!} \log^n |z|^2 \quad \text{and} \quad \lim_{z \rightarrow 0} \mathcal{L}_{w \neq x_0^n}(z) = 0. \quad (2.3.13)$$

The SVHPLs also obey differential equations in \bar{z} . Both sets of equations are represented nicely in terms of the generating function (2.3.8),

$$\frac{\partial}{\partial z} \mathcal{L}(z) = \left(\frac{x_0}{z} + \frac{x_1}{1-z} \right) \mathcal{L}(z) \quad \text{and} \quad \frac{\partial}{\partial \bar{z}} \mathcal{L}(z) = \mathcal{L}(z) \left(\frac{y_0}{\bar{z}} + \frac{y_1}{1-\bar{z}} \right). \quad (2.3.14)$$

2.4 Six-point remainder function in the leading-logarithmic approximation of MRK

The SVHPLs introduced in the previous section provide a convenient basis of functions to describe the six-point remainder function in MRK. In ref. [19], these functions were used to express the result through ten loops in LLA and through nine loops in NLLA. Here we use the SVHPLs to present a formula in LLA to all loop orders.

2.4.1 The all-orders formula

Recall from the previous section that we defined X^* to be the set of all words w in the letters x_0 and x_1 together with the empty word e . Let $\mathbb{C}\langle X \rangle$ be the complex vector space generated by X^* and let $\mathbb{C}\langle \mathcal{L} \rangle$ be the complex vector space spanned by the SVHPLs, \mathcal{L}_w with $w \in X^*$. Denote by $\mathbb{C}\langle X \rangle[[\eta]]$ and $\mathbb{C}\langle \mathcal{L} \rangle[[\eta]]$ the rings of formal power series in the variable $\eta = a \log(1 - u_1)$ with coefficients in $\mathbb{C}\langle X \rangle$ and $\mathbb{C}\langle \mathcal{L} \rangle$, respectively. There is a natural map, ρ , which sends words to the corresponding SVHPLs,

$$\begin{aligned} \rho : \mathbb{C}\langle X \rangle[[\eta]] &\rightarrow \mathbb{C}\langle \mathcal{L} \rangle[[\eta]] \\ w &\mapsto \mathcal{L}_w. \end{aligned} \quad (2.4.1)$$

Using these ingredients, we propose the following formulas for the MHV and NMHV remainder functions in MRK and LLA,

$$R_6^{\text{MHV}}|_{\text{LLA}} = \frac{2\pi i}{\log(1 - u_1)} \rho \left(\mathcal{X} \mathcal{Z}^{\text{MHV}} - \frac{1}{2} x_1 \eta \right), \quad (2.4.2)$$

$$R_6^{\text{NMHV}}|_{\text{LLA}} = \frac{2\pi i}{\log(1 - u_1)} \frac{1}{1 + w^*} \rho \left(x_0 \mathcal{X} \mathcal{Z}^{\text{NMHV}} \right) + \left\{ (w, w^*) \leftrightarrow \left(\frac{1}{w}, \frac{1}{w^*} \right) \right\}. \quad (2.4.3)$$

where the formal power series $\mathcal{X}, \mathcal{Z}^{(\text{N})\text{MHV}} \in \mathbb{C}\langle X \rangle[[\eta]]$ are,

$$\begin{aligned} \mathcal{X} &= e^{\frac{1}{2}x_0\eta} \left[1 - x_1 \left(\frac{e^{x_0\eta} - 1}{x_0} \right) \right]^{-1}, \\ \mathcal{Z}^{\text{MHV}} &= \frac{1}{2} \sum_{k=1}^{\infty} \left(x_1 \sum_{n=0}^{k-1} (-1)^n x_0^{k-n-1} \sum_{m=0}^n \frac{2^{2m-k+1}}{(k-m-1)!} \mathfrak{Z}(n, m) \right) \eta^k, \\ \mathcal{Z}^{\text{NMHV}} &= \frac{1}{2} \sum_{k=2}^{\infty} \left(x_1 \sum_{n=0}^{k-2} (-1)^n x_0^{k-n-2} \sum_{m=0}^n \frac{2^{2m-k+1}}{(k-m-1)!} \mathfrak{Z}(n, m) \right) \eta^k. \end{aligned} \quad (2.4.4)$$

Here, the $\mathfrak{Z}(n, m)$ are particular combinations of ζ values of uniform weight n . They are related to partial Bell polynomials, and are generated by the series,

$$\exp \left[y \sum_{k=1}^{\infty} \zeta_{2k+1} x^{2k+1} \right] \equiv \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \mathfrak{Z}(n, m) x^n y^m. \quad (2.4.5)$$

An explicit formula is,

$$\mathfrak{Z}(n, m) = \sum_{\beta \in P(n, m)} \prod_i \frac{(\zeta_{2i+1})^{\beta_i}}{\beta_i!}, \quad (2.4.6)$$

where $P(n, m)$ is the set of n -tuples of non-negative integers that sum to m , such that the product of ζ values has weight n ,

$$P(n, m) = \left\{ \{\beta_1, \dots, \beta_n\} \mid \beta_i \in \mathbb{N}_0, \sum_{i=1}^n \beta_i = m, \sum_{i=1}^n (2i+1)\beta_i = n \right\}. \quad (2.4.7)$$

Similarly, an expression for the k th term of \mathcal{X} can be given as,

$$\mathcal{X} = \sum_{k=0}^{\infty} \left(\sum_{n=0}^k \frac{x_0^{k-n}}{2^{k-n} (k-n)!} \sum_{\alpha \in Q(n)} \prod_j \frac{x_1 x_0^{\alpha_j-1}}{\alpha_j!} \right) \eta^k, \quad (2.4.8)$$

where $Q(n)$ is the set of integer compositions of n ,

$$Q(n) = \left\{ \{\alpha_1, \alpha_2, \dots, \alpha_m\} \mid \alpha_i \in \mathbb{Z}^+, \sum_{i=1}^m \alpha_i = n \right\}. \quad (2.4.9)$$

Excluding the one-loop term in eq. (2.4.2), the arguments of the ρ functions factorize into the product of a ζ -free function, \mathcal{X} , and a ζ -containing function, $\mathcal{Z}^{(\text{N})\text{MHV}}$. The ζ -free function is simpler and its first few terms read,

$$\begin{aligned} \mathcal{X} = & 1 + \left(\frac{1}{2} x_0 + x_1 \right) \eta + \left(\frac{1}{8} x_0^2 + \frac{1}{2} x_0 x_1 + \frac{1}{2} x_1 x_0 + x_1^2 \right) \eta^2 \\ & + \left(\frac{1}{48} x_0^3 + \frac{1}{8} x_0^2 x_1 + \frac{1}{4} x_0 x_1 x_0 + \frac{1}{2} x_0 x_1^2 + \frac{1}{6} x_1 x_0^2 + \frac{1}{2} x_1 x_0 x_1 + \frac{1}{2} x_1^2 x_0 + x_1^3 \right) \eta^3 \\ & + \dots \end{aligned} \quad (2.4.10)$$

The ζ -containing functions are slightly more complicated. Their first few terms are,

$$\begin{aligned} \mathcal{Z}^{\text{MHV}} &= \frac{1}{2} x_1 \eta + \frac{1}{4} x_1 x_0 \eta^2 + \frac{1}{16} x_1 x_0^2 \eta^3 + \left(\frac{1}{96} x_1 x_0^3 - \frac{1}{8} \zeta_3 x_1 \right) \eta^4 + \dots, \\ \mathcal{Z}^{\text{NMHV}} &= \frac{1}{4} x_1 \eta^2 + \frac{1}{16} x_1 x_0 \eta^3 + \frac{1}{96} x_1 x_0^2 \eta^4 + \left(\frac{1}{768} x_1 x_0^3 - \frac{1}{48} \zeta_3 x_1 \right) \eta^5 + \dots \end{aligned} \quad (2.4.11)$$

Using eqs. (2.4.10) and (2.4.11), one may easily extract $g_{\ell-1}^{(\ell)}$ for $\ell = 1, 2, 3, 4$ (cf. eqs. (2.1.5) and (2.4.2)). The one loop term vanishes, $g_0^{(1)} = 0$, and the other functions

read,

$$\begin{aligned}
g_1^{(2)} &= \frac{1}{4} \mathcal{L}_{0,1} + \frac{1}{4} \mathcal{L}_{1,0} + \frac{1}{2} \mathcal{L}_{1,1}, \\
g_2^{(3)} &= \frac{1}{16} \mathcal{L}_{0,0,1} + \frac{1}{8} \mathcal{L}_{0,1,0} + \frac{1}{4} \mathcal{L}_{0,1,1} + \frac{1}{16} \mathcal{L}_{1,0,0} + \frac{1}{4} \mathcal{L}_{1,0,1} + \frac{1}{4} \mathcal{L}_{1,1,0} + \frac{1}{2} \mathcal{L}_{1,1,1}, \\
g_3^{(4)} &= \frac{1}{96} \mathcal{L}_{0,0,0,1} + \frac{1}{32} \mathcal{L}_{0,0,1,0} + \frac{1}{16} \mathcal{L}_{0,0,1,1} + \frac{1}{32} \mathcal{L}_{0,1,0,0} + \frac{1}{8} \mathcal{L}_{0,1,0,1} + \frac{1}{8} \mathcal{L}_{0,1,1,0} \\
&\quad + \frac{1}{4} \mathcal{L}_{0,1,1,1} + \frac{1}{96} \mathcal{L}_{1,0,0,0} + \frac{1}{12} \mathcal{L}_{1,0,0,1} + \frac{1}{8} \mathcal{L}_{1,0,1,0} + \frac{1}{4} \mathcal{L}_{1,0,1,1} + \frac{1}{16} \mathcal{L}_{1,1,0,0} \\
&\quad + \frac{1}{4} \mathcal{L}_{1,1,0,1} + \frac{1}{4} \mathcal{L}_{1,1,1,0} + \frac{1}{2} \mathcal{L}_{1,1,1,1} - \frac{1}{8} \zeta_3 \mathcal{L}_1.
\end{aligned} \tag{2.4.12}$$

Similarly, one may extract the first few $f^{(\ell)}$ (cf. eqs. (2.2.20) and (2.4.3)), finding $f^{(1)} = 0$ and,

$$\begin{aligned}
f^{(2)} &= \frac{1}{4} \mathcal{L}_{0,1}, \\
f^{(3)} &= \frac{1}{8} \mathcal{L}_{0,0,1} + \frac{1}{16} \mathcal{L}_{0,1,0} + \frac{1}{4} \mathcal{L}_{0,1,1}, \\
f^{(4)} &= \frac{1}{32} \mathcal{L}_{0,0,0,1} + \frac{1}{32} \mathcal{L}_{0,0,1,0} + \frac{1}{8} \mathcal{L}_{0,0,1,1} + \frac{1}{96} \mathcal{L}_{0,1,0,0} + \frac{1}{8} \mathcal{L}_{0,1,0,1} + \frac{1}{16} \mathcal{L}_{0,1,1,0} \\
&\quad + \frac{1}{4} \mathcal{L}_{0,1,1,1}, \\
f^{(5)} &= \frac{1}{192} \mathcal{L}_{0,0,0,0,1} + \frac{1}{128} \mathcal{L}_{0,0,0,1,0} + \frac{1}{32} \mathcal{L}_{0,0,0,1,1} + \frac{1}{192} \mathcal{L}_{0,0,1,0,0} + \frac{1}{16} \mathcal{L}_{0,0,1,0,1} \\
&\quad + \frac{1}{32} \mathcal{L}_{0,0,1,1,0} + \frac{1}{8} \mathcal{L}_{0,0,1,1,1} + \frac{1}{768} \mathcal{L}_{0,1,0,0,0} + \frac{1}{24} \mathcal{L}_{0,1,0,0,1} + \frac{1}{32} \mathcal{L}_{0,1,0,1,0} \\
&\quad + \frac{1}{8} \mathcal{L}_{0,1,0,1,1} + \frac{1}{96} \mathcal{L}_{0,1,1,0,0} + \frac{1}{8} \mathcal{L}_{0,1,1,0,1} + \frac{1}{16} \mathcal{L}_{0,1,1,1,0} + \frac{1}{4} \mathcal{L}_{0,1,1,1,1} \\
&\quad - \frac{1}{48} \zeta_3 \mathcal{L}_{0,1}.
\end{aligned} \tag{2.4.13}$$

We do not offer a proof that eqs. (2.4.2) and (2.4.3) are valid to all orders in perturbation theory. One may easily check that their expansions through low loop orders, as determined by eqs. (2.4.12) and (2.4.13), match the known results [12, 19]. It is also straightforward to extend the above calculations to ten loops and confirm

that the results are in agreement with those of ref. [19]. Moreover, we have verified that the truncated series expansion of eq. (2.4.2) as $|w| \rightarrow 0$ agrees with that of eq. (2.2.16) through 14 loops.

A comparison through such a high loop order is important in order to confirm the absence of multiple zeta values with depth larger than one (hereafter simply “MZVs”). To see why these MZVs should be absent, consider performing the sum of residues in eq. (2.2.16). Transcendental constants can only arise from the evaluation the ψ function and its derivatives at integer values. The latter are given in terms of rational numbers (Euler-Zagier sums) and ordinary ζ values. Therefore, it is impossible for the series expansion of eq. (2.2.16) to contain MZVs.

On the other hand, we would naively expect MZVs to appear in the series expansion of eq. (2.4.2) at 12 loops and beyond. This expectation is due to the fact that, for high weights, the y alphabet of eq. (2.3.10) contains MZVs, and, starting at weight 12, these MZVs begin appearing explicitly in the definitions of the SVHPLs. In order for eq. (2.4.2) to agree with eq. (2.2.16), all the MZVs must conspire to cancel in the particular linear combination of SVHPLs that appears in (2.4.2). We find that this cancellation indeed occurs, at least through 14 loops. It would be interesting to understand the mechanism of this cancellation, but we postpone this study to future work.

2.4.2 Consistency of the MHV and NMHV formulas

The MHV and NMHV remainder functions are related by the differential equation (2.2.21),

$$w^* \frac{\partial}{\partial w^*} R_6^{\text{MHV}}|_{\text{LLA}} = w \frac{\partial}{\partial w} R_6^{\text{NMHV}}|_{\text{LLA}}. \quad (2.4.14)$$

Recalling that $(w, w^*) = (-z, -\bar{z})$, it is straightforward to use the formulas (2.3.14) to check that eqs. (2.4.2) and (2.4.3) obey this differential equation. To see how this works, consider eq. (2.4.2), which we write as,

$$R_6^{\text{MHV}}|_{\text{LLA}} = \frac{2\pi i}{\log(1-u_1)} \rho \left[g_0(x_0, x_1)x_0 + g_1(x_0, x_1)x_1 \right], \quad (2.4.15)$$

for some functions $g_0(x_0, x_1)$ and $g_1(x_0, x_1)$ which can be easily read off from eq. (2.4.2). The w^* derivative acts on SVHPLs by clipping off the last index and multiplying by $1/w^*$ if that index was an x_0 or by $-1/(1+w^*)$ if it was an x_1 . There are also corrections due to the y alphabet at higher weights. Importantly, $y_0 = x_0$, so these corrections only affect the terms with a prefactor $1/(1+w^*)$. This observation allows us to write,

$$\begin{aligned} w^* \frac{\partial}{\partial w^*} R_6^{\text{MHV}}|_{\text{LLA}} &= \frac{2\pi i}{\log(1-u_1)} \rho \left[g_0(x_0, x_1) - \frac{w^*}{1+w^*} \hat{g}_1(x_0, x_1) \right] \\ &= \frac{2\pi i}{\log(1-u_1)} \rho \left[\frac{1}{1+w^*} g_0(x_0, x_1) \right. \\ &\quad \left. + \frac{1}{1+1/w^*} \left(g_0(x_0, x_1) - \hat{g}_1(x_0, x_1) \right) \right]. \end{aligned} \quad (2.4.16)$$

Due to the complicated expression for y_1 , it is difficult to obtain an explicit formula for $\hat{g}_1(x_0, x_1)$. Thankfully, we may employ a symmetry argument to avoid calculating it directly. Referring to eq. (2.2.16), $R_6^{\text{MHV}}|_{\text{LLA}}$ has manifest symmetry under inversion $(w, w^*) \leftrightarrow (1/w, 1/w^*)$, or, equivalently, $(\nu, n) \leftrightarrow (-\nu, -n)$. The differential operator $w^* \partial_{w^*}$ flips the parity, so eq. (2.4.16) should be odd under inversion. Since the two rational prefactors on the second line of eq. (2.4.16) map into one another under inversion, we can infer that their coefficients must be related⁸,

$$g_0 \left(\frac{1}{w}, \frac{1}{w^*} \right) = -g_0(w, w^*) + \hat{g}_1(w, w^*), \quad (2.4.17)$$

where $g_0(w, w^*) = \rho(g_0(x_0, x_1))$ and $\hat{g}_1(w, w^*) = \rho(\hat{g}_1(x_0, x_1))$. It is easy to check that this identity is satisfied for low loop orders⁹.

Using these symmetry properties, we can write,

$$w^* \frac{\partial}{\partial w^*} R_6^{\text{MHV}}|_{\text{LLA}} = \frac{2\pi i}{\log(1-u_1)} \frac{1}{1+w^*} \rho \left[g_0(x_0, x_1) \right] - \left\{ (w, w^*) \leftrightarrow \left(\frac{1}{w}, \frac{1}{w^*} \right) \right\}. \quad (2.4.18)$$

⁸ ρ does not generate any rational functions which might allow these terms to mix together.

⁹A general proof would be tantamount to showing that eq. (2.4.2) is symmetric under inversion. The latter seems to require another intricate cancellation of multiple zeta values. We postpone this investigation to future work.

Turning to the right-hand side of eq. (2.4.14), we observe that the differential operator $w \partial_w$ acts on eq. (2.4.3) by removing the leading x_0 and flipping the sign of the second term,

$$w \frac{\partial}{\partial w} R_6^{\text{NMHV}}|_{\text{LLA}} = \frac{2\pi i}{\log(1-u_1)} \frac{1}{1+w^*} \rho \left[\mathcal{X} \mathcal{Z}^{\text{NMHV}} \right] - \left\{ (w, w^*) \leftrightarrow \left(\frac{1}{w}, \frac{1}{w^*} \right) \right\}. \quad (2.4.19)$$

Comparing eq. (2.4.18) and eq. (2.4.19), we see that eq. (2.4.14) is only satisfied if $g_0(x_0, x_1) = \mathcal{X} \mathcal{Z}^{\text{NMHV}}$. To verify that this is true, we must extract $g_0(x_0, x_1)$ from $R_6^{\text{MHV}}|_{\text{LLA}}$. To this end, collect all terms in the argument of ρ with at least one trailing x_0 and remove that x_0 . This procedure gives,

$$\begin{aligned} g_0(x_0, x_1) &= \frac{1}{2} \mathcal{X} \sum_{k=2}^{\infty} \left(x_1 \sum_{n=0}^{k-2} (-1)^n x_0^{k-n-2} \sum_{m=0}^n \frac{2^{2m-k+1}}{(k-m-1)!} \mathfrak{Z}(n, m) \right) \eta^k \\ &= \mathcal{X} \mathcal{Z}^{\text{NMHV}}, \end{aligned} \quad (2.4.20)$$

so we conclude that eq. (2.4.14) is indeed satisfied.

2.5 Collinear limit

In the previous section, we proposed an all-orders formula for the MHV and NMHV remainder functions in MRK. The expressions are effectively functions of two variables, w and w^* . The single-valuedness condition allows for these functions to be expressed in a compact way, but the result is still somewhat difficult to manipulate.

In this section, we study a simpler kinematical configuration: the collinear corner of MRK phase space. To reach this configuration, we begin in multi-Regge kinematics and then take legs 1 and 6 to be nearly collinear. In terms of the cross ratios u_i , this limit is

$$1 - u_1, u_2, u_3 \sim 0, \quad x \equiv \frac{u_2}{1 - u_1} = \mathcal{O}(1), \quad y \equiv \frac{u_3}{1 - u_1} \sim 0, \quad (2.5.1)$$

or, in terms of the (w, w^*) variables, it is equivalent to,

$$1 - u_1 \sim 0, \quad |w| \sim 0, \quad w \sim w^*. \quad (2.5.2)$$

As we approach the collinear limit, the remainder function can be expanded in powers of w , w^* , and $\log |w|$. The leading power-law behavior is proportional to $(w + w^*)$. Neglecting terms that are suppressed by further powers of $|w|$, the result is effectively a function of a single variable, $\xi = \eta \log |w| = a \log(1 - u_1) \log |w|$, and is simple enough to be computed explicitly, as we show in the following subsections.

2.5.1 MHV

In the MHV helicity configuration, the remainder function is symmetric under conjugation $w \leftrightarrow w^*$. It also vanishes in the strict collinear limit. These conditions suggest a convenient form for the expansion in the near-collinear limit,

$$R_6^{\text{MHV}}|_{\text{LLA, coll.}} = \frac{2\pi i}{\log(1 - u_1)} (w + w^*) \sum_{k=0}^{\infty} \eta^{k+1} r_k^{\text{MHV}}(\eta \log |w|), \quad (2.5.3)$$

for some functions r_k^{MHV} that are analytic in a neighborhood of the origin. We have neglected further power-suppressed terms, *i.e.* terms quadratic or higher in w or w^* . The index k labels the degree to which r_k^{MHV} is subleading in $\log |w|$. For example, the leading logarithms are collected in r_0^{MHV} , the next-to-leading logarithms are collected in r_1^{MHV} , etc.

Starting from eq. (2.4.2), it is possible to obtain an explicit formula for r_k^{MHV} . To begin, we note that it is sufficient to restrict our attention to the terms proportional to w — the conjugation symmetry guarantees that they are equal to the terms proportional to w^* . The main observation is that only a subset of terms in eq. (2.4.2) contributes to the power series expansion at order w . It turns out that the relevant subset is simply the set of SVHPLs with a single x_1 in the weight vector. Roughly speaking, each additional x_1 implies another integration by $1/(1+w)$, which increases the leading power by one.

The equivalent statement is not true for w^* , *i.e.* SVHPLs with an arbitrary number

of x_1 's contribute to the power series expansion at order w^* . This asymmetry can be traced to the differences between the x and y alphabets: referring to eq. (2.3.9), the x alphabet indexes the HPLs with argument w and the y alphabet indexes the HPLs with argument w^* .

We are therefore led to consider the terms in eq. (2.4.2) with exactly one x_1 . Eq. (2.4.4) shows that these terms may be obtained by dropping all x_1 's from \mathcal{X} ,

$$R_6^{\text{MHV}}|_{\text{LLA, coll.}} = \frac{2\pi i}{\log(1-u_1)} \rho\left(e^{\frac{1}{2}x_0\eta} \mathcal{Z}^{\text{MHV}} - \frac{1}{2}x_1\eta\right). \quad (2.5.4)$$

Since no ζ terms appear in SVHPLs with a single x_1 , it is straightforward to express them in terms of HPLs,

$$\mathcal{L}_{x_0^n x_1 x_0^m} = \sum_{j=0}^n \frac{1}{j!} H_{x_0}^j \bar{H}_{x_0^m x_1 x_0^{n-j}} + \sum_{j=0}^m \frac{1}{j!} H_{x_0^n x_1 x_0^{m-j}} \bar{H}_{x_0}^j. \quad (2.5.5)$$

Here we have simplified the notation by defining $H_m \equiv H_m(-w)$ and $\bar{H}_m = H_m(-w^*)$. Next, we recall eq. (2.3.5), in which we used the shuffle algebra to expose the explicit logarithms,

$$H_{x_0^n x_1 x_0^m} = \sum_{j=0}^m \frac{(-1)^j}{(m-j)!} \binom{n+j}{j} H_{x_0}^{m-j} H_{x_0^{n+j} x_1}. \quad (2.5.6)$$

Finally, eqs. (2.3.6) and (2.3.7) implies that the series expansions for small w have leading term,

$$H_{x_0^k x_1}(-w) = -w + \mathcal{O}(w^2). \quad (2.5.7)$$

Combining eqs. (2.5.4)-(2.5.7) and applying some hypergeometric function identities, we arrive at an explicit formula for r_k^{MHV} ,

$$\begin{aligned} r_k^{\text{MHV}}(x) &= \frac{1}{2} \delta_{0,k} \\ &+ \sum_{n=0}^k \sum_{m=0}^n \sum_{j=k-m}^{2k-n-m} \frac{(-2)^{2m+j-k-1}}{(m+j-k)!} \mathfrak{Z}(n, m) x^{m-k+j/2} P_j^{(k-j-n, k-j-m)}(0) I_j(2\sqrt{x}). \end{aligned} \quad (2.5.8)$$

In this expression, the I_j are modified Bessel functions and the $P_j^{(a,b)}$ are Jacobi polynomials, which can be defined for non-negative integers j by the generating function,

$$\sum_{j=0}^{\infty} P_j^{(a,b)}(z) t^j = \frac{2^{a+b} \left(1 - t + \sqrt{t^2 - 2tz + 1}\right)^{-a} \left(1 + t + \sqrt{t^2 - 2tz + 1}\right)^{-b}}{\sqrt{t^2 - 2tz + 1}}. \quad (2.5.9)$$

It is easy to extract the first few terms,

$$\begin{aligned} r_0^{\text{MHV}}(x) &= \frac{1}{2} [1 - I_0(2\sqrt{x})], \\ r_1^{\text{MHV}}(x) &= -\frac{1}{4} I_2(2\sqrt{x}), \\ r_2^{\text{MHV}}(x) &= \frac{1}{4x} I_2(2\sqrt{x}) - \frac{1}{16} I_4(2\sqrt{x}). \end{aligned} \quad (2.5.10)$$

The leading term, r_0^{MHV} , corresponds to the double-leading-logarithmic approximation (DLLA) of ref. [70],

$$R_6^{\text{MHV}}|_{\text{DLLA}} = i\pi a(w + w^*) \left[1 - I_0\left(2\sqrt{\eta \log |w|}\right)\right], \quad (2.5.11)$$

and is in agreement with the results of that reference.

Only for $k > 2$ do ζ values begin to appear in r_k^{MHV} . Moreover, modified Bessel functions with odd indices only appear in the ζ -containing terms. To see this, notice that the ζ -free terms of eq. (2.5.8) arise from the boundary of the sum with $n = m = 0$, in which case $a = b = k - j$ in eq. (2.5.9). When $a = b$, $P_j^{a,b}(0) = 0$ for odd j since eq. (2.5.9) reduces to a function of t^2 in this case. It follows that the ζ -free pieces of r_k^{MHV} have no modified Bessel functions with odd indices.

Equations (2.5.3) and (2.5.8) provide an explicit formula for the six-point remainder function in the near-collinear limit of the LL approximation of MRK. If the sum in eq. (2.5.3) converges sufficiently quickly, then it should be possible to evaluate the function numerically by truncating the sum at a finite value of k , k_{max} . A numerical analysis indicates that for $|w| < 1$ and $\eta \lesssim 20$, $k_{\text{max}} \simeq 100$ is adequate to ensure convergence.

The numerical analysis also indicates that $R_6^{\text{MHV}}|_{\text{LLA, coll.}}$ increases exponentially

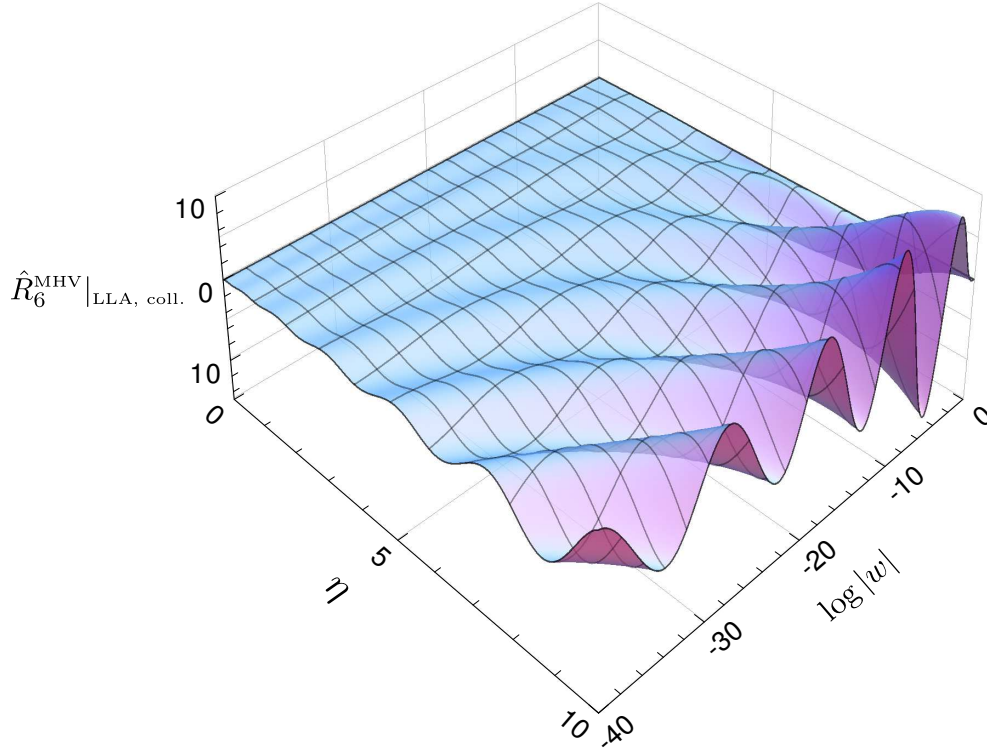


Figure 2.1: The MHV remainder function in the near-collinear limit of the LL approximation of MRK. It has been rescaled by an exponential damping factor. See eq. (2.5.12).

as a function of η , and that the extent of this increase depends strongly on the value of $\log |w|$. We find empirically that the rescaled function

$$\hat{R}_6^{\text{MHV}}|_{\text{LLA, coll.}} = \exp\left(-\frac{\eta}{\sqrt[4]{-\log |w|}}\right) \frac{\log(1-u_1)}{2\pi i(w+w^*)} R_6^{\text{MHV}}|_{\text{LLA, coll.}} \quad (2.5.12)$$

attains reasonable uniformity in the region $0 < \eta < 10$ and $-40 < \log |w| < 0$. This particular rescaling carries no special significance, as alternatives are possible and may be more appropriate in different regions. In eq. (2.5.12) we have also divided by the overall prefactor of eq. (2.5.3) so that $\hat{R}_6^{\text{MHV}}|_{\text{LLA, coll.}}$ is truly a function of the two variables η and $\log |w|$. The results are displayed in fig. 2.1.

2.5.2 NMHV

A similar analysis can be performed for the NMHV helicity configuration. The situation is slightly more complicated in this case because the NMHV remainder function is not symmetric under conjugation $w \leftrightarrow w^*$. One consequence is that its expansion in the collinear limit requires two sequences of functions, which we choose to parameterize by r_k^{NMHV} and $\tilde{r}_k^{\text{NMHV}}$,

$$R_6^{\text{NMHV}}|_{\text{LLA, coll.}} = \frac{2\pi i}{\log(1-u_1)} \left[(w+w^*) \sum_{k=0}^{\infty} \eta^{k+2} r_k^{\text{NMHV}}(\eta \log |w|) + w^* \sum_{k=0}^{\infty} \eta^k \tilde{r}_k^{\text{NMHV}}(\eta \log |w|) \right]. \quad (2.5.13)$$

Contributions to the power series at order w arise from the first term of eq. (2.4.3) (the second term has an overall factor of w^*), and, as in the MHV case, only from the subset of SVHPLs with a single x_1 in the weight vector. It is therefore possible to reuse eqs. (2.5.5)-(2.5.7) and obtain an explicit formula for the coefficient of w , r_k^{NMHV} . The result is,

$$r_k^{\text{NMHV}}(x) = \sum_{n=0}^k \sum_{m=0}^n \sum_{j=k-m}^{2k-n-m} \left[\frac{(-2)^{2m+j-k}}{(m+j-k)!} \mathfrak{Z}(n, m) x^{m-k+(j-1)/2} \times P_{j+2}^{(k-j-n-1, k-j-m-1)}(0) I_{j+1}(2\sqrt{x}) \right]. \quad (2.5.14)$$

The first few terms are

$$\begin{aligned} r_0^{\text{NMHV}}(x) &= -\frac{1}{4\sqrt{x}} I_1(2\sqrt{x}), \\ r_1^{\text{NMHV}}(x) &= -\frac{1}{8\sqrt{x}} I_3(2\sqrt{x}), \\ r_2^{\text{NMHV}}(x) &= \frac{3}{16x^{3/2}} I_3(2\sqrt{x}) - \frac{1}{32\sqrt{x}} I_5(2\sqrt{x}). \end{aligned} \quad (2.5.15)$$

As previously mentioned, it is not so straightforward to extract the coefficient of

w^* in this way. We can instead make progress by exploiting the differential equation (2.2.21). In terms of the functions r_k^{MHV} , r_k^{NMHV} , and $\tilde{r}_k^{\text{NMHV}}$, the equations read,

$$\begin{aligned}\partial_x r_k^{\text{MHV}}(x) &= 2 r_k^{\text{NMHV}}(x) + \partial_x r_{k-1}^{\text{NMHV}}(x) \\ \partial_x \tilde{r}_k^{\text{NMHV}}(x) &= 2 r_k^{\text{MHV}}(x) + 2 r_{k-1}^{\text{NMHV}}(x).\end{aligned}\tag{2.5.16}$$

The first of these equations is automatically satisfied and confirms the consistency of eq. (2.5.8) and eq. (2.5.14). The second equation determines $\tilde{r}_k^{\text{NMHV}}$ up to a constant of integration which can be determined by examining the $n = -1$ term of eq. (2.2.19). The solution is,

$$\begin{aligned}\tilde{r}_k^{\text{NMHV}}(x) = x \delta_{0,k} - \sum_{n=0}^k \sum_{m=0}^n \sum_{j=k-m}^{2k-n-m} &\left[\frac{(-2)^{2m+j-k}}{(m+j-k)!} \mathfrak{Z}(n, m) x^{m-k+(j+1)/2} \right. \\ &\left. \times P_j^{(k-j-n, k-j-m)}(0) I_{j-1}(2\sqrt{x}) \right].\end{aligned}\tag{2.5.17}$$

The first few terms are

$$\begin{aligned}\tilde{r}_0^{\text{NMHV}}(x) &= x - \sqrt{x} I_1(2\sqrt{x}), \\ \tilde{r}_1^{\text{NMHV}}(x) &= -\frac{1}{2} \sqrt{x} I_1(2\sqrt{x}), \\ \tilde{r}_2^{\text{NMHV}}(x) &= \frac{1}{2\sqrt{x}} I_1(2\sqrt{x}) - \frac{1}{8} \sqrt{x} I_3(2\sqrt{x}).\end{aligned}\tag{2.5.18}$$

Modified Bessel functions with even indices only appear in the ζ -containing terms of r_k^{NMHV} and $\tilde{r}_k^{\text{NMHV}}$. The explanation of this fact is the same as in the MHV case, except that the parity is flipped due to the shifts of the indices of the modified Bessel functions in eq. (2.5.14) and eq. (2.5.17).

2.5.3 The real part of the MHV remainder function in NLLA

As described in section 2.2, the real part of the MHV remainder function in NLLA is related to its imaginary part in LLA. In the collinear limit, the relation (2.2.15) may

be written as,

$$\begin{aligned} \text{Re} \left(R_6^{\text{MHV}}|_{\text{NLLA, coll.}} \right) &= \frac{2\pi i}{\log(1-u_1)} \left(\frac{1}{2} \eta^2 \frac{\partial}{\partial \eta} \frac{1}{\eta} - \frac{1}{2} \eta \log |w| \right) R_6^{\text{MHV}}|_{\text{LLA, coll.}} \\ &\quad - \frac{\pi^2}{\log^2(1-u_1)} \eta^2 \log |w|. \end{aligned} \quad (2.5.19)$$

Since $R_6^{\text{MHV}}|_{\text{LLA}}$ vanishes like $(w + w^*)$ in the strict collinear limit, the quadratic term $(R_6^{\text{MHV}}|_{\text{LLA}})^2$ in eq. (2.2.15) only contributes to further power-suppressed terms in the near-collinear limit and is therefore omitted from eq. (2.5.19)¹⁰. We may write eq. (2.5.19) as,

$$\text{Re} \left(R_6^{\text{MHV}}|_{\text{NLLA, coll.}} \right) = -\frac{4\pi^2}{\log^2(1-u_1)} (w + w^*) \sum_{k=0}^{\infty} \eta^{k+1} q_k(\eta \log |w|), \quad (2.5.20)$$

where,

$$q_k(x) = \frac{1}{4} x \delta_{0,k} + \frac{1}{2} (k-x) r_k^{\text{MHV}}(x) + \frac{1}{2} x \partial_x r_k^{\text{MHV}}(x). \quad (2.5.21)$$

The leading term, q_0 , corresponds to the real part of the next-to-double-leading-logarithmic approximation (NDLLA) of ref. [70]. Our results agree¹¹ with that reference and read,

$$\begin{aligned} \text{Re} \left(R_6^{\text{MHV}}|_{\text{NDLLA}} \right) &= \frac{\pi^2 (w + w^*) \eta}{\log^2(1-u_1)} \left[-\eta \log |w| I_0 \left(2\sqrt{\eta \log |w|} \right) \right. \\ &\quad \left. + \sqrt{\eta \log |w|} I_1 \left(2\sqrt{\eta \log |w|} \right) \right]. \end{aligned} \quad (2.5.22)$$

2.6 Conclusions

In this article, we studied the six-point amplitude of planar $\mathcal{N} = 4$ super-Yang-Mills theory in the leading-logarithmic approximation of multi-Regge kinematics. In this limit, the remainder function assumes a particularly simple form, which we exposed

¹⁰As a consequence, eq. (2.5.19) does not depend on the conventions used to define R , i.e. the equation is equally valid if R is replaced by $\exp(R)$.

¹¹The agreement requires a few typos to be corrected in eq. (A.16) of ref. [70].

to all loop orders in terms of the single-valued harmonic polylogarithms introduced by Brown. The SVHPLs provide a natural basis of functions for the remainder function in MRK because the single-valuedness condition maps nicely onto a physical constraint imposed by unitarity. Previously, these functions had been used to calculate the remainder function in LLA through ten loops. In this work, we extended these results to all loop orders.

In MRK, the tree amplitudes in the MHV and NMHV helicity configurations are identical. This observation motivates the definition of an NMHV remainder function in analogy with the MHV case. We examined both remainder functions in this article, and proposed all-order formulas for each case. In fact, these formulas are related: as described in ref. [18], the two remainder functions are linked by a simple differential equation. We employed this differential equation to verify the consistency of our results.

We also investigated the behavior of our formulas in the near-collinear limit of MRK. The additional large logarithms that arise in this limit impose a hierarchical organization of the resulting expansions. We derived explicit all-orders expressions for the terms of this logarithmic expansion. The results are given in terms of modified Bessel functions.

We did not provide a proof of the all-orders result, but we verified that it agrees through 14 loops with an integral formula of Lipatov and Prygarin. The agreement of these formulas at 12 loops and beyond requires an intricate cancellation of multiple zeta values. It would be interesting to understand the mechanism of this cancellation. There are several other potential directions for future research. For example, in refs. [38–40], Alday, Gaiotto, Maldacena, Sever, and Vieira performed an OPE analysis of hexagonal Wilson loops which in principle should provide additional cross-checks of our results. It should also be possible to study the all-orders formula as a function of the coupling and, in particular, to examine its strong-coupling expansion. We have begun this study in the collinear limit and presented our initial results in fig. 2.1. A first attempt to compare the six-point remainder function in MRK at strong and weak coupling was made by Bartels, Kotanski, and Schomerus [11]. Further analysis of our all-orders formula should allow for an important comparison with this string-theoretic

calculation.

Chapter 3

Leading singularities and off-shell conformal integrals

3.1 Introduction

The work presented in this paper is motivated by recent progress in planar $\mathcal{N} = 4$ super Yang-Mills (SYM) theory in four dimensions, although the methods that we exploit and further develop should be of much wider applicability.

$\mathcal{N} = 4$ SYM theory has many striking properties due to its high degree of symmetry; for instance it is conformally invariant, even as a quantum theory [88], and the spectrum of anomalous dimensions of composite operators can be found from an integrable system [89]. Most strikingly perhaps, it is related to IIB string theory on $\text{AdS}_5 \times \text{S}^5$ by the AdS/CFT correspondence [90]. This is a weak/strong coupling duality in which the same physical system is conveniently described by the field theory picture at weak coupling, while the string theory provides a way of capturing its strong coupling regime. The strong coupling limit of scattering amplitudes in the model has been elaborated in ref. [21] from a string perspective. The formulae take the form of vacuum expectation values of polygonal Wilson loops with light-like edges.

This duality between amplitudes and Wilson loops remains true at weak coupling [1, 2, 24, 25], extending to the finite terms in $\mathcal{N} = 4$ SYM previously known relations between the infrared divergences of scattering amplitudes and the ultra-violet divergences of (light-like) Wilson lines in QCD [91]. Furthermore, it was recently discovered that both sides of this correspondence can be generated from n -point correlation functions of stress-tensor multiplets by taking a certain light-cone limit [92].

The four-point function of stress-tensor multiplets was intensely studied in the early days of the AdS/CFT duality, in the supergravity approximation [93] as well as at weak coupling. The one-loop [94] and two-loop [95] corrections are given by conformal ladder integrals.

A Feynman-graph based three-loop result has never become available because of the formidable size and complexity of multi-leg multi-loop computations. Already the two parallel two-loop calculations [95] drew heavily upon superconformal symmetry. However, a formulation on a maximal (‘analytic’) superspace [96, 97] makes it apparent that the loop corrections to the lowest x -space component are given by a product of a certain polynomial with linear combinations of conformal integrals, cf. ref. [98–101]. Then in ref. [102, 103], using a hidden symmetry permuting integration variables and external variables, the problem of finding the three-loop integrand was reduced down to just four unfixed coefficients without any calculation and further down to only one overall coefficient after a little further analysis. This single overall coefficient can then easily be fixed e.g. by comparing to the MHV four-point three-loop amplitude [32] via the correlator/amplitude duality or by requiring the exponentiation of logarithms in a double OPE limit [102].

Beyond the known ladder and the ‘tennis court’, the off-shell three-loop four-point correlator contains two unknown integrals termed ‘Easy’ and ‘Hard’ in ref. [102]. In this work we embark on an analytic evaluation of the Easy and Hard integrals postulating that

- the integrals are sums $\sum_i R_i F_i$, where R_i are rational functions and F_i are *pure functions*, i.e. \mathbb{Q} -linear combinations of logarithms and multiple polylogarithms [104],

- the rational functions R_i are given by the so-called *leading singularities* (i.e. residues of global poles) of the integrals [105],
- the symbol of each F_i can be pinned down by appropriate constraints and then integrated to a unique transcendental function.

The principle of *uniform transcendentality*, innate to the planar $\mathcal{N} = 4$ SYM theory, implies that the symbols of all the pure functions are tensors of uniform rank six. Our strategy will be to make an ansatz for the entries that can appear in the symbols of the pure functions and to write down the most general tensor of uniform rank six of this form. We then impose a set of constraints on this general tensor to pin down the symbols of the pure functions. First of all, the tensor needs to satisfy the *integrability condition*, a criterion for a general tensor to correspond to the symbol of a transcendental function. Next the symmetries of the integrals induce additional constraints, and finally we equate with single variable expansions corresponding to Euclidean coincidence limits. The latter were elaborated for the Easy and Hard integrals in ref. [106, 107] using the method of *asymptotic expansion of Feynman integrals* [108]. This expansion technique reduces the original higher-point integrals to two-point integrals, albeit with high exponents of the denominator factors and complicated numerators.

To be specific, up to three loops the off-shell four-point correlator is given by [94, 95, 102]

$$G_4(1, 2, 3, 4) = G_4^{(0)} + \frac{2(N_c^2 - 1)}{(4\pi^2)^4} R(1, 2, 3, 4) [aF^{(1)} + a^2F^{(2)} + a^3F^{(3)} + O(a^4)] , \quad (3.1.1)$$

Here N_c denotes the number of colors and a is the 't Hooft coupling. $G_4^{(0)}$ represents the tree-level contribution and $R(1, 2, 3, 4)$ is a universal prefactor, in particular taking into account the different $SU(4)$ flavors which can appear (see ref. [102, 103] for details). Our focus here is on the loop corrections. These can be written in the

compact form (exposing the hidden $S_{4+\ell}$ symmetry) as

$$F^{(\ell)}(x_1, x_2, x_3, x_4) = \frac{x_{12}^2 x_{13}^2 x_{14}^2 x_{23}^2 x_{24}^2 x_{34}^2}{\ell! (\pi^2)^\ell} \int d^4 x_5 \dots d^4 x_{4+\ell} \hat{f}^{(\ell)}(x_1, \dots, x_{4+\ell}), \quad (3.1.2)$$

where

$$\hat{f}^{(1)}(x_1, \dots, x_5) = \frac{1}{\prod_{1 \leq i < j \leq 5} x_{ij}^2}, \quad (3.1.3)$$

$$\hat{f}^{(2)}(x_1, \dots, x_6) = \frac{\frac{1}{48} x_{12}^2 x_{34}^2 x_{56}^2 + S_6 \text{ permutations}}{\prod_{1 \leq i < j \leq 6} x_{ij}^2}, \quad (3.1.4)$$

$$\hat{f}^{(3)}(x_1, \dots, x_7) = \frac{\frac{1}{20} (x_{12}^2)^2 (x_{34}^2 x_{45}^2 x_{56}^2 x_{67}^2 x_{73}^2) + S_7 \text{ permutations}}{\prod_{1 \leq i < j \leq 7} x_{ij}^2}. \quad (3.1.5)$$

Writing out the sum over permutations in the above expressions, these are written as follows

$$F^{(1)} = g_{1234}, \quad (3.1.6)$$

$$\begin{aligned} F^{(2)} &= h_{12;34} + h_{34;12} + h_{23;14} + h_{14;23} \\ &+ h_{13;24} + h_{24;13} + \frac{1}{2} \leftrightarrow x_{12}^2 x_{34}^2 + x_{13}^2 x_{24}^2 + x_{14}^2 x_{23}^2 [g_{1234}]^2, \end{aligned} \quad (3.1.7)$$

$$\begin{aligned} F^{(3)} &= [L_{12;34} + 5 \text{ perms}] + [T_{12;34} + 11 \text{ perms}] \\ &+ [E_{12;34} + 11 \text{ perms}] + \frac{1}{2} [x_{14}^2 x_{23}^2 H_{12;34} + 11 \text{ perms}] \\ &+ [(g \times h)_{12;34} + 5 \text{ perms}], \end{aligned} \quad (3.1.8)$$

which involve the following integrals:

$$\begin{aligned} g_{1234} &= \frac{1}{\pi^2} \int \frac{d^4 x_5}{x_{15}^2 x_{25}^2 x_{35}^2 x_{45}^2}, \\ h_{12;34} &= \frac{x_{34}^2}{\pi^4} \int \frac{d^4 x_5 d^4 x_6}{(x_{15}^2 x_{35}^2 x_{45}^2) x_{56}^2 (x_{26}^2 x_{36}^2 x_{46}^2)}. \end{aligned} \quad (3.1.9)$$

At three-loop order we encounter

$$\begin{aligned}
 (g \times h)_{12;34} &= \frac{x_{12}^2 x_{34}^4}{\pi^6} \int \frac{d^4 x_5 d^4 x_6 d^4 x_7}{(x_{15}^2 x_{25}^2 x_{35}^2 x_{45}^2)(x_{16}^2 x_{36}^2 x_{46}^2)(x_{27}^2 x_{37}^2 x_{47}^2) x_{67}^2}, \\
 L_{12;34} &= \frac{x_{34}^4}{\pi^6} \int \frac{d^4 x_5 d^4 x_6 d^4 x_7}{(x_{15}^2 x_{35}^2 x_{45}^2) x_{56}^2 (x_{36}^2 x_{46}^2) x_{67}^2 (x_{27}^2 x_{37}^2 x_{47}^2)}, \\
 T_{12;34} &= \frac{x_{34}^2}{\pi^6} \int \frac{d^4 x_5 d^4 x_6 d^4 x_7 x_{17}^2}{(x_{15}^2 x_{35}^2)(x_{16}^2 x_{46}^2)(x_{37}^2 x_{27}^2 x_{47}^2) x_{56}^2 x_{57}^2 x_{67}^2}, \\
 E_{12;34} &= \frac{x_{23}^2 x_{24}^2}{\pi^6} \int \frac{d^4 x_5 d^4 x_6 d^4 x_7 x_{16}^2}{(x_{15}^2 x_{25}^2 x_{35}^2) x_{56}^2 (x_{26}^2 x_{36}^2 x_{46}^2) x_{67}^2 (x_{17}^2 x_{27}^2 x_{47}^2)}, \\
 H_{12;34} &= \frac{x_{34}^2}{\pi^6} \int \frac{d^4 x_5 d^4 x_6 d^4 x_7 x_{57}^2}{(x_{15}^2 x_{25}^2 x_{35}^2 x_{45}^2) x_{56}^2 (x_{36}^2 x_{46}^2) x_{67}^2 (x_{17}^2 x_{27}^2 x_{37}^2 x_{47}^2)}.
 \end{aligned} \tag{3.1.10}$$

Here g, h, L are recognized as the one-loop, two-loop and three-loop ladder integrals, respectively, the dual graphs of the off-shell box, double-box and triple-box integrals. Off-shell, the ‘tennis court’ integral T can be expressed as the three-loop ladder integral L by using the conformal flip properties¹ of a two-loop ladder sub-integral [22]. The only new integrals are thus E and H (see fig. 3.1).

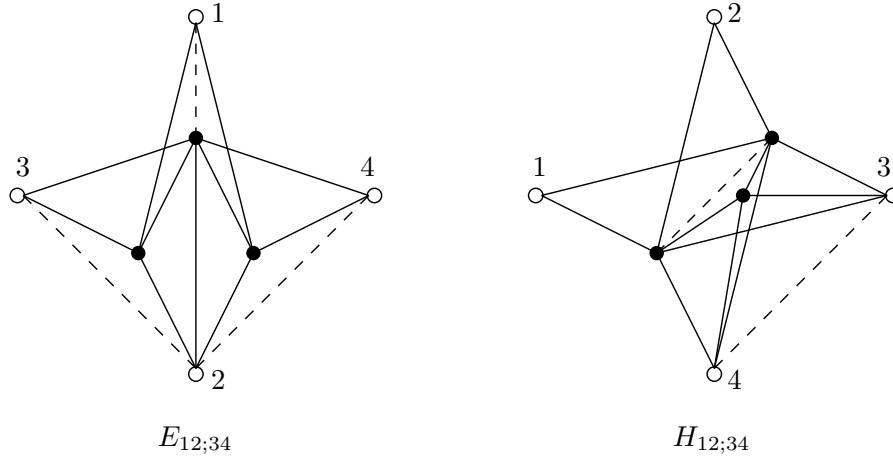


Figure 3.1: The Easy and Hard integrals contributing to the correlator of stress tensor multiplets at three loops.

¹Such identities rely on manifest conformal invariance and will be broken by the introduction of most regulators. For instance, the equivalence of T and L is not true for the dimensionally regulated on-shell integrals.

Conformal four-point integrals are given by a factor carrying their conformal weight, say, $(x_{13}^2 x_{24}^2)^n$ times some function of the two cross ratios

$$u = \frac{x_{12}^2 x_{34}^2}{x_{13}^2 x_{24}^2} = x \bar{x}, \quad v = \frac{x_{14}^2 x_{23}^2}{x_{13}^2 x_{24}^2} = (1-x)(1-\bar{x}). \quad (3.1.11)$$

Ladder integrals are explicitly known for any number of loops, see ref. [109] where they are very elegantly expressed as one-parameter integrals. Integration is simplified by the change of variables from the cross-ratios (u, v) to (x, \bar{x}) as defined in the last equation. The unique rational prefactor, $x_{13}^2 x_{24}^2 (x - \bar{x})$, is common to all cases and can be computed by the leading singularity method as we illustrate shortly. This is multiplied by pure polylogarithm functions which fit with the classification of single-valued harmonic polylogarithms (SVHPLs) in ref. [47]. The associated symbols of the ladder integrals are then tensors composed of the four letters $\{x, \bar{x}, 1-x, 1-\bar{x}\}$.

On the other hand, for generic conformal four-point integrals (of which the Easy and Hard integrals are the first examples) there are no explicit results. Fortunately, in recent years a formalism has been developed in the context of scattering amplitudes to find at least the rational prefactors (i.e. the leading singularities), which are given by the residues of the integrals [105]. There is one leading singularity for each global pole of the integrand and it is obtained by deforming the contour of integration to lie on a maximal torus surrounding the pole in question, i.e. by computing the residue at the global pole. As an illustration², let us apply this technique to the massive one-loop box integral g_{1234} defined in eq. (3.1.9). Its leading singularity is obtained by shifting the contour to encircle one of the global poles of the integrand, where all four terms in the denominator vanish. To find this let us consider a change of coordinates from x_5^μ to $p_i = x_{i5}^2$. The Jacobian for this change of variables is

$$J = \det \left(\frac{\partial p_i}{\partial x_5^\mu} \right) = \det (-2x_{i5}^\mu), \quad J^2 = \det (4x_{i5} \cdot x_{j5}) = 16 \det (x_{ij}^2 - x_{i5}^2 - x_{j5}^2), \quad (3.1.12)$$

where the second identity follows by observing that $\det(M) = \sqrt{\det(MM^T)}$. Using

²The massless box-integral (i.e. the same integral in the limit $x_{i,i+1}^2 \rightarrow 0$) is discussed in ref. [80] in terms of twistor variables as the simplest example of a ‘Schubert problem’ in projective geometry. The off-shell case that we discuss here was also recently discussed by S. Caron-Huot (see [110]).

this change of variables the massive box becomes

$$g_{1234} = \frac{1}{\pi^2} \int \frac{d^4 p_i}{p_1 p_2 p_3 p_4 J} . \quad (3.1.13)$$

To find its leading singularity we simply compute the residue around all four poles at $p_i = 0$ (divided by $2\pi i$). We obtain

$$g_{1234} \rightarrow \frac{1}{4\pi^2 \lambda_{1234}} , \quad \lambda_{1234} = \sqrt{\det(x_{ij}^2)_{i,j=1..4}} = x_{13}^2 x_{24}^2 (x - \bar{x}) \quad (3.1.14)$$

in full agreement with the analytic result [109].

Note that we do not consider explicitly a contour around the branch cut associated with the square root factor J in the denominator of (3.1.13). Because there is no pole at infinity, the residue theorem guarantees that such a contour is equivalent to the one we already considered. On the other hand, in higher-loop examples, Jacobians from previous integrations cannot be discarded in this manner. In all the examples we consider, these Jacobians always collapse to become simple poles when evaluated on the zero loci of the other denominators and thereby contribute non-trivially to the leading singularity.

The main results of this paper are the analytic evaluations of the Easy and Hard integrals. Due to Jacobian poles, the Easy integral has three distinct leading singularities, out of which only two are algebraically independent, though. The Hard integral has two distinct leading singularities, too. Armed with this information we then attempt to find the pure polylogarithmic functions multiplying these rational factors. Our main inputs for this are analytic expressions for the integrals in the limit $\bar{x} \rightarrow 0$ obtained from the results in [107]. Matching these asymptotic expressions with an ansatz for the symbol of the pure functions we obtain unique answers for the pure functions.

The pure functions contributing to the Easy integral are given by SVHPLs, corresponding to a symbol with entries drawn from the set $\{x, 1-x, \bar{x}, 1-\bar{x}\}$. In this case there is a very straightforward method for obtaining the corresponding function from its asymptotics, by essentially lifting HPLs to SVHPLs as we explain in the

next section. However, the SVHPLs are not capable of meeting all constraints for the pure functions contributing to the Hard integral, so that we need to enlarge the set of letters. A natural guess is to include $x - \bar{x}$ (cf. ref. [106]) since it also occurs in the rational factors, and indeed this turns out to be correct. Ultimately, one of the pure functions is found to have a four-letter symbol corresponding to SVHPLs, but the symbol of the other function contains the new letter: the corresponding function cannot be expressed through SVHPLs alone, but it belongs to a more general class of multiple polylogarithms.

Let us stress that the analytic evaluation of the Easy and Hard integrals completes the derivation of the three-loop four-point correlator of stress-tensor multiplets in $\mathcal{N} = 4$ SYM. The multiple polylogarithms that we find can be numerically evaluated to very high precision, which paves the way for tests of future integrable system predictions for the four-point function, or for instance for further analyses of the operator product expansion.

Finally, since our set of methods has allowed to obtain the analytic result for the Easy and Hard integrals in a relatively straightforward way (despite the fact that these are not at all simple to evaluate by conventional techniques) we wish to investigate whether this can be repeated to still higher orders. We examine a first relatively simple looking, but non-trivial, four-loop example from the list of integrals contributing to the four-point correlator at that order [103]:

$$I_{14;23}^{(4)} = \frac{1}{\pi^8} \int \frac{d^4x_5 d^4x_6 d^4x_7 d^4x_8 x_{14}^2 x_{24}^2 x_{34}^2}{x_{15}^2 x_{18}^2 x_{25}^2 x_{26}^2 x_{37}^2 x_{38}^2 x_{45}^2 x_{46}^2 x_{47}^2 x_{48}^2 x_{56}^2 x_{67}^2 x_{78}^2} . \quad (3.1.15)$$

The computation of its unique leading singularity follows the same lines as at three loops. However, just as for the Hard integral, the alphabet $\{x, 1 - x, \bar{x}, 1 - \bar{x}\}$ and the corresponding function space are too restrictive. Interestingly, this integral is related to the Easy integral by a differential equation of Laplace type. Solving this equation promotes the denominator factor $1 - u$ of the leading singularities of the Easy integral to a new entry in the symbol of the four-loop integral. Note that it is at least conceivable that the letter $x - \bar{x}$ arrives in the symbol of the Hard integral due to a similar mechanism, although admittedly not every integral obeys a simple

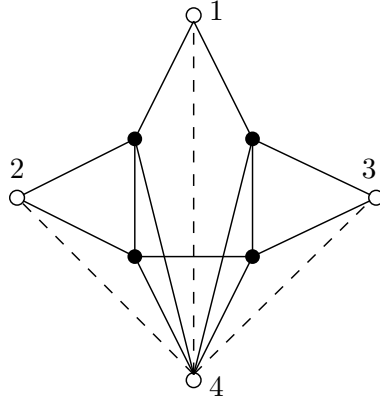


Figure 3.2: The four-loop integral $I_{14;23}^{(4)}$ defined in eq. (3.1.15).

differential equation.

The paper is organized as follows:

- In section 3.2, we give definitions of the concepts introduced here: symbols, harmonic polylogarithms, SVHPLs, multiple polylogarithms and so on.
- In section 3.3, we comment on the asymptotic expansion of Feynman integrals.
- In sections 3.4 and 3.5 we derive the leading singularities, symbols and ultimately the pure functions corresponding to the Easy and Hard integrals. We also present numerical data indicating the correctness of our results.
- In section 3.7, we perform a similar calculation for the four-loop integral, $I^{(4)}$.
- Finally we draw some conclusions. We include several appendices collecting some formulae for the asymptotic expansions of the integrals and alternative ways how to derive the analytic results.

3.2 Conformal four-point integrals and single-valued polylogarithms

The ladder-type integrals that contribute to the correlator are known. More precisely, if we write

$$\begin{aligned} g_{13;24} &= \frac{1}{x_{13}^2 x_{24}^2} \Phi^{(1)}(u, v), \\ h_{13;24} &= \frac{1}{x_{13}^2 x_{24}^2} \Phi^{(2)}(u, v), \\ l_{13;24} &= \frac{1}{x_{13}^2 x_{24}^2} \Phi^{(3)}(u, v), \end{aligned} \tag{3.2.1}$$

then the functions $\Phi^{(L)}(u, v)$ are given by the well-known result [109],

$$\begin{aligned} \Phi^{(L)}(u, v) &= -\frac{1}{L!(L-1)!} \int_0^1 \frac{d\xi}{v\xi^2 + (1-u-v)\xi + u} \log^{L-1} \xi \\ &\quad \times \left(\log \frac{v}{u} + \log \xi \right)^{L-1} \left(\log \frac{v}{u} + 2 \log \xi \right) \\ &= -\frac{1}{x - \bar{x}} f^{(L)} \left(\frac{x}{x-1}, \frac{\bar{x}}{\bar{x}-1} \right), \end{aligned} \tag{3.2.2}$$

where the conformal cross ratios are given by eq. (3.1.11) and where we defined the pure function

$$f^{(L)}(x, \bar{x}) = \sum_{r=0}^L \frac{(-1)^r (2L-r)!}{r!(L-r)!L!} \log^r(x\bar{x}) (\text{Li}_{2L-r}(x) - \text{Li}_{2L-r}(\bar{x})). \tag{3.2.3}$$

At this stage, the variables (x, \bar{x}) are simply a convenient parameterization which rationalizes the two roots of the quadratic polynomial in the denominator of eq. (3.2.2). We note that x and \bar{x} are complex conjugate to each other if we work in Euclidean space while they are both real in Minkowski signature.

The particular combination of polylogarithms that appears in eq. (3.2.2) is not random, but it has a particular mathematical meaning: in Euclidean space, where x and \bar{x} are complex conjugate to each other, the functions $\Phi^{(L)}$ are single-valued

functions of the complex variable x . In other words, the combination of polylogarithms that appears in the ladder integrals is such that they have no branch cuts in the complex x plane. In order to understand the reason for this, it is useful to look at the symbols of the ladder integrals.

3.2.1 The symbol

One possible way to define the symbol of a transcendental function is to consider its total differential. More precisely, if F is a function whose differential satisfies

$$dF = \sum_i F_i d \log R_i, \quad (3.2.4)$$

where the R_i are rational functions, then we can define the symbol of F recursively by [36]

$$\mathcal{S}(F) = \sum_i \mathcal{S}(F_i) \otimes R_i. \quad (3.2.5)$$

As an example, the symbols of the classical polylogarithms and the ordinary logarithms are given by

$$\mathcal{S}(\text{Li}_n(z)) = -(1-z) \otimes \underbrace{z \otimes \dots \otimes z}_{(n-1) \text{ times}} \quad \text{and} \quad \mathcal{S}\left(\frac{1}{n!} \ln^n z\right) = \underbrace{z \otimes \dots \otimes z}_{n \text{ times}}. \quad (3.2.6)$$

In addition the symbol satisfies the following identities,

$$\begin{aligned} \dots \otimes (a \cdot b) \otimes \dots &= \dots \otimes a \otimes \dots + \dots \otimes b \otimes \dots, \\ \dots \otimes (\pm 1) \otimes \dots &= 0, \\ \mathcal{S}(FG) &= \mathcal{S}(F) \amalg \mathcal{S}(G), \end{aligned} \quad (3.2.7)$$

where \amalg denotes the shuffle product on tensors. Furthermore, all multiple zeta values are mapped to zero by the symbol map. Conversely, an arbitrary tensor

$$\sum_{i_1, \dots, i_n} c_{i_1 \dots i_n} \omega_{i_1} \otimes \dots \otimes \omega_{i_n} \quad (3.2.8)$$

whose entries are rational functions is the symbol of a function only if the following *integrability condition* is fulfilled,

$$\sum_{i_1, \dots, i_n} c_{i_1 \dots i_n} d \log \omega_{i_k} \wedge d \log \omega_{i_{k+1}} \omega_{i_1} \otimes \dots \otimes \omega_{i_{k-1}} \otimes \omega_{i_{k+2}} \otimes \dots \otimes \omega_{i_n} = 0, \quad (3.2.9)$$

for all consecutive pairs (i_k, i_{k+1}) .

The symbol of a function also encodes information about the discontinuities of the function. More precisely, the singularities (i.e. the zeroes or infinities) of the first entries of a symbol determine the branching points of the function, and the symbol of the discontinuity across the branch cut is obtained by dropping this first entry from the symbol. As an example, consider a function $F(x)$ whose symbol has the form

$$\mathcal{S}(F(x)) = (a_1 - x) \otimes \dots \otimes (a_n - x), \quad (3.2.10)$$

where the a_i are independent of x . Then $F(x)$ has a branching point at $x = a_1$, and the symbol of the discontinuity across the branch cut is given by

$$\mathcal{S}[\text{disc}_{a_1} F(x)] = 2\pi i (a_2 - x) \otimes \dots \otimes (a_n - x). \quad (3.2.11)$$

If F is a Feynman integral, then the branch cuts of F are dictated by Cutkosky's rules. In particular, for Feynman integrals without internal masses the branch cuts extend between points where one of the Mandelstam invariants becomes zero or infinity. As a consequence, the first entries of the symbol of a Feynman integral must necessarily be Mandelstam invariants [40]. In the case of the four-point position space integrals we are considering in this paper, the first entries of the symbol must then be distances between two points, x_{ij}^2 for $i, j = 1 \dots 4$. Combined with conformal invariance, this implies that the first entries of the symbols of conformally invariant four-point functions can only be cross ratios. As an example, consider the symbol of the one-loop four-point function,

$$\mathcal{S}[f^{(1)}(x, \bar{x})] = u \otimes \frac{1-x}{1-\bar{x}} + v \otimes \frac{\bar{x}}{x}. \quad (3.2.12)$$

The first entry condition puts strong constraints on the transcendental functions that can contribute to a conformal four-point function. In order to understand this better let us consider a function whose symbol can be written in the form

$$\mathcal{S}(F) = u \otimes S_u + v \otimes S_v = (x\bar{x}) \otimes S_u + [(1-x)(1-\bar{x})] \otimes S_v, \quad (3.2.13)$$

where S_u and S_v are tensors of lower rank. Let us assume we work in Euclidean space where x and \bar{x} are complex conjugate to each other. It then follows from the previous discussion that F has potential branching points in the complex x plane at $x \in \{0, 1, \infty\}$. Let us compute for example the discontinuity of F around $x = 0$. Only the first term in eq. (3.2.13) can give rise to a non-zero contribution, and x and \bar{x} contribute with opposite signs. So we find

$$\mathcal{S}[\text{disc}_0(F)] = 2\pi i S_u - 2\pi i S_u = 0. \quad (3.2.14)$$

The argument for the discontinuities around $x = 1$ and $x = \infty$ is similar. We thus conclude that F is single-valued in the whole complex x plane. This observation puts strong constraints on the pure functions that might appear in the analytical result for a conformal four-point function. In particular, the ladder integrals $\Phi^{(L)}$ are related to the single-valued analogues of the *classical* polylogarithms,

$$D_n(x) = \Re_n \sum_{k=0}^{n-1} \frac{B_k 2^k}{k!} \log^k |x| \text{Li}_{n-k}(x), \quad (3.2.15)$$

where \Re_n denotes the real part for n odd and the imaginary part otherwise and B_k are the Bernoulli numbers. For example, we have

$$f^{(1)}(x, \bar{x}) = 4i D_2(x). \quad (3.2.16)$$

3.2.2 Single-Valued Harmonic Polylogarithms (SVHPLs)

For more general conformal four-point functions more general classes of polylogarithms may appear. The simplest extension of the classical polylogarithms are the

so-called harmonic polylogarithms (HPLs), defined by the iterated integrals³ [48]

$$H(a_1, \dots, a_n; x) = \int_0^x dt f_{a_1}(t) H(a_2, \dots, a_n; t), \quad a_i \in \{0, 1\}, \quad (3.2.17)$$

with

$$f_0(x) = \frac{1}{x} \quad \text{and} \quad f_1(x) = \frac{1}{1-x}. \quad (3.2.18)$$

By definition, $H(x) = 1$ and in the case where all the a_i are zero, we use the special definition

$$H(\vec{0}_n; x) = \frac{1}{n!} \log^n x. \quad (3.2.19)$$

The number n of indices of a harmonic polylogarithm is called its *weight*. Note that the harmonic polylogarithms contain the classical polylogarithms as special cases,

$$H(\vec{0}_{n-1}, 1; x) = \text{Li}_n(x). \quad (3.2.20)$$

In ref. [111] it was shown that infinite classes of generalized ladder integrals can be expressed in terms of single-valued combinations of HPLs. Single-valued analogues of HPLs were studied in detail in ref. [47], and an explicit construction valid for all weights was presented. Here it suffices to say that for every harmonic polylogarithm of the form $H(\vec{a}; x)$ there is a function $\mathcal{L}_{\vec{a}}(x)$ with essentially the same properties as the ordinary harmonic polylogarithms, but in addition it is single-valued in the whole complex x plane. We will refer to these functions as *single-valued harmonic polylogarithms* (SVHPLs). Explicitly, the functions $\mathcal{L}_{\vec{a}}(x)$ can be expressed as

$$\mathcal{L}_{\vec{a}}(x) = \sum_{i,j} c_{ij} H(\vec{a}_i; x) H(\vec{a}_j; \bar{x}), \quad (3.2.21)$$

where the coefficients c_{ij} are polynomials of multiple ζ values such that all branch cuts cancel.

There are two natural symmetry groups acting on the space of SVHPLs. The first symmetry group acts by complex conjugation, i.e., it exchanges x and \bar{x} . The

³In the following we use the word *harmonic polylogarithm* in a restricted sense, and only allow for singularities at $x \in \{0, 1\}$ inside the iterated integrals.

conformal four-point functions we are considering are real, and thus eigenfunctions under complex conjugation, while the SVHPLs defined in ref. [47] in general are not. It is therefore convenient to diagonalize the action of this symmetry by defining

$$\begin{aligned} L_{\vec{a}}(x) &= \frac{1}{2} [\mathcal{L}_{\vec{a}}(x) - (-1)^{|\vec{a}|} \mathcal{L}_{\vec{a}}(\bar{x})] , \\ \bar{L}_{\vec{a}}(x) &= \frac{1}{2} [\mathcal{L}_{\vec{a}}(x) + (-1)^{|\vec{a}|} \mathcal{L}_{\vec{a}}(\bar{x})] , \end{aligned} \quad (3.2.22)$$

where $|\vec{a}|$ denotes the weight of $\mathcal{L}_{\vec{a}}(x)$. Note that we have apparently doubled the number of functions, so not all the functions $L_{\vec{a}}(x)$ and $\bar{L}_{\vec{a}}(x)$ can be independent. Indeed, one can observe that

$$\bar{L}_{\vec{a}}(x) = [\text{product of lower weight SVHPLs of the form } L_{\vec{a}}(x)] . \quad (3.2.23)$$

The functions $\bar{L}_{\vec{a}}(x)$ can thus always be rewritten as linear combinations of products of SVHPLs of lower weights. In other words, the multiplicative span of the functions $L_{\vec{a}}(x)$ and multiple zeta values spans the whole algebra of SVHPLs. As an example, in this basis the ladder integrals take the very compact form

$$f^{(L)}(x, \bar{x}) = (-1)^{L+1} 2 \underbrace{L_{0, \dots, 0, 0, 1, 0, \dots, 0}}_{L-1}(x) . \quad (3.2.24)$$

While we present most of our result in terms of the $L_{\vec{a}}(x)$, we occasionally find it convenient to employ the $\bar{L}_{\vec{a}}(x)$ and the $\mathcal{L}_{\vec{a}}(x)$ to obtain more compact expressions.

The second symmetry group is the group S_3 which acts via the transformations of the argument

$$\begin{aligned} x &\rightarrow x, & x &\rightarrow 1-x, & x &\rightarrow 1/(1-x), \\ x &\rightarrow 1/x, & x &\rightarrow 1-1/x, & x &\rightarrow x/(x-1). \end{aligned} \quad (3.2.25)$$

This action of S_3 permutes the three singularities $\{0, 1, \infty\}$ in the integral representations of the harmonic polylogarithms. In addition, this action has also a physical

interpretation. The different cross ratios one can form out of four points x_i are parameterized by the group $S_4/(\mathbb{Z}_2 \times \mathbb{Z}_2) \simeq S_3$. The action (3.2.25) is the representation of this group on the cross ratios in the parameterization (3.1.11).

3.2.3 The $\bar{x} \rightarrow 0$ limit of SVHPLs

We will be using knowledge of the asymptotic expansions of integrals in the limit $\bar{x} \rightarrow 0$ in order to constrain, and even determine, the integrals themselves. If the function lives in the space of SVHPLs there is a very direct and simple way to obtain the full function from its asymptotic expansion.

This direct procedure relies on the close relation between the series expansion of SVHPLs around $\bar{x} = 0$ and ordinary HPLs. In the case where SVHPLs are analytic at $(x, \bar{x}) = 0$ (i.e. when the corresponding word ends in a ‘1’) then

$$\lim_{\bar{x} \rightarrow 0} \mathcal{L}_w(x) = H_w(x) . \quad (3.2.26)$$

Similar results exist in the case where $\mathcal{L}_w(x)$ is not analytic at the origin. In that case the limit does strictly speaking not exist, but we can, nevertheless, represent the function in a neighborhood of the origin as a polynomial in $\log u$, whose coefficients are analytic functions. More precisely, using the shuffle algebra properties of SVHPLs, we have a unique decomposition

$$\mathcal{L}_w(x) = \sum_{p, w'} a_{p, w'} \log^p u \mathcal{L}_{w'}(x) , \quad (3.2.27)$$

where $a_{p, w'}$ are integer numbers and $\mathcal{L}_{w'}(x)$ are analytic at the origin $(x, \bar{x}) = 0$.

Conversely, if we are given a function $f(x, \bar{x})$ that around $\bar{x} = 0$ admits the asymptotic expansion

$$f(x, \bar{x}) = \sum_{p, w} a_{p, w} \log^p u H_w(x) + \mathcal{O}(\bar{x}) , \quad (3.2.28)$$

where the $a_{p, w}$ are independent of (x, \bar{x}) and w are words made out of the letters 0 and 1 ending in a 1, there is a unique function $f_{\text{SVHPL}}(x, \bar{x})$ which is a linear combination of

products of SVHPLs that has the same asymptotic expansion around $\bar{x} = 0$ as $f(x, \bar{x})$. Moreover, this function is simply obtained by replacing the HPLs in eq. (3.2.28) by their single-valued analogues,

$$f_{\text{SVHPL}}(x, \bar{x}) = \sum_{p,w} a_{p,w} \log^p u \mathcal{L}_w(x) . \quad (3.2.29)$$

In other words, $f(x, \bar{x})$ and $f_{\text{SVHPL}}(x, \bar{x})$ agree in the limit $\bar{x} \rightarrow 0$ up to power-suppressed terms.

It is often the case that we find simpler expressions by expanding out all products, i.e. by not explicitly writing the powers of logarithms of u . More precisely, replacing $\log u$ by $\log x + \log \bar{x}$ in eq. (3.2.28) and using the shuffle product for HPLs, we can write eq. (3.2.28) in the form

$$f(x, \bar{x}) = \sum_w a_w H_w(x) + \log \bar{x} P(x, \log \bar{x}) + \mathcal{O}(\bar{x}) , \quad (3.2.30)$$

where $P(x, \log \bar{x})$ is a polynomial in $\log \bar{x}$ whose coefficients are HPLs in x . From the previous discussion we know that there is a linear combination of SVHPLs that agrees with $f(x, \bar{x})$ up to power-suppressed terms. In fact, this function is independent of the actual form of the polynomial P , and is completely determined by the first term in the left-hand side of eq. (3.2.30),

$$f_{\text{SVHPL}}(x, \bar{x}) = \sum_w a_w \mathcal{L}_w(x) . \quad (3.2.31)$$

So far we have only described how we can always construct a linear combination of SVHPLs that agrees with a given function in the limit $\bar{x} \rightarrow 0$ up to power-suppressed terms. The inverse is obviously not true, and we will encounter such a situation for the Hard integral. In such a case we need to enlarge the space of functions to include more general classes of multiple polylogarithms. Indeed, while SVHPLs have symbols whose entries are all drawn from the set $\{x, \bar{x}, 1-x, 1-\bar{x}\}$, it was observed in ref. [106] that the symbols of three-mass three-point functions (which are related to conformal four-point functions upon sending a point to infinity) in dimensional regularization

involve functions whose symbols also contain the entry $x - \bar{x}$. Function of this type cannot be expressed in terms of HPLs alone, but they require more general classes of multiple polylogarithms, defined recursively by $G(x) = 1$ and,

$$G(a_1, \dots, a_n; x) = \int_0^x \frac{dt}{t - a_1} G(a_2, \dots, a_n; t), \quad G(\vec{0}_p; x) = \frac{\log^p(x)}{p!}, \quad (3.2.32)$$

where $a_i \in \mathbb{C}$. We will encounter such functions in later sections when constructing the analytic results for the Easy and Hard integrals.

3.3 The short-distance limit

In this section we sketch how the method of ‘asymptotic expansion of Feynman integrals’ can deliver asymptotic series for the $\bar{x} \rightarrow 0$ limit of the Easy and the Hard integral. These expansions contain enough information about the integrals to eventually fix ansätze for the full expressions.

In ref. [107, 112] asymptotic expansions were derived for both the Easy and Hard integrals in the limits where one of the cross ratios, say u , tends to zero. The limit $u \rightarrow 0, v \rightarrow 1$ can be described as a short-distance limit, $x_2 \rightarrow x_1$. Let us assume that we have got rid of the coordinate x_4 by sending it to infinity and that we are dealing with a function of three coordinates, x_1, x_2, x_3 , one of which, say x_1 , can be set to zero. The short-distance limit we are interested in then corresponds to $x_2 \rightarrow 0$, so that the coordinate x_2 is small (soft) and the coordinate x_3 is large (hard). This is understood in the Euclidean sense, i.e. x_2 tends to zero precisely when each of its component tends to zero. One can formalize this by multiplying x_2 by a parameter ρ and then considering the limit $\rho \rightarrow 0$ upon which $u \sim \rho^2, v - 1 \sim \rho$.

For a Euclidean limit in momentum space, one can apply the well-known formulae for the corresponding asymptotic expansion written in graph-theoretical language (see ref. [108] for a review). One can also write down similar formulae in position space. In practice, it is often more efficient to apply the prescriptions of the strategy of expansion by regions [108, 113] (see also chapter 9 of ref. [114] for a recent review), which are equivalent to the graph-theoretical prescriptions in the case of Euclidean

limits. The situation is even simpler in position space where we work with propagators $1/x_{ij}^2$. It turns out that in order to reveal all the regions contributing to the asymptotic expansion of a position-space Feynman integral it is sufficient to consider each of the integration coordinates x_i either soft (i.e. of order x_2) or hard (i.e. of order x_3). Ignoring vanishing contributions, which correspond to integrals without scale, one obtains a set of regions relevant to the given limit. One can reveal this set of regions automatically, using the code described in refs. [115, 116].

The most complicated contributions in the expansion correspond to regions where the internal coordinates are either all hard or soft. For the Easy and Hard integrals, this gives three-loop two-point integrals with numerators. In ref. [112], these integrals were evaluated by treating three numerators as extra propagators with negative exponents, so that the number of the indices in the given family of integrals was increased from nine to twelve. The integrals were then reduced to master integrals using integration-by-parts (IBP) identities using the `c++` version of the code `FIRE` [117]. While this procedure is not optimal, it turned out to be sufficient for the computation in ref. [112]. In ref. [107], a more efficient way was chosen: performing a tensor decomposition and reducing the problem to evaluating integrals with nine indices by the well-known `MINCER` program [118], which is very fast because it is based on a hand solution of the IBP relations for this specific family of integrals. This strategy has given the possibility to evaluate much more terms of the asymptotic expansion.

It turns out that the expansion we consider includes, within dimensional regularization, the variable u raised to powers involving an amount proportional to $\epsilon = (4 - d)/2$. A characteristic feature of asymptotic expansions is that individual contributions may exhibit poles. Since the conformal integrals we are dealing with are finite in four dimensions, the poles necessarily cancel, leaving behind some logarithms. The resulting expansions contain powers and logarithms of u times polynomials in $v - 1$. Instead of the variable v , we turn to the variables (x, \bar{x}) defined in eq. (3.1.11). Note that it is easy to see that in terms of these variables the limit $u \rightarrow 0, v \rightarrow 1$ corresponds to both x and \bar{x} becoming small.

In fact, we only need the leading power term with respect to u and *all* the terms with respect to x . The results of ref. [107] were presented in terms of infinite sums

involving harmonic numbers, i.e., for each inequivalent permutation of the external points, it was shown that one can write

$$I(u, v) = \sum_{k=0}^3 \log^k u f_k(x) + \mathcal{O}(u), \quad (3.3.1)$$

where $I(u, v)$ denotes either the Easy or the Hard integral, and $v = 1 - x + \mathcal{O}(\bar{x})$. The coefficients $f_k(x)$ were expressed as combinations of terms of the form

$$\sum_{s=1}^{\infty} \frac{x^{s-1}}{s^i} S_{\vec{j}}(s) \quad \text{or} \quad \sum_{s=1}^{\infty} \frac{x^{s-1}}{(1+s)^i} S_{\vec{j}}(s), \quad (3.3.2)$$

where $S_{\vec{j}}(s)$ are nested harmonic sums [52],

$$S_i(s) = \sum_{n=1}^s \frac{1}{n^i} \quad \text{and} \quad S_{i\vec{j}}(s) = \sum_{n=1}^s \frac{S_{\vec{j}}(n)}{n^i}. \quad (3.3.3)$$

To arrive at such explicit results for the coefficients $f_k(x)$ a kind of experimental mathematics suggested in ref. [119] was applied: the evaluation of the first terms in the expansion in x gave a hint about the possible dependence of the coefficient at the n -th power of x . Then an ansatz in the form of a linear combination of nested sums was constructed and the coefficients in this ansatz were fixed by the information about the first terms. Finally, the validity of the ansatz was confirmed using information about the next terms. The complete x -expansion was thus inferred from the leading terms.

For the purpose of this paper, it is more convenient to work with polylogarithmic functions in x rather than harmonic sums. Indeed, sums of the type (3.3.2) can easily be performed in terms of harmonic polylogarithms using the algorithms described in ref. [61]. We note, however, that during the summation process, sums of the type (3.3.2) with $i = 0$ are generated. Sums of this type are strictly speaking not covered by the algorithms of ref. [61], but we can easily reduce them to the case $i \neq 0$

using the following procedure,

$$\sum_{s=1}^{\infty} x^{s-1} S_{ij}(s) = \frac{1}{x} \sum_{s=1}^{\infty} x^s \sum_{n=1}^s \frac{1}{n_1^i} S_j(n) = \frac{1}{x} \sum_{s=0}^{\infty} x^s \sum_{n=0}^s \frac{1}{n^i} S_j(n), \quad (3.3.4)$$

where the last step follows from $S_j(0) = 0$. Reshuffling the sum by letting $s = n_1 + n$, we obtain the following relation which is a special case of eq. (96) in ref. [119]:

$$\sum_{s=1}^{\infty} x^{s-1} S_{ij}(s) = \frac{1}{x} \sum_{n_1=0}^{\infty} x^{n_1} \sum_{n=0}^{\infty} \frac{x^n}{n^i} S_j(n) = \frac{1}{1-x} \sum_{s=1}^{\infty} \frac{x^{s-1}}{s^i} S_j(s). \quad (3.3.5)$$

The last sum is now again of the type (3.3.2) and can be dealt with using the algorithms of ref. [61].

Performing all the sums that appear in the results of ref. [107], we find for example

$$\begin{aligned} x_{13}^2 x_{24}^2 E_{14;23} &= \frac{\log u}{x} \left(H_{2,2,1} - H_{2,1,2} + H_{1,3,1} + 2H_{1,2,1,1} - H_{1,1,3} - 2H_{1,1,1,2} \right. \\ &\quad - 6\zeta_3 H_2 - 6\zeta_3 H_{1,1} \Big) - \frac{2}{x} \left(2\zeta_3 H_{2,1} - 4\zeta_3 H_{1,2} + 4\zeta_3 H_{1,1,1} + H_{3,2,1} \right. \\ &\quad - H_{3,1,2} + H_{2,3,1} - H_{2,1,3} + 2H_{1,4,1} + 2H_{1,3,1,1} + 2H_{1,2,2,1} - 2H_{1,1,4} \\ &\quad \left. - 2H_{1,1,2,2} - 2H_{1,1,1,3} - 6\zeta_3 H_3 \right) + \mathcal{O}(u), \end{aligned} \quad (3.3.6)$$

$$\begin{aligned} x_{13}^4 x_{24}^4 H_{12;34} &= \frac{4 \log u}{x^2} \left(H_{1,1,2,1} - H_{1,1,1,2} - 6\zeta_3 H_{1,1} \right) - \frac{2}{x^2} \left(4H_{2,1,2,1} - 4H_{2,1,1,2} \right. \\ &\quad \left. + 4H_{1,1,3,1} - H_{1,1,2,1,1} - 4H_{1,1,1,3} + H_{1,1,1,2,1} - 24\zeta_3 H_{2,1} + 6\zeta_3 H_{1,1,1} \right) \\ &\quad + \mathcal{O}(u), \end{aligned} \quad (3.3.7)$$

where we used the compressed notation, e.g., $H_{2,1,1,2} \equiv H(0, 1, 1, 1, 0, 1; x)$. The results for the other orientations are rather lengthy, so we do not show them here, but we collect them in appendix B.1. Let us however comment about the structure of the functions $f_k(x)$ that appear in the expansions. The functions $f_k(x)$ can always be written in the form

$$f_k(x) = \sum_l R_{k,l}(x) \times [\text{HPLs in } x], \quad (3.3.8)$$

where $R_{k,l}(x)$ may represent any of the following rational functions

$$\frac{1}{x^2}, \quad \frac{1}{x}, \quad \frac{1}{x(1-x)}. \quad (3.3.9)$$

We note that the last rational function only enters the asymptotic expansion of $H_{13;24}$.

The aim of this paper is to compute the Easy and Hard integrals by writing for each integral an ansatz of the form

$$\sum_i R_i(x, \bar{x}) P_i(x, \bar{x}), \quad (3.3.10)$$

and to fix the coefficients that appear in the ansatz by matching the limit $\bar{x} \rightarrow 0$ to the asymptotic expansions presented in this section. In the previous section we argued that a natural space of functions for the polylogarithmic part $P_i(x, \bar{x})$ are functions that are single-valued in the complex x plane in Euclidean space. We however still need to determine the rational prefactors $R_i(x, \bar{x})$, which are not constrained by single-valuedness.

A natural ansatz would consist in using the same rational prefactors as those appearing in the ladder type integrals. For ladder type integrals we have

$$R_i^{\text{ladder}}(x, \bar{x}) = \frac{1}{(x - \bar{x})^\alpha}, \quad \alpha \in \mathbb{N}, \quad (3.3.11)$$

plus all possible transformations of this function obtained from the action of the S_3 symmetry (3.2.25). Then in the limit $u \rightarrow 0$ we obtain

$$\lim_{\bar{x} \rightarrow 0} R_i^{\text{ladder}}(x, \bar{x}) = \frac{1}{x^\alpha}. \quad (3.3.12)$$

We see that the rational prefactors that appear in the ladder-type integrals can only give rise to rational prefactors in the asymptotic expansions with are pure powers of x , and so they can never account for the rational function $1/(x(1-x))$ that appears in the asymptotic expansion of $H_{13;24}$. We thus need to consider more general prefactors than those appearing in the ladder-type integrals. This issue will be addressed in the next sections.

3.4 The Easy integral

3.4.1 Residues of the Easy integral

The Easy integral is defined as

$$E_{12;34} = \frac{x_{23}^2 x_{24}^2}{\pi^6} \int \frac{d^4 x_5 d^4 x_6 d^4 x_7 x_{16}^2}{(x_{15}^2 x_{25}^2 x_{35}^2) x_{56}^2 (x_{26}^2 x_{36}^2 x_{46}^2) x_{67}^2 (x_{17}^2 x_{27}^2 x_{47}^2)} . \quad (3.4.1)$$

To find all its leading singularities we order the integrations as follows

$$E_{12;34} = \frac{x_{23}^2 x_{24}^2}{\pi^6} \left[\int \frac{d^4 x_6 x_{16}^2}{x_{26}^2 x_{36}^2 x_{46}^2} \left(\int \frac{d^4 x_5}{x_{15}^2 x_{25}^2 x_{35}^2 x_{56}^2} \right) \left(\int \frac{d^4 x_7}{x_{17}^2 x_{27}^2 x_{47}^2 x_{67}^2} \right) \right] . \quad (3.4.2)$$

First the x_7 and x_5 integrations: they are both the same as the massive box computed in the Introduction and thus give leading singularities (see eq. (3.1.14))

$$\pm \frac{1}{4 \lambda_{1236}} \quad \pm \frac{1}{4 \lambda_{1246}} , \quad (3.4.3)$$

respectively. So we can move directly to the final x_6 integration

$$\frac{1}{16 \pi^6} \int \frac{d^4 x_6 x_{16}^2}{x_{26}^2 x_{36}^2 x_{46}^2 \lambda_{1236} \lambda_{1246}} . \quad (3.4.4)$$

Here there are five factors in the denominator and we want to take the residues when four of them vanish to compute the leading singularity, so there are various choices to consider. The simplest option is to cut the three propagators $1/x_{i6}^2$. Then on this cut we have $\lambda_{1236|cut} = \pm x_{16}^2 x_{23}^2$ and $\lambda_{1246|cut} = \pm x_{16}^2 x_{24}^2$, where the vertical line indicates the value on the cut, and the integral reduces to the massive box. This simplification of the λ factors is similar to the phenomenon of composite leading singularities [120]. Thus cutting either of the two λ s will result in⁴

$$\text{leading singularity \#1 of } E_{12;34} = \pm \frac{1}{64 \pi^6 \lambda_{1234}} . \quad (3.4.5)$$

⁴With a slight abuse of language, in the following we use the word ‘cut’ to designate that we look at the zeroes of a certain denominator factor.

The only other possibility is cutting both λ 's. There are then three possibilities, firstly we could cut x_{26}^2 and x_{36}^2 as well as the two λ 's. On this cut λ_{1236} reduces to $\pm x_{16}^2 x_{23}^2$ and one obtains residue #1 again. Similarly in the second case where we cut x_{26}^2, x_{46}^2 and the two λ s.

So finally we consider the case where we cut x_{36}^2, x_{46}^2 and the two λ 's. In this case $\lambda_{1236|cut} = \pm(x_{16}^2 x_{23}^2 - x_{13}^2 x_{26}^2)$ and $\lambda_{1246|cut} = \pm(x_{16}^2 x_{24}^2 - x_{14}^2 x_{26}^2)$. Notice that setting $\lambda_{1236} = \lambda_{1246} = 0$ means setting $x_{16}^2 = x_{26}^2 = 0$. We then need to compute the Jacobian associated with cutting $x_{36}^2, x_{46}^2, \lambda_{1236}, \lambda_{1246}$

$$\begin{aligned}
 & \det \left(\frac{\partial(x_{36}^2, x_{46}^2, \lambda_{1236}, \lambda_{1246})}{\partial x_6^\mu} \right) \Big|_{cut} \\
 &= \pm 16 \det \left(x_{36}^\mu, x_{46}^\mu, x_{16}^\mu x_{23}^2 - x_{13}^2 x_{26}^\mu, x_{16}^\mu x_{24}^2 - x_{14}^2 x_{26}^\mu \right) \Big|_{cut} \\
 &= \pm 16 \det(x_{36}^\mu, x_{46}^\mu, x_{16}^\mu, x_{26}^\mu) (x_{23}^2 x_{14}^2 - x_{24}^2 x_{13}^2) \Big|_{cut} \\
 &= \pm 4 \lambda_{1234} (x_{23}^2 x_{14}^2 - x_{24}^2 x_{13}^2) ,
 \end{aligned} \tag{3.4.6}$$

The result of the x_6 integral (3.4.4) is

$$\frac{1}{64 \pi^6} \frac{x_{16}^2}{x_{26}^2 \lambda_{1234} (x_{23}^2 x_{14}^2 - x_{24}^2 x_{13}^2)} \Big|_{cut} \tag{3.4.7}$$

At this point there is a subtlety, since on the cut we have simultaneously $x_{16}^2 x_{23}^2 - x_{13}^2 x_{26}^2 = x_{16}^2 x_{24}^2 - x_{14}^2 x_{26}^2 = 0$, i.e. $x_{16}^2 = x_{26}^2 = 0$ and so $\frac{x_{16}^2}{x_{26}^2}$ is undefined. More specifically, the integral depends on whether we take $x_{16}^2 x_{23}^2 - x_{13}^2 x_{26}^2 = 0$ first or $x_{16}^2 x_{24}^2 - x_{14}^2 x_{26}^2 = 0$ first. So we get two possibilities (after multiplying by the external factors $x_{23}^2 x_{24}^2$ in eq. (3.4.1)) :

$$\text{leading singularity \#2 of } E_{12;34} = \pm \frac{x_{13}^2 x_{24}^2}{64 \pi^6 \lambda_{1234} (x_{23}^2 x_{14}^2 - x_{24}^2 x_{13}^2)} \tag{3.4.8}$$

$$\text{leading singularity \#3 of } E_{12;34} = \pm \frac{x_{14}^2 x_{23}^2}{64 \pi^6 \lambda_{1234} (x_{23}^2 x_{14}^2 - x_{24}^2 x_{13}^2)} . \tag{3.4.9}$$

We conclude that the Easy integral takes the ‘leading singularity times pure function’ form⁵

$$E_{12;34} = \frac{1}{x_{13}^2 x_{24}^2} \left[\frac{E^{(a)}(x, \bar{x})}{x - \bar{x}} + \frac{E^{(b)}(x, \bar{x})}{(x - \bar{x})(v - 1)} + \frac{v E^{(c)}(x, \bar{x})}{(x - \bar{x})(v - 1)} \right]. \quad (3.4.10)$$

We note that the $x_3 \leftrightarrow x_4$ symmetry relates $E^{(b)}$ and $E^{(c)}$. Furthermore, putting everything over a common denominator it is easy to see that $E^{(a)}$ can be absorbed into the other two functions. We conclude that there is in fact only one independent function, and the Easy integral can be written in terms of a single pure function $E(x, \bar{x})$ as

$$E_{12;34} = \frac{1}{x_{13}^2 x_{24}^2 (x - \bar{x})(v - 1)} \left[E(x, \bar{x}) + v E\left(\frac{x}{x - 1}, \frac{\bar{x}}{\bar{x} - 1}\right) \right]. \quad (3.4.11)$$

The function $E(x, \bar{x})$ is antisymmetric under the interchange of x, \bar{x}

$$E(\bar{x}, x) = -E(x, \bar{x}), \quad (3.4.12)$$

to ensure that $E_{12;34}$ is a symmetric function of x, \bar{x} , but it possesses no other symmetry.

The other two orientations of the Easy integral are then found by permuting various points and are given by

$$E_{13;24} = \frac{1}{x_{13}^2 x_{24}^2 (x - \bar{x})(u - v)} \left[u E\left(\frac{1}{x}, \frac{1}{\bar{x}}\right) + v E\left(\frac{1}{1 - x}, \frac{1}{1 - \bar{x}}\right) \right], \quad (3.4.13)$$

$$E_{14;23} = \frac{1}{x_{13}^2 x_{24}^2 (x - \bar{x})(1 - u)} \left[E(1 - x, 1 - \bar{x}) + u E\left(1 - \frac{1}{x}, 1 - \frac{1}{\bar{x}}\right) \right]. \quad (3.4.14)$$

It is thus enough to have an expression for $E(x, \bar{x})$ to determine all possible orientations of the Easy integral. The functional form of $E(x, \bar{x})$ will be the purpose of the rest of this section.

⁵A similar form of the Easy leading singularities, as well as those of the Hard integral discussed in the next section, was independently obtained by S. Caron-Huot [121].

3.4.2 The symbol of $E(x, \bar{x})$

In this subsection we determine the symbol of $E(x, \bar{x})$, and in the next section we describe its uplift to a function. This strategy seems over-complicated in the case at hand, because $E(x, \bar{x})$ can in fact directly be obtained in terms of SVHPLs of weight six from its asymptotic expansion using the method described in section 3.2.3. The two-step derivation (symbol and subsequent uplift) is included mainly for pedagogical purposes because it equally applies to the Hard integral and our four-loop example, where the functions are not writable in terms of SVHPLs only so that a direct method yet has to be found.

Returning to the Easy integral, we start by writing down the most general tensor of rank six that

- has all its entries drawn from the set $\{x, 1-x, \bar{x}, 1-\bar{x}\}$,
- satisfies the first entry condition, i.e. the first factors in each tensor are either $x\bar{x}$ or $(1-x)(1-\bar{x})$,
- is odd under an exchange of x and \bar{x} .

This results in a tensor that depends on $2 \cdot 4^5/2 = 1024$ free coefficients (which we assume to be rational numbers). Imposing the integrability condition (3.2.9) reduces the number of free coefficients to 28, which is the number of SVHPLs of weight six that are odd under an exchange of x and \bar{x} . The remaining free coefficients can be fixed by matching to the limit $u \rightarrow 0, v \rightarrow 1$, or equivalently $\bar{x} \rightarrow 0$.

In order to take the limit, we drop every term in the symbol containing an entry $1-\bar{x}$ and we replace $\bar{x} \rightarrow u/x$, upon which the singularity is hidden in u . As a result, every permutation of our ansatz yields a symbol composed of the three letters $\{u, x, 1-x\}$. This tensor can immediately be matched to the symbol of the asymptotic

expansion of the Easy integral discussed in section 3.3. Explicitly, the limits

$$x_{13}^2 x_{24}^2 E_{12;34} \rightarrow -\frac{1}{x^2} \left[\lim_{\bar{x} \rightarrow 0} E(x, \bar{x}) + \lim_{\bar{x} \rightarrow 0} E\left(\frac{x}{x-1}, \frac{\bar{x}}{\bar{x}-1}\right) \right] + \frac{1}{x} \lim_{\bar{x} \rightarrow 0} E\left(\frac{x}{x-1}, \frac{\bar{x}}{\bar{x}-1}\right) \quad (3.4.15)$$

$$x_{13}^2 x_{24}^2 E_{13;24} \rightarrow -\frac{1}{x} \lim_{\bar{x} \rightarrow 0} E\left(\frac{1}{1-x}, \frac{1}{1-\bar{x}}\right) \quad (3.4.16)$$

$$x_{13}^2 x_{24}^2 E_{14;23} \rightarrow \frac{1}{x} \lim_{\bar{x} \rightarrow 0} E(1-x, 1-\bar{x}) \quad (3.4.17)$$

can be matched with the asymptotic expansions recast as HPLs. All three conditions are consistent with our ansatz; each of them on its own suffices to determine all remaining constants. The resulting symbol is a linear combination of 1024 tensors with entries drawn from the set $\{x, 1-x, \bar{x}, 1-\bar{x}\}$ and with coefficients $\{\pm 1, \pm 2\}$.

Note that the uniqueness of the uplift procedure for SVHPLs given in section 3.2.3 implies that each asymptotic limit is sufficient to fix the symbol.

3.4.3 The analytic result for $E(x, \bar{x})$: uplifting from the symbol

In this section we determine the function $E(x, \bar{x})$ defined in eq. (3.4.11) starting from its symbol. As the symbol has all its entries drawn from the set $\{x, 1-x, \bar{x}, 1-\bar{x}\}$, the function $E(x, \bar{x})$ can be expressed in terms of the SVHPLs classified in [47]. Additional single-valued terms⁶ proportional to zeta values can be fixed by again appealing to the asymptotic expansion of the integral.

We start by writing down an ansatz for $E(x, \bar{x})$ as a linear combination of weight six of SVHPLs that is odd under exchange of x and \bar{x} . Note that we have some freedom w.r.t. the basis for our ansatz. In the following we choose basis elements containing a single factor of the form $L_{\bar{a}}(x)$. This ensures that all the terms are linearly independent.

⁶In principle we cannot exclude at this stage more complicated functions of weight less than six multiplied by zeta values.

Next we fix the free coefficients in our ansatz by requiring its symbol to agree with that of $E(x, \bar{x})$ determined in the previous section. As we had started from SVHPLs with the correct symmetries and weight, all coefficients are fixed in a unique way. We arrive at the following expression for $E(x, \bar{x})$:

$$\begin{aligned} E(x, \bar{x}) = & 4L_{2,4} - 4L_{4,2} - 2L_{1,3,2} + 2L_{2,1,3} - 2L_{3,1,2} + 4L_{3,2,0} \\ & - 2L_{2,2,1,0} + 8L_{3,1,0,0} + 2L_{3,1,1,0} - 2L_{2,1,1,1,0} \end{aligned} \quad (3.4.18)$$

For clarity, we suppressed the argument of the L functions and we employed the compressed notation for HPLs, e.g., $L_{3,2,1} \equiv L_{0,0,1,0,1,1}(x, \bar{x})$. The asymptotic limits of the last expression correctly reproduce the terms proportional to zeta values in eq. (3.3.7) and the formulae in appendix B.1.

3.4.4 The analytic result for $E(x, \bar{x})$: the direct approach

Here we quickly give the direct method for obtaining $E(x, \bar{x})$ explicitly from its asymptotics via the method outlined in section 3.2.3.

The asymptotic value of the Easy integral in the permutation $E_{12;34}$ is given in appendix B.1. Comparing eq. (B.1.1) with eq. (3.4.15) and further writing $\log u = \log x + \log \bar{x}$ and expanding out products of functions we find for the asymptotic value of $E(x, \bar{x})$:

$$\begin{aligned} E(x, \bar{x}) = & 4\zeta_3 H_{2,1} + 2H_{2,4} - 2H_{4,2} + H_{1,2,3} - H_{1,3,2} - 2H_{1,4,0} + H_{2,1,3} - H_{3,1,2} \\ & + 2H_{3,2,0} - H_{1,3,1,0} + H_{2,1,2,0} - 2H_{2,2,0,0} - H_{2,2,1,0} + H_{3,1,1,0} + 2H_{1,2,0,0,0} \\ & + H_{1,2,1,0,0} - H_{2,1,1,0,0} - 20\zeta_5 H_1 + 8\zeta_3 H_3 + 2\zeta_3 H_{1,2} \\ & + \log \bar{x} P(x, \log \bar{x}) + \mathcal{O}(\bar{x}), \end{aligned} \quad (3.4.19)$$

where P is a polynomial in $\log \bar{x}$ with coefficients that are HPLs in x . From the discussion in section 3.2.3 we know that there is a unique combination of SVHPLs

with this precise asymptotic behavior, and so we find a natural ansatz for $E(x, \bar{x})$,

$$\begin{aligned}
 E(x, \bar{x}) = & 4\zeta_3 \mathcal{L}_{2,1} + 2\mathcal{L}_{2,4} - 2\mathcal{L}_{4,2} + \mathcal{L}_{1,2,3} - \mathcal{L}_{1,3,2} - 2\mathcal{L}_{1,4,0} + \mathcal{L}_{2,1,3} - \mathcal{L}_{3,1,2} + 2\mathcal{L}_{3,2,0} \\
 & - \mathcal{L}_{1,3,1,0} + \mathcal{L}_{2,1,2,0} - 2\mathcal{L}_{2,2,0,0} - \mathcal{L}_{2,2,1,0} + \mathcal{L}_{3,1,1,0} + 2\mathcal{L}_{1,2,0,0,0} + \mathcal{L}_{1,2,1,0,0} \\
 & - \mathcal{L}_{2,1,1,0,0} - 20\zeta_5 \mathcal{L}_1 + 8\zeta_3 \mathcal{L}_3 + 2\zeta_3 \mathcal{L}_{1,2} .
 \end{aligned} \tag{3.4.20}$$

We have lifted this function from its asymptotics in just one limit $\bar{x} \rightarrow 0$ while we also know two other limits of this function given in eq. (3.3.7) and appendix B.1. Remarkably, eq. (3.4.20) is automatically consistent with these two limits, giving a strong indication that it is indeed the right function. Furthermore, eq. (3.4.20) can then in turn be rewritten in a way that makes the antisymmetry under exchange of x and \bar{x} manifest, and we recover eq. (3.4.18). Note also that antisymmetry in $x \leftrightarrow \bar{x}$ was not input anywhere, and the fact that the resulting function is indeed antisymmetric is a non-trivial consistency check.

As an aside we also note here that the form of $E(x, \bar{x})$, expressed in the particular basis of SVHPLs we chose to work with, is very simple, having only coefficients ± 1 or ± 2 for the polylogarithms of weight six. Indeed other orientations of E have even simpler forms, for instance

$$\begin{aligned}
 E(1/x, 1/\bar{x}) = & \mathcal{L}_{2,4} - \mathcal{L}_{3,3} - \mathcal{L}_{1,2,3} + \mathcal{L}_{1,3,2} - \mathcal{L}_{1,4,0} - \mathcal{L}_{2,1,3} + \mathcal{L}_{3,1,2} - \mathcal{L}_{4,0,0} + \mathcal{L}_{4,1,0} \\
 & + \mathcal{L}_{1,3,0,0} + \mathcal{L}_{1,3,1,0} - \mathcal{L}_{2,1,2,0} + \mathcal{L}_{2,2,1,0} + \mathcal{L}_{3,0,0,0} - \mathcal{L}_{3,1,1,0} - \mathcal{L}_{1,2,1,0,0} \\
 & - \mathcal{L}_{2,1,0,0,0} + \mathcal{L}_{2,1,1,0,0} + 8\zeta_3 \mathcal{L}_3 - 2\zeta_3 \mathcal{L}_{1,2} - 6\zeta_3 \mathcal{L}_{2,0} - 4\zeta_3 \mathcal{L}_{2,1} ,
 \end{aligned} \tag{3.4.21}$$

with all coefficients of the weight six SVHPLs being ± 1 , or in the manifestly antisymmetric form with all weight six SVHPLs with coefficient $+1$

$$\begin{aligned}
 E(1/x, 1/\bar{x}) = & L_{2,4} + L_{1,3,2} + L_{3,1,2} + L_{4,1,0} + L_{1,3,0,0} + L_{1,3,1,0} \\
 & + L_{2,2,1,0} + L_{3,0,0,0} + L_{2,1,1,0,0} + 6\zeta_3 L_3 - 2\zeta_3 L_{2,1} .
 \end{aligned} \tag{3.4.22}$$

3.4.5 Numerical consistency tests for E

We have determined the analytic result for the Easy integral relying on the knowledge of its residues, symbol and asymptotic expansions. In order to check the correctness of the result, we evaluated $E_{14;23}$ numerically⁷ and compared it to a direct numerical evaluation of the coordinate space integral using **FIESTA** [122, 123].

To be specific, we evaluate the conformally-invariant function $x_{13}^2 x_{24}^2 E_{14;23}$. Applying a conformal transformation to send x_4 to infinity, the integral takes the simplified form,

$$\lim_{x_4 \rightarrow \infty} x_{13}^2 x_{24}^2 E_{14;23} = \frac{1}{\pi^6} \int \frac{d^4 x_5 d^4 x_6 d^4 x_7 x_{13}^2 x_{16}^2}{(x_{15}^2 x_{25}^2) x_{56}^2 (x_{26}^2 x_{36}^2) x_{67}^2 (x_{17}^2 x_{37}^2)}, \quad (3.4.23)$$

with only 8 propagators. We use the remaining freedom to fix $x_{13}^2 = 1$ so that $u = x_{12}^2$ and $v = x_{23}^2$. Other numerical values for x_{13}^2 are possible, of course, but we found that this choice yields relatively stable numerics.

After Feynman parameterization, the integral is only seven-dimensional and can be evaluated with off-the-shelf software. We generate the integrand with **FIESTA** and perform the numerical integration with a stand-alone version of **CIntegrate**. Using the algorithm Divonne⁸, we obtain roughly five digits of precision after five million function evaluations.

In total, we checked 40 different pairs of values for the cross ratios and we found very good agreement in all cases. A sample of the numerical checks is shown in Table 3.1. Note that δ denotes the relative error between the analytic result and the number obtained by **FIESTA**,

$$\delta = \left| \frac{N_{analytic} - N_{FIESTA}}{N_{analytic} + N_{FIESTA}} \right|. \quad (3.4.24)$$

⁷All polylogarithms appearing in this paper have been evaluated numerically using the **GINAC** [66] and **HPL** [68] packages.

⁸Experience shows that Divonne outperforms other algorithms of the Cuba library for problems roughly this size.

u	v	Analytic	FIESTA	δ
0.1	0.2	82.3552	82.3553	6.6e-7
0.2	0.3	57.0467	57.0468	3.2e-8
0.3	0.1	90.3540	90.3539	5.9e-8
0.4	0.5	37.1108	37.1108	1.9e-8
0.5	0.6	31.9626	31.9626	1.9e-8
0.6	0.2	54.2881	54.2881	6.9e-8
0.7	0.3	42.6519	42.6519	4.4e-8
0.8	0.9	23.0199	23.0199	1.7e-8
0.9	0.5	30.8195	30.8195	2.4e-8

Table 3.1: Numerical comparison of the analytic result for $x_{13}^2 x_{24}^2 E_{14;23}$ against FIESTA for several values of the conformal cross ratios.

3.5 The Hard integral

3.5.1 Residues of the Hard integral

To find all the leading singularities we consider each integration sequentially as follows

$$H_{12;34} = \frac{x_{34}^2}{\pi^6} \left\{ \int \frac{d^4 x_6}{x_{16}^2 x_{26}^2 x_{36}^2 x_{46}^2} \left[\int \frac{d^4 x_5 x_{56}^2}{x_{15}^2 x_{25}^2 x_{35}^2 x_{45}^2} \left(\int \frac{d^4 x_7}{x_{37}^2 x_{47}^2 x_{57}^2 x_{67}^2} \right) \right] \right\}. \quad (3.5.1)$$

Let us start with the x_7 integration,

$$\int \frac{d^4 x_7}{x_{37}^2 x_{47}^2 x_{57}^2 x_{67}^2}. \quad (3.5.2)$$

This is simply the off-shell box considered in section 3.1, and so its leading singularities are (see eq. (3.1.14))

$$\pm \frac{1}{4 \lambda_{3456}}. \quad (3.5.3)$$

Next we turn to the x_5 integration, which now takes the form

$$\int \frac{d^4 x_5 x_{56}^2}{x_{15}^2 x_{25}^2 x_{35}^2 x_{45}^2 \lambda_{3456}}. \quad (3.5.4)$$

There are five factors in the denominator, and we want to cut four of them to compute the leading singularity. The simplest option is to cut the four propagators $1/x_{i5}^2$. Doing so would yield a new Jacobian factor $1/\lambda_{1234}$ (exactly as in the previous subsection) and freeze $\lambda_{3456|cut} = \pm x_{56}^2 x_{34}^2$. This latter factor simply cancels the numerator and we are left with the final x_6 integration being that of the box in the Introduction. Putting everything together, the leading singularity for this choice is

$$\text{leading singularity \#1 of } H_{12;34} = \pm \frac{1}{64\pi^6 \lambda_{1234}^2} . \quad (3.5.5)$$

Returning to the x_5 integration, eq. (3.5.4), we must consider the possibility of cutting λ_{3456} and three other propagators. Cutting x_{35}^2 and x_{45}^2 immediately freezes $\lambda_{3456|cut} = \pm x_{56}^2 x_{34}^2$ which is canceled by the numerator. Thus it is not possible to cut these two propagators and λ_{3456} . However, cutting $x_{15}^2, x_{25}^2, x_{35}^2$ and λ_{3456} is possible (the only other possibility, i.e. cutting $x_{15}^2, x_{25}^2, x_{45}^2$ and λ_{3456} , gives the same result by by invariance of the integral under exchange of x_3 and x_4). Indeed one finds that when $x_{35}^2 = 0$,

$$\lambda_{3456} = \pm (x_{45}^2 x_{36}^2 - x_{56}^2 x_{34}^2) . \quad (3.5.6)$$

To compute the leading singularity associated with this pole we need to compute the Jacobian

$$J = \det \left(\frac{\partial(x_{15}^2, x_{25}^2, x_{35}^2, \lambda_{3456})}{\partial x_5^\mu} \right) , \quad (3.5.7)$$

As in the box case, it is useful to consider the square of J (on the cut),

$$J^2 = 16 \det \begin{pmatrix} x_{ij}^2 & -2x_i \cdot \partial \lambda_{3456} / \partial x_5 \\ -2x_i \cdot \partial \lambda_{3456} / \partial x_5 & (\partial \lambda_{3456} / \partial x_5)^2 \end{pmatrix} . \quad (3.5.8)$$

The result of the x_5 integration is then simply

$$\left. \frac{x_{56}^2}{J x_{45}^2} \right|_{cut} = \left. \frac{x_{36}^2}{J x_{34}^2} \right|_{cut} , \quad (3.5.9)$$

where the second equality follows since x_{56}^2 and x_{45}^2 are to be evaluated on the cut

(indicated by the vertical line) for which $x_{45}^2 x_{36}^2 - x_{56}^2 x_{34}^2 = 0$. Finally we need to turn to the remaining x_6 integral. We are simply left with

$$\frac{1}{16\pi^6} \int \frac{d^4 x_6}{x_{16}^2 x_{26}^2 x_{46}^2 J} \Big|_{\text{cut}}, \quad (3.5.10)$$

where we note that the x_{36}^2 propagator term has canceled with the numerator in eq. (3.5.9). So we have no choice left for the quadruple cut as there are only four poles. In fact on the other cut of the three propagators we find $J_{\text{cut}} = 4(x_{14}^2 x_{23}^2 - x_{13}^2 x_{24}^2) x_{36}^2$, and so this brings back the propagator x_{36}^2 .

Computing the Jacobian associated with this final integration thus yields the final result for the leading singularity,

$$\text{leading singularity \#2 of } H_{12;34} = \pm \frac{1}{64\pi^6 (x_{14}^2 x_{23}^2 - x_{13}^2 x_{24}^2) \lambda_{1234}}. \quad (3.5.11)$$

We conclude that the Hard integral can be written as these leading singularities times pure functions, i.e. it has the form

$$H_{12;34} = \frac{1}{x_{13}^4 x_{24}^4} \left[\frac{H^{(a)}(x, \bar{x})}{(x - \bar{x})^2} + \frac{H^{(b)}(x, \bar{x})}{(v - 1)(x - \bar{x})} \right], \quad (3.5.12)$$

where $H^{(a),(b)}$ are pure polylogarithmic functions. The pure functions must furthermore satisfy the following properties

$$\begin{aligned} H^{(a)}(x, \bar{x}) &= H^{(a)}(\bar{x}, x), & H^{(b)}(x, \bar{x}) &= -H^{(b)}(\bar{x}, x), \\ H^{(a)}(x, \bar{x}) &= H^{(a)}(x/(x-1), \bar{x}/(\bar{x}-1)), & H^{(b)}(x, \bar{x}) &= H^{(b)}(x/(x-1), \bar{x}/(\bar{x}-1)), \end{aligned} \quad (3.5.13)$$

in order that $H_{12;34}$ be symmetric in x, \bar{x} and under the permutation $x_1 \leftrightarrow x_2$. Furthermore we would expect that $H^{(a)}(x, x) = 0$ in order to cancel the pole at $x - \bar{x}$. In fact it will turn out in this section that even without imposing this condition by hand we will arrive at a unique result which nevertheless has this particular property.

By swapping the points around we automatically get

$$H_{13;24} = \frac{1}{x_{13}^4 x_{24}^4} \left[\frac{H^{(a)}(1/x, 1/\bar{x})}{(x - \bar{x})^2} + \frac{H^{(b)}(1/x, 1/\bar{x})}{(u - v)(x - \bar{x})} \right], \quad (3.5.14)$$

$$H_{14;23} = \frac{1}{x_{13}^4 x_{24}^4} \left[\frac{H^{(a)}(1 - x, 1 - \bar{x})}{(x - \bar{x})^2} + \frac{H^{(b)}(1 - x, 1 - \bar{x})}{(1 - u)(x - \bar{x})} \right]. \quad (3.5.15)$$

3.5.2 The symbols of $H^{(a)}(x, \bar{x})$ and $H^{(b)}(x, \bar{x})$

In order to determine the pure functions contributing to the Hard integral, we proceed just like for the Easy integral and first determine the symbol. For the Hard integral we have to start from two ansätze for the symbols $\mathcal{S}[H^{(a)}(x, \bar{x})]$ and $\mathcal{S}[H^{(b)}(x, \bar{x})]$. While both pure functions are invariant under the exchange $x_1 \leftrightarrow x_2$, $\mathcal{S}[H^{(a)}]$ must be symmetric under the exchange of x, \bar{x} and $\mathcal{S}[H^{(b)}]$ has to be antisymmetric, cf. eq. (3.5.13). Going through exactly the same steps as for E we find that the single-variable limits of the symbols *cannot* be matched against the data from the asymptotic expansions using only entries from the set $\{x, 1 - x, \bar{x}, 1 - \bar{x}\}$. We thus need to enlarge the ansatz.

Previously, the letter $x - \bar{x} \sim \lambda_{1234}$ has been encountered in ref. [106, 124] in a similar context. We therefore consider all possible integrable symbols made from the letters $\{x, 1 - x, \bar{x}, 1 - \bar{x}, x - \bar{x}\}$ which obey the initial entry condition (3.2.13). In the case of the Easy integral, the integrability condition only implied that terms depending on both x and \bar{x} come from products of single-variable functions. Here, on the other hand, the condition is more non-trivial since, for example,

$$\begin{aligned} d \log \frac{x}{\bar{x}} \wedge d \log(x - \bar{x}) &= d \log x \wedge d \log \bar{x}, \\ d \log \frac{1 - x}{1 - \bar{x}} \wedge d \log(x - \bar{x}) &= d \log(1 - x) \wedge d \log(1 - \bar{x}). \end{aligned} \quad (3.5.16)$$

We summarize the dimensions of the spaces of such symbols, split according to parity under exchange of x and \bar{x} , in Table 3.2.

Given our ansatz for the symbols of the functions we are looking for, we then match against the twist two asymptotics as described previously. We find a unique solution for the symbols of both $H^{(a)}$ and $H^{(b)}$ compatible with all asymptotic limits.

Weight	Even	Odd
1	2	0
2	3	1
3	6	3
4	12	9
5	28	24
6	69	65

Table 3.2: Dimensions of the spaces of integrable symbols with entries drawn from the set $\{x, 1-x, \bar{x}, 1-\bar{x}, x-\bar{x}\}$ and split according to the parity under exchange of x and \bar{x} .

Interestingly, the limit of $H_{13;24}$ leaves one undetermined parameter in $\mathcal{S}[H^{(a)}]$, which we may fix by appealing to another limit. In the resulting symbols, the letter $x - \bar{x}$ occurs only in the last two entries of $\mathcal{S}[H^{(a)}]$ while it is absent from $\mathcal{S}[H^{(b)}]$. Although we did not impose this as a constraint, $\mathcal{S}[H^{(a)}]$ goes to zero when $x \rightarrow \bar{x}$, which is necessary since the integral cannot have a pole at $x = \bar{x}$.

3.5.3 The analytic results for $H^{(a)}(x, \bar{x})$ and $H^{(b)}(x, \bar{x})$

In this section we integrate the symbol of the Hard integral to a function, i.e. we determine the full answers for the *functions* $H^{(a)}(x, \bar{x})$ and $H^{(b)}(x, \bar{x})$ that contribute to the Hard integral $H_{12;34}$.

In the previous section we already argued that the symbol of $H^{(b)}(x, \bar{x})$ has all its entries drawn from the set $\{x, 1-x, \bar{x}, 1-\bar{x}\}$, and so it is reasonable to assume that $H^{(b)}(x, \bar{x})$ can be expressed in terms of SVHPLs only. We may therefore proceed by lifting directly from the asymptotic form as we did in section 3.4.4 for the Easy integral. By comparing the form of $H_{13;24}$, eq. (3.5.14), with its asymptotic value (3.1.14) we can read off the asymptotic form of $H(1/x, 1/\bar{x})$. Writing $\log u$ as $\log x + \log \bar{x}$, expanding out all the functions and neglecting $\log \bar{x}$ terms, we can lift directly to

the full function by simply converting HPLs to SVHPLs. In this way we arrive at

$$\begin{aligned}
H^{(b)}(1/x, 1/\bar{x}) = & 2\mathcal{L}_{2,4} - 2\mathcal{L}_{3,3} - 2\mathcal{L}_{1,1,4} - 2\mathcal{L}_{1,4,0} + 2\mathcal{L}_{1,4,1} - 2\mathcal{L}_{2,3,1} + 2\mathcal{L}_{3,1,2} \\
& - 2\mathcal{L}_{4,0,0} + 2\mathcal{L}_{4,1,0} + 2\mathcal{L}_{1,1,1,3} + 2\mathcal{L}_{1,1,3,0} + 2\mathcal{L}_{1,3,0,0} - 2\mathcal{L}_{1,3,1,1} \\
& - 2\mathcal{L}_{2,1,1,2} + 2\mathcal{L}_{2,1,2,1} + 2\mathcal{L}_{3,0,0,0} - 2\mathcal{L}_{3,1,1,0} - 2\mathcal{L}_{1,1,1,2,1} - 2\mathcal{L}_{1,1,2,1,0} \\
& + 2\mathcal{L}_{1,1,2,1,1} - 2\mathcal{L}_{1,2,1,0,0} + 2\mathcal{L}_{1,2,1,1,0} - 2\mathcal{L}_{2,1,0,0,0} + 2\mathcal{L}_{2,1,1,0,0} \\
& + 16\zeta_3\mathcal{L}_3 - 16\zeta_3\mathcal{L}_{2,1} .
\end{aligned} \tag{3.5.17}$$

Other orientations although still quite simple do not all share the property that they only have coefficients ± 2 . Using the basis of SVHPLs that makes the parity under exchange of x and \bar{x} explicit, we can write the last equation in the equivalent form

$$\begin{aligned}
H^{(b)}(x, \bar{x}) = & 16L_{2,4} - 16L_{4,2} - 8L_{1,3,2} - 8L_{1,4,1} + 8L_{2,1,3} - 8L_{2,2,2} + 8L_{2,3,1} - 8L_{3,1,2} \\
& + 16L_{3,2,0} + 8L_{3,2,1} - 8L_{4,1,1} + 4L_{1,2,2,1} - 8L_{1,3,1,1} - 4L_{2,1,1,2} + 8L_{2,1,2,1} \\
& - 8L_{2,2,1,0} - 4L_{2,2,1,1} + 8L_{3,1,1,0} - 4L_{1,1,2,1,1} - 24L_{2,1,1,1,0} .
\end{aligned} \tag{3.5.18}$$

Next, we turn to the function $H^{(a)}(x, \bar{x})$. As the symbol of $H^{(a)}(x, \bar{x})$ contains the entry $x - \bar{x}$, it cannot be expressed through SVHPLs only. Single-valued functions whose symbols have entries drawn from the set $\{x, 1-x, \bar{x}, 1-\bar{x}, x-\bar{x}\}$ have been studied up to weight four in ref. [106], and a basis for the corresponding space of functions was constructed. The resulting single-valued functions are combinations of logarithms of x and \bar{x} and multiple polylogarithms $G(a_1, \dots, a_n; 1)$, with $a_i \in \{0, 1/x, 1/\bar{x}\}$. Note that the harmonic polylogarithms form a subalgebra of this class of functions, because we have, e.g.,

$$G\left(0, \frac{1}{x}, \frac{1}{x}; 1\right) = H(0, 1, 1; x) . \tag{3.5.19}$$

This class of single-valued functions thus provides a natural extension of the SVHPLs we have encountered so far. In the following we show how we can integrate the symbol of $H^{(a)}(x, \bar{x})$ in terms of these functions. The basic idea is the same as for the case

of the SVHPLs: we would like to write down the most general linear combination of multiple polylogarithms of this type and fix their coefficients by matching to the symbol and the asymptotic expansion of $H^{(a)}(x, \bar{x})$. Unlike the SVHPL case, however, some of the steps are technically more involved, and we therefore discuss these points in detail.

Let us denote by \mathcal{G} the algebra generated by $\log x$ and $\log \bar{x}$ and by multiple polylogarithms $G(a_1, \dots, a_n; 1)$, with $a_i \in \{0, 1/x, 1/\bar{x}\}$, with coefficients that are polynomials in multiple zeta values. Note that without loss of generality we may assume that $a_n \neq 0$. In the following we denote by \mathcal{G}^\pm the linear subspaces of \mathcal{G} of the functions that are respectively even and odd under an exchange of x and \bar{x} . Our first goal will be to construct a basis for the algebra \mathcal{G} , as well as for its even and odd subspaces. As we know the generators of the algebra \mathcal{G} , we automatically know a basis for the underlying vector space for every weight. It is however often desirable to choose a basis that “recycles” as much as possible information from lower weights, i.e. we would like to choose a basis that explicitly includes all possible products of lower weight basis elements. Such a basis can always easily be constructed: indeed, a theorem by Radford [125] states that every shuffle algebra is isomorphic to the polynomial algebra constructed out of its Lyndon words. In our case, we immediately obtain a basis for \mathcal{G} by taking products of $\log x$ and $\log \bar{x}$ and $G(a_1, \dots, a_n; 1)$, where (a_1, \dots, a_n) is a Lyndon word in the three letters $\{0, 1/x, 1/\bar{x}\}$. Next, we can easily construct a basis for the eigenspaces \mathcal{G}^\pm by decomposing each (indecomposable) basis function into its even and odd parts. In the following we use the shorthands

$$G_{m_1, \dots, m_k}^\pm(x_1, \dots, x_k) = \frac{1}{2} G\left(\underbrace{0, \dots, 0}_{m_1-1}, \frac{1}{x_1}, \dots, \underbrace{0, \dots, 0}_{m_k-1}, \frac{1}{x_k}; 1\right) \pm (x \leftrightarrow \bar{x}). \quad (3.5.20)$$

In doing so we have seemingly doubled the number of basis functions, and so not all the eigenfunctions corresponding to Lyndon words can be independent. Indeed, we have for example

$$G_{1,1}^+(x, \bar{x}) = \frac{1}{2} G_1^+(x)^2 - \frac{1}{2} G_1^-(x)^2. \quad (3.5.21)$$

It is easy to check this relation by computing the symbol of both sides of the equation. Similar relations can be obtained without much effort for higher weight functions. The resulting linearly independent set of functions are the desired bases for the eigenspaces. We can now immediately write down the most general linear combination of elements of weight six in \mathcal{G}^+ and determine the coefficients by matching to the symbol of $H^{(a)}(x, \bar{x})$. As we are working with a basis, all the coefficients are fixed uniquely.

At this stage we have determined a function in \mathcal{G}^+ whose symbol matches the symbol of $H^{(a)}(x, \bar{x})$. We have however not yet fixed the terms proportional to zeta values. We start by parameterizing these terms by writing down all possible products of zeta values and basis functions in \mathcal{G}^+ . Some of the free parameters can immediately be fixed by requiring the function to vanish for $x = \bar{x}$ and by matching to the asymptotic expansion. Note that our basis makes it particularly easy to compute the leading term in the limit $\bar{x} \rightarrow 0$, because

$$\lim_{\bar{x} \rightarrow 0} G_m^\pm(\dots, \bar{x}, \dots) = 0. \quad (3.5.22)$$

In other words, the small u limit can easily be approached by dropping all terms which involve (non-trivial) basis functions that depend on \bar{x} . The remaining terms only depend on $\log \bar{x}$ and harmonic polylogarithms in x . However, unlike for SVHPLs, matching to the asymptotic expansions does not fix uniquely the terms proportional to zeta values. The reason for this is that, while in the SVHPL case we could rely on our knowledge of a basis for the single-valued subspace of harmonic polylogarithms, in the present case we have been working with a basis for the full space, and so the function we obtain might still contain non-trivial discontinuities. In the remainder of this section we discuss how one can fix this ambiguity.

In ref. [106] a criterion was given that allows one to determine whether a given function is single-valued. In order to understand the criterion, let us consider the algebra $\overline{\mathcal{G}}$ generated by multiple polylogarithms $G(a_1, \dots, a_n; a_{n+1})$, with $a_i \in \{0, 1/x, 1/\bar{x}\}$ and $a_{n+1} \in \{0, 1, 1/x, 1/\bar{x}\}$, with coefficients that are polynomials in multiple zeta values. Note that $\overline{\mathcal{G}}$ contains \mathcal{G} as a subalgebra. The reason to consider the larger

algebra $\overline{\mathcal{G}}$ is that $\overline{\mathcal{G}}$ carries a Hopf algebra structure⁹ [126], i.e. $\overline{\mathcal{G}}$ can be equipped with a coproduct $\Delta : \overline{\mathcal{G}} \rightarrow \overline{\mathcal{G}} \otimes \overline{\mathcal{G}}$. Consider now the subspace \mathcal{G}_{SV} of $\overline{\mathcal{G}}$ consisting of single-valued functions. It is easy to see that \mathcal{G}_{SV} is a subalgebra of $\overline{\mathcal{G}}$. However, it is not a sub-Hopf algebra, but rather \mathcal{G}_{SV} is a $\overline{\mathcal{G}}$ -comodule, i.e. $\Delta : \mathcal{G}_{SV} \rightarrow \overline{\mathcal{G}} \otimes \mathcal{G}_{SV}$. In other words, when acting with the coproduct on a single-valued function, the first factor in the coproduct must itself be single-valued. As a simple example, we have

$$\Delta(L_2) = \frac{1}{2}L_0 \otimes \log \frac{1-x}{1-\bar{x}} + \frac{1}{2}L_1 \otimes \log \frac{\bar{x}}{x}. \quad (3.5.23)$$

Note that this is a natural extension of the first entry condition discussed in section 1.3. This criterion can now be used to recursively fix the remaining ambiguities to obtain a single-valued function. In particular, in ref. [106] an explicit basis up to weight four was constructed for \mathcal{G}_{SV} . We extended this construction and obtained a complete basis at weight five, and we refer to ref. [106] about the construction of the basis. All the remaining ambiguities can then easily be fixed by requiring that after acting with the coproduct, the first factor can be decomposed into the basis of \mathcal{G}_{SV} up to weight five. We then finally arrive at

$$\begin{aligned} H^{(a)}(x, \bar{x}) = & \mathcal{H}(x, \bar{x}) - \frac{28}{3}\zeta_3 L_{1,2} + 164\zeta_3 L_{2,0} + \frac{136}{3}\zeta_3 L_{2,1} - \frac{160}{3}L_3 L_{2,1} - 66L_0 L_{1,4} \\ & - \frac{148}{3}L_0 L_{2,3} + \frac{64}{3}L_2 L_{3,1} + \frac{52}{3}L_0 L_{3,2} + 16L_1 L_{3,2} + 36L_0 L_{4,1} + 64L_1 L_{4,1} \\ & + \frac{70}{3}L_0 L_{1,2,2} + 24L_0 L_{1,3,1} + \frac{26}{3}L_1 L_{1,3,1} - 8L_2 L_{2,1,1} + 64L_0 L_{2,1,2} \\ & - \frac{58}{3}L_0 L_{2,2,0} - 4L_0 L_{2,2,1} + \frac{50}{3}L_1 L_{2,2,1} - 12L_0 L_{3,1,0} - \frac{88}{3}L_0 L_{3,1,1} \\ & + 18L_1 L_{3,1,1} - \frac{32}{3}L_0 L_{1,1,2,1} - 18L_0 L_{1,2,1,1} + \frac{166}{3}L_0 L_{2,1,1,0} - 8L_0 L_{2,1,1,1} \\ & + 328\zeta_3 L_3 + 32L_3^2 - 64L_2 L_4. \end{aligned} \quad (3.5.24)$$

The function $\mathcal{H}(x, \bar{x})$ is a single-valued combination of multiple polylogarithms that

⁹Note that we consider a slightly extended version of the Hopf algebra considered in ref. [126] that allows us to include consistently multiple zeta values of even weight, see ref. [63, 64].

cannot be expressed through SVHPLs alone,

$$\begin{aligned}
 \mathcal{H}(x, \bar{x}) = & -128G_{4,2}^+ - 512G_{5,\bar{1}}^+ - 64G_{3,1,2}^+ + 64G_{3,\bar{1},2}^+ - 64G_{3,\bar{1},\bar{2}}^+ - 128G_{3,2,\bar{1}}^+ \\
 & + 64G_{4,1,\bar{1}}^+ - 64G_{4,\bar{1},1}^+ - 448G_{4,\bar{1},\bar{1}}^+ + 64G_{2,\bar{1},2,1}^+ + 64G_{2,\bar{1},\bar{2},\bar{1}}^+ + 64G_{2,2,1,\bar{1}}^+ + 64G_{2,2,\bar{1},1}^+ \\
 & - 64G_{2,2,\bar{1},\bar{1}}^+ + 128G_{2,\bar{2},1,1}^+ + 128G_{2,\bar{2},\bar{1},\bar{1}}^+ + 256G_{3,1,1,\bar{1}}^+ + 128G_{3,1,\bar{1},1}^+ - 128G_{3,1,\bar{1},\bar{1}}^+ \\
 & + 192G_{3,\bar{1},1,1}^+ - 64G_{3,\bar{1},1,\bar{1}}^+ - 64G_{3,\bar{1},\bar{1},1}^+ + 192G_{3,\bar{1},\bar{1},\bar{1}}^+ + 128H_{2,4}^+ - 128H_{4,2}^+ \\
 & + \frac{640}{3}H_{2,1,3}^+ - \frac{64}{3}H_{2,3,1}^+ - \frac{256}{3}H_{3,1,2}^+ + 64H_{2,1,1,2}^+ - 64H_{2,2,1,1}^+ + 64L_0G_{3,2}^+ \quad (3.5.25)
 \end{aligned}$$

$$\begin{aligned}
 & + 256L_0G_{4,\bar{1}}^+ + 32L_0G_{2,1,\bar{2}}^+ + 64L_0G_{2,2,\bar{1}}^+ + 96L_0G_{3,1,\bar{1}}^+ + 32L_0G_{3,\bar{1},1}^+ + 96L_0G_{3,\bar{1},\bar{1}}^+ \\
 & - 64L_0G_{2,1,1,\bar{1}}^+ + 64L_0G_{2,\bar{1},1,\bar{1}}^+ - 32L_1G_{3,2}^+ - 128L_1G_{4,\bar{1}}^+ - 16L_1G_{2,1,\bar{2}}^+ \\
 & - 32L_1G_{2,2,\bar{1}}^+ - 80L_1G_{3,1,\bar{1}}^+ - 16L_1G_{3,\bar{1},1}^+ - 16L_1G_{3,\bar{1},\bar{1}}^+ - 64L_2G_{2,\bar{1},\bar{1}}^- + 64L_4G_{1,\bar{1}}^- \\
 & + 32L_{2,2}G_{1,\bar{1}}^- - \frac{32}{3}H_2^+H_{2,2}^+ - 64H_2^+H_{2,1,1}^+ - 128H_2^+H_4^+ - 64H_1^-L_0G_{2,\bar{1},\bar{1}}^- \\
 & - 32L_0^2G_{3,\bar{1}}^+ - 32L_0^2G_{2,\bar{1},\bar{1}}^+ + 32L_0^2G_{1,1,1,\bar{1}}^+ + 32L_1L_0G_{3,\bar{1}}^+ + 16L_1L_0G_{2,1,\bar{1}}^+ \\
 & + 16L_1L_0G_{2,\bar{1},\bar{1}}^+ - \frac{80}{3}H_1^-L_0L_{2,2} - 48H_1^-L_0L_{2,1,1} + 12H_1^-L_1L_{2,2} + 16L_0^2H_{2,2}^+ \\
 & + 32L_0^2H_{2,1,1}^+ - 64H_1^-L_4L_0 + 16H_1^-L_1L_4 + 64L_3G_{1,1,\bar{1}}^+ - \frac{640}{3}H_3^-H_{2,1}^- \\
 & + 64(H_{2,1}^-)^2 + 128(H_3^-)^2 + 32L_0L_2G_{2,\bar{1}}^- - 32L_0L_2G_{1,1,\bar{1}}^- - 16L_1L_2G_{2,\bar{1}}^- \\
 & + \frac{16}{3}L_0L_2H_{2,1}^- + 16H_1^-L_2L_{2,1} - \frac{112}{3}H_2^+L_0L_{2,1} - 8H_2^+L_1L_{2,1} - 32H_3^-L_0L_2 \\
 & - 48H_1^-L_3L_2 + 32H_2^+L_0L_3 + 16H_2^+L_1L_3 + 32H_1^-L_0^2G_{2,\bar{1}}^- - 16H_1^-L_1L_0G_{2,\bar{1}}^- \\
 & + \frac{16}{3}L_0^3G_{2,\bar{1}}^+ + \frac{16}{3}L_0^3G_{1,1,\bar{1}}^+ - 8L_1L_0^2G_{2,\bar{1}}^+ - 8L_1L_0^2G_{1,1,\bar{1}}^+ + \frac{16}{3}H_1^-L_0^2H_{2,1}^- \\
 & - 16(H_1^-)^2L_0L_{2,1} - 32H_1^-H_3^-L_0^2 + \frac{8}{3}(H_1^-)^2L_3L_0 - 12(H_1^-)^2L_1L_3 + 28H_2^+L_2^2 \\
 & + \frac{368(H_2^+)^3}{9} - 16L_0^2L_2G_{1,\bar{1}}^- - 8L_0L_1L_2G_{1,\bar{1}}^- + \frac{56}{3}H_1^-H_2^+L_0L_2 - 8H_1^-H_2^+L_1L_2 \\
 & + 8(H_1^-)^2L_2^2 + 8(H_2^+)^2L_0^2 + 8(H_2^+)^2L_0L_1 + \frac{28}{3}(H_1^-)^2H_2^+L_0^2 - 4(H_1^-)^2H_2^+L_0L_1 \\
 & - 96H_2^-(H_1^-)^3L_0 + \frac{160}{3}(H_1^-)^3L_0L_2 + \frac{52}{3}H_1^-L_0^3L_2 + 4H_1^-L_0L_1^2L_2
 \end{aligned}$$

$$\begin{aligned}
 & + 4H_1^- L_0^2 L_1 L_2 + H_2^+ L_0 L_1^3 + \frac{2}{3} H_2^+ L_0^2 L_1^2 - 8H_2^+ L_0^3 L_1 + \frac{148}{3} (H_1^-)^4 L_0^2 \\
 & + \frac{10}{3} (H_1^-)^2 L_0^4 + 5(H_1^-)^2 L_0^2 L_1^2 - \frac{10}{3} (H_1^-)^2 L_0^3 L_1 - 128\zeta_3 G_{2,\bar{1}}^+ - 128\zeta_3 G_{1,1,\bar{1}}^+ \\
 & + \frac{16}{3} \zeta_3 (H_1^-)^2 L_0 + 24\zeta_3 (H_1^-)^2 L_1 + \frac{64}{3} \zeta_3 H_1^- L_2,
 \end{aligned}$$

where we used the obvious shorthand

$$H_{\vec{m}}^\pm \equiv \frac{1}{2} H_{\vec{m}}(x) \pm (x \leftrightarrow \bar{x}). \quad (3.5.26)$$

and similarly for $G_{\vec{m}}^\pm$. In addition, for $G_{\vec{m}}^\pm$ the position of \bar{x} is indicated by the bars in the indices, e.g.,

$$G_{1,\bar{2},\bar{3}}^\pm \equiv G_{1,2,3}^\pm(x, \bar{x}, \bar{x}). \quad (3.5.27)$$

Note that we have expressed $\mathcal{H}(x, \bar{x})$ entirely using the basis of \mathcal{G}^+ constructed at the beginning of this section. As a consequence, all the terms are linearly independent and there can be no cancellations among different terms.

3.5.4 Numerical consistency checks for H

In the previous section we have determined the analytic result for the Hard integral. In order to check that our method indeed produced the correct result for the integral, we have compared our expression numerically against **FIESTA**. Specifically, we evaluate the conformally-invariant function $x_{13}^4 x_{24}^4 H_{13;24}$. Applying a conformal transformation to send x_4 to infinity, the integral takes the simplified form,

$$\lim_{x_4 \rightarrow \infty} x_{13}^4 x_{24}^4 H_{13;24} = \frac{1}{\pi^6} \int \frac{d^4 x_5 d^4 x_6 d^4 x_7 x_{13}^4 x_{57}^2}{(x_{15}^2 x_{25}^2 x_{35}^2) x_{56}^2 (x_{36}^2) x_{67}^2 (x_{17}^2 x_{27}^2 x_{37}^2)}, \quad (3.5.28)$$

with 9 propagators. As we did for $E_{14;23}$, we use the remaining freedom to fix $x_{13}^2 = 1$ so that $u = x_{12}^2$ and $v = x_{23}^2$, and perform the numerical evaluation using the same setup. We compare at 40 different values, and find excellent agreement in all cases. A small sample of the numerical checks is shown in Table 3.3.

u	v	Analytic	FIESTA	δ
0.1	0.2	269.239	269.236	6.4e-6
0.2	0.3	136.518	136.518	1.9e-6
0.3	0.1	204.231	204.230	1.3e-6
0.4	0.5	61.2506	61.2505	5.0e-7
0.5	0.6	46.1929	46.1928	3.5e-7
0.6	0.2	82.7081	82.7080	7.4e-7
0.7	0.3	57.5219	57.5219	4.7e-7
0.8	0.9	24.6343	24.6343	2.0e-7
0.9	0.5	34.1212	34.1212	2.6e-7

Table 3.3: Numerical comparison of the analytic result for $x_{13}^4 x_{24}^4 H_{13;24}$ against FIESTA for several values of the conformal cross ratios.

3.6 The analytic result for the three-loop correlator

In the previous sections we computed the Easy and Hard integrals analytically. Using eq. (3.1.8), we can therefore immediately write down the analytic answer for the three-loop correlator of four stress tensor multiplets. We find

$$\begin{aligned}
 x_{13}^2 x_{24}^2 F_3 = & \frac{6}{x - \bar{x}} \left[f^{(3)}(x) + f^{(3)}\left(1 - \frac{1}{x}\right) + f^{(3)}\left(\frac{1}{1-x}\right) \right] \\
 & + \frac{2}{(x - \bar{x})^2} f^{(1)}(x) \left[v f^{(2)}(x) + f^{(2)}\left(1 - \frac{1}{x}\right) + u f^{(2)}\left(\frac{1}{1-x}\right) \right] \\
 & + \frac{4}{x - \bar{x}} \left[\frac{1}{v-1} E(x) + \frac{v}{v-1} E\left(\frac{x}{x-1}\right) + \frac{1}{1-u} E(1-x) \right. \\
 & \quad \left. + \frac{u}{1-u} E\left(1 - \frac{1}{x}\right) + \frac{u}{u-v} E\left(\frac{1}{x}\right) + \frac{v}{u-v} E\left(\frac{1}{1-x}\right) \right] \\
 & + \frac{1}{(x - \bar{x})^2} \left[(1+v) H^{(a)}(x) + (1+u) H^{(a)}(1-x) + (u+v) H^{(a)}\left(\frac{1}{x}\right) \right]
 \end{aligned} \tag{3.6.1}$$

$$+ \frac{1}{x - \bar{x}} \left[\frac{v+1}{v-1} H^{(b)}(x) + \frac{1+u}{1-u} H^{(b)}(1-x) + \frac{u+v}{u-v} H^{(b)}\left(\frac{1}{x}\right) \right].$$

The pure functions appearing in the correlator are defined in eqs. (3.2.3), (3.4.18), (3.5.17) and (3.5.24). For clarity, we suppressed the dependence of the pure functions on \bar{x} , i.e. we write $f^{(L)}(x) \equiv f^{(L)}(x, \bar{x})$ and so on. All the pure functions can be expressed in terms of SVHPLs, except for $H^{(a)}$ which contains functions whose symbols involve $x - \bar{x}$ as an entry. We checked that these contributions do not cancel in the sum over all contributions to the correlator.

3.7 A four-loop example

In this section we will discuss a four-loop integral to illustrate how our techniques can be applied at higher loops. The example we consider contributes to the four-loop four-point function of stress-tensor multiplets in $\mathcal{N} = 4$ SYM. Specifically, we consider the Euclidean, conformal, four-loop integral,

$$I_{14;23}^{(4)} = \frac{1}{\pi^8} \int \frac{d^4 x_5 d^4 x_6 d^4 x_7 d^4 x_8 x_{14}^2 x_{24}^2 x_{34}^2}{x_{15}^2 x_{18}^2 x_{25}^2 x_{26}^2 x_{37}^2 x_{38}^2 x_{45}^2 x_{46}^2 x_{47}^2 x_{48}^2 x_{56}^2 x_{67}^2 x_{78}^2} = \frac{1}{x_{13}^2 x_{24}^2} f(u, v), \quad (3.7.1)$$

where the cross ratios u and v are defined by eq. (3.1.11). As we will demonstrate in the following sections, this integral obeys a second-order differential equation whose solution is uniquely specified by imposing single-valued behavior, similar to the generalized ladders considered in ref. [111].

The four-loop contribution to the stress-tensor four-point function in $\mathcal{N} = 4$ SYM contains some integrals that do not obviously obey any such differential equations, and with the effort presented here we also wanted to learn to what extent the two-step procedure of deriving symbols and subsequently uplifting them to functions can be repeated for those cases. Our results are encouraging: the main technical obstacle is obtaining sufficient data from the asymptotic expansions; we show that this step is indeed feasible, at least for $I^{(4)}$, and present the results in section 3.7.1. Ultimately we find it simpler to evaluate $I^{(4)}$ by solving a differential equation, and in this case

the asymptotic expansions provide stringent consistency checks.

3.7.1 Asymptotic expansions

Let us first consider the limits of the four-loop integral (3.7.1) and its point permutations for $x_{12}, x_{34} \rightarrow 0$. We derive expressions for its asymptotic expansion in the limit where $u \rightarrow 0, v \rightarrow 1$ similar to those for the Easy and Hard integrals obtained in section 3.3. The logarithmic terms can be fully determined, while the non-logarithmic part of the expansion requires four-loop IBP techniques that allow us to reach spin 15. This contains enough information to fix the $\zeta_n \log^0(u)$ terms (important for beyond-the-symbol contributions) while the purely rational part of the asymptotic series remains partially undetermined. However, our experience with Easy and Hard has shown that each of the three coincidence limits is (almost) sufficient to pin down the various symbols. Inverting the integrals from one orientation to another ties non-logarithmic terms in one expansion to logarithmic ones in another, so that we do in fact command over much more data than it superficially seems. It is also conceivable to take into account more than the lowest order in u .

We start by investigating the asymptotic expansion of the integral $I_{14;23}^{(4)}$ whose coincidence limit $x_{12}, x_{34} \rightarrow 0$ diverges as $\log^2 u$. There are three contributing regions: while in the first two regions the original integral factors into a product of two two-loop integrals or a one-loop integral and a trivial three-loop integral, the third part corresponds to the four-loop ‘hard’ region in which the original integral is simply expanded in the small distances. The coefficients of the logarithmically divergent terms in the asymptotic expansion, i.e. the coefficients of $\log^2 u$ and $\log u$, can be worked out from the first two regions alone. It is easy to reach high powers in x and we obtain a safe match onto harmonic series of the type (3.3.2) with $i > 1$. Similar to the case of the Easy and Hard integrals discussed in section 3.3, we can sum up the harmonic sums in terms of HPLs. Note that the absence of harmonic sums with $i = 1$ implies the absence of HPLs of the form $H_{1,\dots}(x)$.

In the hard region, we have explicitly worked out the contribution from spin zero through eight, i.e., up to and including terms of $\mathcal{O}(x^8)$. By what has been said above

about the form of the series, this amount of data is sufficient to pin down the terms involving zeta values, while we cannot hope to fix the purely rational part where the dimension of the ansatz is larger than the number of constraints we can obtain. The linear combination displayed below was found from the limit $\bar{x} \rightarrow 0$ of the symbol of the four-loop integral derived in subsequent sections. Its expansion around $x = 0$ reproduces the asymptotic expansion of the integral up to $O(x^8)$. We find

$$\begin{aligned}
x_{13}^2 x_{24}^2 I_{14;23}^{(4)} = & \quad (3.7.2) \\
& \frac{1}{2x} \log^2 u \left[H_{2,1,3} - H_{2,3,1} + H_{3,1,2} - H_{3,2,1} + 2H_{2,1,1,2} - 2H_{2,2,1,1} + \zeta_3(6H_3 + 6H_{2,1}) \right] + \\
& \frac{1}{x} \log u \left[-4H_{2,1,4} + 4H_{2,4,1} - 3H_{3,1,3} + 3H_{3,3,1} - 3H_{4,1,2} + 3H_{4,2,1} - 4H_{2,1,1,3} - 4H_{2,1,2,2} \right. \\
& \left. + 4H_{2,2,2,1} + 4H_{2,3,1,1} - 2H_{3,1,1,2} + 2H_{3,2,1,1} + \zeta_3(-18H_4 - 8H_{2,2} - 2H_{3,1} + 8H_{2,1,1}) \right] + \\
& \frac{1}{x} \left[10H_{2,1,5} + 2H_{2,2,4} - 2H_{2,3,3} - 10H_{2,5,1} + 8H_{3,1,4} - 8H_{3,4,1} + 6H_{4,1,3} - 6H_{4,3,1} \right. \\
& + 6H_{5,1,2} - 6H_{5,2,1} + 8H_{2,1,1,4} + 6H_{2,1,2,3} + 8H_{2,1,3,2} - 2H_{2,1,4,1} + 2H_{2,2,2,2} - 4H_{2,2,3,1} \\
& - 4H_{2,3,1,2} - 10H_{2,3,2,1} - 4H_{2,4,1,1} + 4H_{3,1,1,3} + 6H_{3,1,2,2} - 6H_{3,2,2,1} - 4H_{3,3,1,1} + 4H_{2,1,1,2,2} \\
& - 4H_{2,1,2,2,1} - 4H_{2,2,1,1,2} + 4H_{2,2,2,1,1} + \zeta_3(36H_5 + 8H_{2,3} + 12H_{3,2} - 12H_{4,1} - 4H_{2,1,2} \\
& \left. - 16H_{2,2,1} - 8H_{3,1,1}) + \zeta_5(10H_3 + 10H_{2,1}) \right] + \mathcal{O}(u).
\end{aligned}$$

Next we turn to the asymptotic expansion of the orientation $I_{12;34}^{(4)}$. Here the Euclidean coincidence limit $x_{12}, x_{34} \rightarrow 0$ is finite, and thus the only region we need to analyze is the four-loop hard region, for which we have determined the asymptotic expansion up to and including terms of $\mathcal{O}(x^{15})$. Just like for the non-logarithmic part in the asymptotic expansion of $I_{14;23}^{(4)}$, eq. (3.7.2), we have fixed the terms proportional to zeta values by matching an ansatz in terms of HPLs onto this data, and once again, the terms not containing zeta values are taken from the relevant limit of the symbol. We find

$$x_{13}^2 x_{24}^2 I_{12;34}^{(4)} = \quad (3.7.3)$$

$$\begin{aligned}
 & \frac{1}{x} \left[4H_{1,3,4} - 4H_{1,5,2} + 2H_{1,1,2,4} - 2H_{1,1,4,2} + 2H_{1,2,1,4} - 2H_{1,2,3,2} + 2H_{1,3,1,3} + 2H_{1,3,3,1} \right. \\
 & - 2H_{1,4,1,2} - 2H_{1,5,1,1} + H_{1,1,2,1,3} + H_{1,1,2,3,1} - H_{1,1,3,1,2} - H_{1,1,3,2,1} + H_{1,2,1,1,3} + H_{1,2,1,3,1} \\
 & - H_{1,2,2,1,2} + H_{1,2,2,2,1} - 2H_{1,2,3,1,1} + H_{1,3,1,2,1} - H_{1,3,2,1,1} + H_{1,2,1,1,2,1} - H_{1,2,1,2,1,1} + \\
 & \left. \zeta_3(8H_{1,1,3} - 8H_{1,2,2} + 4H_{1,1,2,1} - 4H_{1,2,1,1}) + 70\zeta_7 H_1 \right] + \mathcal{O}(u).
 \end{aligned}$$

The expansion around $x = 0$ of this expression reproduces the asymptotic expansion of the integral up to $\mathcal{O}(x^{15})$.

The most complicated integrals appearing in the asymptotic expansion of $I_{14;23}^{(4)}$ and $I_{12;34}^{(4)}$ are four-loop two-point dimensionally regularized (in position space) integrals which belong to the family of integrals contributing to the evaluation of the five-loop contribution to the Konishi anomalous dimension [112],

$$\begin{aligned}
 G(a_1, \dots, a_{14}) = & \int \frac{d^d x_6 d^d x_7 d^d x_8 d^d x_9}{(x_{16}^2)^{a_1} (x_{17}^2)^{a_2} (x_{18}^2)^{a_3} (x_{19}^2)^{a_4} (x_6^2)^{a_5} (x_7^2)^{a_6} (x_8^2)^{a_7}} \\
 & \times \frac{1}{(x_9^2)^{a_8} (x_{67}^2)^{a_9} (x_{68}^2)^{a_{10}} (x_{69}^2)^{a_{11}} (x_{78}^2)^{a_{12}} (x_{79}^2)^{a_{13}} (x_{89}^2)^{a_{14}}}, \quad (3.7.4)
 \end{aligned}$$

with various integer indices a_1, \dots, a_{14} and $d = 4 - 2\epsilon$.

The complexity of the IBP reduction to master integrals is determined, in a first approximation, by the number of positive indices and the maximal deviation from the corner point of a sector, which has indices equal to 0 or 1 for non-positive and positive indices, correspondingly. This deviation can be characterized by the number $\sum_{i \in \nu_+} (a_i - 1) - \sum_{i \in \nu_-} a_i$ where ν_{\pm} are sets of positive (negative) indices. So the most complicated (for an IBP reduction) integrals appearing in the contribution of spin s to the asymptotic expansion in the short-distance limit have nine positive indices and the deviation from the corner point is equal to $2s - 2$. It was possible to get results up to spin 15.

As in ref. [112] the IBP reduction was performed by the `c++` version of the code `FIRE` [117]. The master integrals of this family either reduce, via a dual transformation, to the corresponding momentum space master integrals [127, 128] or can be taken from ref. [112]. To arrive at contributions corresponding to higher spin values, `FIRE` was combined with a recently developed alternative code to solve IBP relations

LiteRed [129] based on the algebraic properties of IBP relations revealed in ref. [130]. (See ref. [131] where this combination was presented within the `Mathematica` version of FIRE.)

3.7.2 A differential equation

We can use the magic identity [22] on the two-loop ladder subintegral

$$I^{(2)}(x_1, x_2, x_4, x_7) = h_{14;27} = \frac{1}{\pi^4} \int \frac{d^4 x_5 d^4 x_6 x_{24}^2}{x_{15}^2 x_{25}^2 x_{26}^2 x_{45}^2 x_{46}^2 x_{67}^2 x_{56}^2}. \quad (3.7.5)$$

The magic identity reads

$$I^{(2)}(x_1, x_2, x_4, x_7) = I^{(2)}(x_2, x_1, x_7, x_4), \quad (3.7.6)$$

and using it on the four-loop integral we find

$$\begin{aligned} I_{14;23}^{(4)} &= \frac{1}{\pi^4} \int \frac{d^4 x_7 d^4 x_8}{x_{18}^2 x_{37}^2 x_{38}^2 x_{47}^2 x_{48}^2 x_{78}^2} I^{(2)}(x_1, x_2, x_4, x_7) \\ &= \frac{1}{\pi^4} \int \frac{d^4 x_7 d^4 x_8}{x_{18}^2 x_{37}^2 x_{38}^2 x_{47}^2 x_{48}^2 x_{78}^2} I^{(2)}(x_2, x_1, x_7, x_4) \\ &= \frac{1}{\pi^8} \int \frac{d^4 x_5 d^4 x_6 d^4 x_7 d^4 x_8 x_{17}^2 x_{14}^2 x_{34}^2}{x_{18}^2 x_{37}^2 x_{38}^2 x_{47}^2 x_{48}^2 x_{78}^2 x_{25}^2 x_{15}^2 x_{16}^2 x_{75}^2 x_{76}^2 x_{64}^2 x_{56}^2}. \end{aligned} \quad (3.7.7)$$

The resulting integral (3.7.7) is ‘boxable’, i.e. we may apply the Laplace operator at the point x_2 . The only propagator which depends on x_2 is the one connected to the point x_5 and we have

$$\square_2 \frac{1}{x_{25}^2} = -4\pi^2 \delta^4(x_{25}). \quad (3.7.8)$$

The effect of the Laplace operator is therefore to reduce the loop order by one [22]. Thus on the full integral $I^{(4)}$ we have

$$\begin{aligned} \square_2 I_{14;23}^{(4)} &= -\frac{4}{\pi^6} \int \frac{d^4 x_6 d^4 x_7 d^4 x_8 x_{17}^2 x_{14}^2 x_{34}^2}{x_{18}^2 x_{37}^2 x_{38}^2 x_{47}^2 x_{48}^2 x_{78}^2 x_{12}^2 x_{16}^2 x_{72}^2 x_{76}^2 x_{64}^2 x_{26}^2} \\ &= -4 \frac{x_{14}^2}{x_{12}^2 x_{24}^2} E_{14;23}, \end{aligned} \quad (3.7.9)$$

where we have recognized the Easy integral,

$$E_{14;23} = \frac{1}{\pi^6} \int \frac{d^4x_6 d^4x_7 d^4x_8 x_{34}^2 x_{24}^2 x_{17}^2}{x_{18}^2 x_{37}^2 x_{38}^2 x_{47}^2 x_{48}^2 x_{78}^2 x_{16}^2 x_{72}^2 x_{76}^2 x_{64}^2 x_{26}^2} = \frac{1}{x_{13}^2 x_{24}^2} f_E(u, v). \quad (3.7.10)$$

The differential equation (3.7.9) becomes an equation for the function f ,

$$\square_2 \frac{1}{x_{13}^2 x_{24}^2} f(u, v) = -4 \frac{x_{14}^2}{x_{12}^2 x_{13}^2 x_{24}^4} f_E(u, v). \quad (3.7.11)$$

Applying the chain rule we obtain the following equation in terms of u and v ,

$$\Delta^{(2)} f(u, v) = -\frac{4}{u} f_E(u, v), \quad (3.7.12)$$

where

$$\Delta^{(2)} = 4[2(\partial_u + \partial_v) + u\partial_u^2 + v\partial_v^2 - (1 - u - v)\partial_u\partial_v]. \quad (3.7.13)$$

In terms of (x, \bar{x}) we have

$$x\bar{x}\partial_x\partial_{\bar{x}}\hat{f}(x, \bar{x}) = -\hat{f}_E(x, \bar{x}), \quad (3.7.14)$$

where

$$\hat{f}(x, \bar{x}) = -(x - \bar{x})f(u, v) \quad (3.7.15)$$

and similarly for \hat{f}_E . Note that $\hat{f}(x, \bar{x}) = -\hat{f}(\bar{x}, x)$. Now we recall that the function $f_E(u, v)$ defined by eq. (3.7.10) in the orientation $E_{14;23}$ is of the form

$$f_E(u, v) = \frac{1}{(x - \bar{x})(1 - x\bar{x})} \left[E(1 - x, 1 - \bar{x}) + x\bar{x}E\left(1 - \frac{1}{x}, 1 - \frac{1}{\bar{x}}\right) \right]. \quad (3.7.16)$$

Hence we find the following equation for \hat{f} ,

$$(1 - x\bar{x})x\bar{x}\partial_x\partial_{\bar{x}}\hat{f}(x, \bar{x}) = -\left[E(1 - x, 1 - \bar{x}) + x\bar{x}E\left(1 - \frac{1}{x}, 1 - \frac{1}{\bar{x}}\right) \right]. \quad (3.7.17)$$

Without examining the equation in great detail we can immediately make the following observations about \hat{f} .

- The function \hat{f} is a pure function of weight eight. From eq. (3.7.15) the only leading singularity of the four-loop integral $I^{(4)}$ is therefore of the $1/(x - \bar{x})$ type, just as for the ladders.
- The final entries of the symbol of $\hat{f}(x, \bar{x})$ can be written as functions only of x or of \bar{x} , but not both together. This follows because the right-hand side of eq. (3.7.17) contains only functions of weight six, whereas there would be a contribution of weight seven if the final entries could not be separated into functions of x or \bar{x} separately.
- The factor $(1 - x\bar{x})$ on the left-hand side implies that the next-to-final entries in the symbol of $\hat{f}(x, \bar{x})$ contain the letter $(1 - x\bar{x})$.

In ref. [111], slightly simpler, but very similar, equations were analyzed for a class of generalized ladder integrals. The analysis of ref. [111] can be adapted to the case of the four-loop integral $I^{(4)}$ and, as in ref. [111], the solution to the equation (3.7.17) is uniquely determined by imposing single-valued behavior on \hat{f} .

First of all we note that any expression of the form $h(x) - h(\bar{x})$ obeys the homogeneous equation and antisymmetry under the exchange of x and \bar{x} and hence can be added to any solution of eq. (3.7.17). However, the conditions of single-valuedness,

$$[\text{disc}_x - \text{disc}_{\bar{x}}]\hat{f}(x, \bar{x}) = 0, \quad [\text{disc}_{1-x} - \text{disc}_{1-\bar{x}}]\hat{f}(x, \bar{x}) = 0, \quad (3.7.18)$$

and that 0 and 1 are the only singular points, fix this ambiguity.

Let us see how the ambiguity is fixed. Imagine that we have a single-valued solution and we try to add $h(x) - h(\bar{x})$ to it so that it remains a single-valued solution. Then the conditions (3.7.18) on the discontinuities tell us that h can have no branch cuts at $x = 0$ or $x = 1$. Since these are the only places that the integral has any singularities, we conclude it has no branch cuts at all. Since the only singularities of the integral are logarithmic branch points, h has no singularities at all and the only allowed possibility is that h is constant, which drops out of the combination $h(x) - h(\bar{x})$. Thus there is indeed a unique single-valued solution to eq. (3.7.17). The argument we have just outlined is identical to the one used in ref. [111] to solve for

the generalized ladders.

A direct way of obtaining the symbol of the single-valued solution to eq. (3.7.17) is to make an ansatz of weight eight from the five letters

$$\{x, 1-x, \bar{x}, 1-\bar{x}, 1-x\bar{x}\}, \quad (3.7.19)$$

and impose integrability and the initial entry condition. Then imposing that the differential equation is satisfied directly at symbol level leads to a unique answer.

3.7.3 An integral solution

Now let us look at the differential equation (3.7.17) in detail and construct the single-valued solution. It will be convenient to organize the right-hand side of the differential equation (3.7.17) according to symmetry under $x \leftrightarrow 1/x$. We define

$$\begin{aligned} E_+(x, \bar{x}) &= \frac{1}{2} \left[E(1-x, 1-\bar{x}) + E\left(1-\frac{1}{x}, 1-\frac{1}{\bar{x}}\right) \right], \\ E_-(x, \bar{x}) &= \frac{1}{2} \left[E(1-x, 1-\bar{x}) - E\left(1-\frac{1}{x}, 1-\frac{1}{\bar{x}}\right) \right]. \end{aligned} \quad (3.7.20)$$

Then the differential equation reads

$$(1-x\bar{x})x\bar{x}\partial_x\partial_{\bar{x}}\hat{f}(x, \bar{x}) = -(1-x\bar{x})E_-(x, \bar{x}) - (1+x\bar{x})E_+(x, \bar{x}). \quad (3.7.21)$$

We may now split the equation (3.7.21) into two parts

$$x\bar{x}\partial_x\partial_{\bar{x}}f_a(x, \bar{x}) = -E_-(x, \bar{x}), \quad (3.7.22)$$

$$(1-x\bar{x})x\bar{x}\partial_x\partial_{\bar{x}}f_b(x, \bar{x}) = -(1+x\bar{x})E_+(x, \bar{x}). \quad (3.7.23)$$

Note that we may take both f_a and f_b to be antisymmetric under $x \leftrightarrow 1/x$.

The equation (3.7.22) is of exactly the same form as the equations considered in ref. [111]. Following the prescription given in ref. [111], section 6.1, it is a simple

matter to find a single-valued solution to the equation (3.7.22) in terms of single-valued polylogarithms. We find

$$\begin{aligned} f_a(x, \bar{x}) = & L_{3,4,0} - 2L_{4,3,0} + L_{5,2,0} + 2L_{3,2,2,0} - 2L_{4,1,2,0} - L_{4,2,0,0} - 2L_{4,2,1,0} + L_{5,0,0,0} \\ & + 2L_{5,1,0,0} + 2L_{5,1,1,0} + 2L_{4,1,1,0,0} - 4\zeta_3(\bar{L}_5 - 2\bar{L}_{3,2} + 2\bar{L}_{4,0} + 3\bar{L}_{4,1}) \end{aligned} \quad (3.7.24)$$

We now treat the equation (3.7.23) for f_b . Let us split it into two parts so that $f_b(x, \bar{x}) = f_1(x, \bar{x}) + f_2(x, \bar{x})$,

$$\begin{aligned} (1 - x\bar{x})x\bar{x}\partial_x\partial_{\bar{x}}f_1(x, \bar{x}) &= -E_+(x, \bar{x}), \\ (1 - x\bar{x})\partial_x\partial_{\bar{x}}f_2(x, \bar{x}) &= -E_+(x, \bar{x}). \end{aligned} \quad (3.7.25)$$

We may write integral solutions

$$f_1(x, \bar{x}) = - \int_1^x \frac{dt}{t} \int_1^{\bar{x}} \frac{d\bar{t}}{\bar{t}} \frac{E_+(t, \bar{t})}{1 - t\bar{t}} \quad (3.7.26)$$

and

$$f_2(x, \bar{x}) = -f_1(1/x, 1/\bar{x}) = - \int_1^x dt \int_1^{\bar{x}} d\bar{t} \frac{E_+(t, \bar{t})}{1 - t\bar{t}} \quad (3.7.27)$$

which obey the equations (3.7.25).

It follows that the full function \hat{f} is given by

$$\hat{f}(x, \bar{x}) = f_a(x, \bar{x}) + f_1(x, \bar{x}) + f_2(x, \bar{x}) + h(x) - h(\bar{x}) \quad (3.7.28)$$

for some holomorphic function h . We note that $\hat{f}(x, 1) - f_a(x, 1) = h(x) - h(1)$.

Now we examine the function f_2 in more detail. Writing,

$$E_+(t, \bar{t}) = \sum_i H_{w_i}(t) H_{w'_i}(\bar{t}), \quad (3.7.29)$$

we find,

$$f_2(x, \bar{x}) = \sum_i \int_1^x \frac{dt}{t} H_{w_i}(t) I_{w'_i}(t, \bar{x}) \quad (3.7.30)$$

where, for a word w made of the letters 0 and 1,

$$I_w(x, \bar{x}) = \int_1^{\bar{x}} \frac{d\bar{t}}{\bar{t} - 1/x} H_w(\bar{t}) = (-1)^d \left(G(\frac{1}{x}, w; \bar{x}) - G(\frac{1}{x}, w; 1) \right). \quad (3.7.31)$$

We may now calculate the symbol of f_2 . We note that

$$df_2(x, \bar{x}) = d \log x \sum_i H_{w_i}(x) I_{w'_i}(x, \bar{x}) - (x \leftrightarrow \bar{x}). \quad (3.7.32)$$

The symbol of I_w is obtained recursively using

$$\mathcal{S}(I_w(x, \bar{x})) = \mathcal{S}(H_w(\bar{x})) \otimes \frac{1 - x\bar{x}}{1 - xa_0} - (-1)^{a_0} \mathcal{S}(I_{w'}(x, \bar{x})) \otimes \frac{x}{1 - xa_0}, \quad (3.7.33)$$

where $w = a_0 w'$. When w is the empty word $I(x, \bar{x})$ is a logarithm,

$$I(x, \bar{x}) = \log \frac{1 - x\bar{x}}{1 - x}. \quad (3.7.34)$$

Using the relations (3.7.32, 3.7.33, 3.7.34) we obtain the symbol of $f_2(x, \bar{x})$. One finds that the result does not obey the initial entry condition (i.e. the first letters in the symbol are not only of the form $u = x\bar{x}$ or $v = (1 - x)(1 - \bar{x})$). However, the initial entry condition can be uniquely restored by adding the symbols of single-variable functions in the form $\mathcal{S}(h_2(x)) - \mathcal{S}(h_2(\bar{x}))$. Inverting $x \leftrightarrow 1/x$ we may similarly treat $f_1(x, \bar{x}) = -f_2(1/x, 1/\bar{x})$. Combining everything we obtain the symbol

$$\mathcal{S}(\hat{f}(x, \bar{x})) = \mathcal{S}(f_a(x, \bar{x}) + f_2(x, \bar{x}) + h_2(x) - h_2(\bar{x}) - f_2(1/x, 1/\bar{x}) - h_2(1/x) + h_2(1/\bar{x})). \quad (3.7.35)$$

The symbol obtained this way agrees with that obtained by imposing the differential equation on an ansatz as described around eq. (3.7.19).

Given that single-valuedness uniquely determines the solution of the differential equation (3.7.17) one might suspect that we can use this property to give an explicit representation of the function $h_2(x)$. Indeed this is the case. The integral formula (3.7.27) can, in principle, have discontinuities around any of the five divisors obtained by setting a letter from the set (3.7.19) to zero.

Let us consider the discontinuity of $f_2(x, \bar{x})$ at $x = 1/\bar{x}$,

$$\begin{aligned} \text{disc}_{x=1/\bar{x}} f_2(x, \bar{x}) &= \int_{1/\bar{x}}^x dt \text{disc}_{t=1/\bar{x}} \int_1^{\bar{x}} d\bar{t} \frac{E_+(t, \bar{t})}{1 - t\bar{t}} \\ &= \int_{1/\bar{x}}^x dt \text{disc}_{\bar{x}=1/t} \int_1^{\bar{x}} d\bar{t} \frac{E_+(t, \bar{t})}{1 - t\bar{t}} \\ &= - \int_{1/\bar{x}}^x \frac{dt}{t} (2\pi i) E_+(t, 1/t). \end{aligned} \quad (3.7.36)$$

The above expression vanishes due to the symmetry of E_+ under $x \leftrightarrow 1/x$ and the antisymmetry under $x \leftrightarrow \bar{x}$. The absence of such discontinuities is the reason that we split the original equation into two pieces, one for f_a and one for f_b .

Now let us consider the discontinuity around $x = 1$. We find

$$\begin{aligned} \text{disc}_{1-x} f_2(x, \bar{x}) &= - \int_1^x \frac{dt}{t} \text{disc}_{1-t} \int_1^{\bar{x}} \frac{d\bar{t}}{\bar{t} - 1/t} E_+(t, \bar{t}) \\ &= -(2\pi i) \int_1^x \frac{dt}{t} E_+(t, 1/t) + \int_1^x dt \int_1^{\bar{x}} d\bar{t} \frac{\text{disc}_{1-t} E_+(t, \bar{t})}{1 - t\bar{t}}. \end{aligned} \quad (3.7.37)$$

The first term above again vanishes due to the symmetries of E_+ . The second term will cancel against the corresponding term involving $\text{disc}_{1-\bar{t}} E_+(t, \bar{t})$ in the integrand when we take the combination $[\text{disc}_{1-x} - \text{disc}_{1-\bar{x}}] f_2(x, \bar{x})$. The discontinuities at $x = 1$ and $\bar{x} = 1$ of f_2 therefore satisfy the single-valuedness conditions (3.7.18) since E_+ does.

For the discontinuities at $x = 0$ we find

$$\text{disc}_x f_2(x, \bar{x}) = \int_0^x dt \text{disc}_t \int_1^{\bar{x}} d\bar{t} \frac{E_+(t, \bar{t})}{1 - t\bar{t}} = \int_0^x dt \int_1^{\bar{x}} \frac{d\bar{t}}{1 - t\bar{t}} \text{disc}_t E_+(t, \bar{t}). \quad (3.7.38)$$

Now writing the \bar{t} integral above as $\int_1^{\bar{x}} = \int_0^{\bar{x}} - \int_0^1$ and using $[\text{disc}_t - \text{disc}_{\bar{t}}] E_+(t, \bar{t}) = 0$ we find

$$\begin{aligned} [\text{disc}_x - \text{disc}_{\bar{x}}] f_2(x, \bar{x}) &= \left[- \int_0^x dt \int_0^1 \frac{d\bar{t}}{1 - t\bar{t}} \text{disc}_t E_+(t, \bar{t}) \right] + (x \leftrightarrow \bar{x}) \\ &= \text{disc}_x \left[- \int_0^x dt \int_0^1 \frac{d\bar{t}}{1 - t\bar{t}} E_+(t, \bar{t}) \right] + (x \leftrightarrow \bar{x}) \end{aligned} \quad (3.7.39)$$

Thus $f_2(x, \bar{x})$ is not single-valued by itself since the above combination of discontinuities (3.7.39) does not vanish. Note however that eq. (3.7.39) is of the form $k(x) + k(\bar{x})$, as necessary in order for it to be canceled by adding a term of the form $h_2(x) - h_2(\bar{x})$ to $f_2(x, \bar{x})$. We now construct such a function $h_2(x)$.

Let

$$h_2^0(x) = \int_0^x dt \int_0^1 \frac{d\bar{t}}{1 - t\bar{t}} E_+(t, \bar{t}). \quad (3.7.40)$$

Writing $E_+(t, \bar{t}) = \sum_i H_{w_i}(t) H_{w'_i}(\bar{t})$ we find

$$h_2^0(x) = - \int_0^x \frac{dt}{t} \sum_i H(w_i; t) \int_0^1 \frac{d\bar{t}}{\bar{t} - 1/t} H(w'_i; \bar{t}). \quad (3.7.41)$$

We can write

$$\int_0^1 \frac{d\bar{t}}{\bar{t} - 1/t} H_{w'_i}(\bar{t}) = (-1)^d G(1/t, w'_i(0, 1); 1), \quad (3.7.42)$$

where we have made explicit that w'_i is a word in the letters 0 and 1 and d is the number of 1 letters. One can always rewrite this in terms of HPLs at argument t . Indeed we can recursively apply the formula

$$G\left(\frac{1}{t}, a_2, a_3, \dots, a_n; 1\right) = \int_0^t \frac{dr}{r-1} G\left(\frac{a_2}{r}, a_3, \dots, a_n; 1\right) - \int_0^t \frac{dr}{r} G\left(\frac{1}{r}, a_3, \dots, a_n; 1\right). \quad (3.7.43)$$

to achieve this. Note that $a_i \in \{0, 1\}$ in the above formula. We also need

$$G\left(\frac{1}{t}, 0_q; 1\right) = (-1)^{q+1} H_{q+1}(t). \quad (3.7.44)$$

Once this has been done, one can use standard HPL relations to calculate the products

$$H_{w_i}(t) G(1/t, w'_i; 1) \quad (3.7.45)$$

and perform the remaining integral from 0 to x w.r.t. t . We thus obtain a function h_2^0 whose discontinuity at $x = 0$ is minus that of the x -dependent contribution to $[\text{disc}_x - \text{disc}_{\bar{x}}]f_2(x, \bar{x})$.

In ref. [111] an explicit projection operator \mathcal{F} was introduced which removes the discontinuity at $x = 0$ of a linear combination of HPLs while preserving the discontinuity at $x = 1$. The orthogonal projector $(1 - \mathcal{F})$ removes the discontinuity at $x = 1$ while preserving that at $x = 0$. We define

$$h_2(x) = (1 - \mathcal{F})h_2^0(x). \quad (3.7.46)$$

Explicitly we find

$$\begin{aligned} h_2(x) = & \frac{151}{16}\zeta_6 H_2 + \frac{15}{2}\zeta_3^2 H_2 - \frac{3}{2}\zeta_2 \zeta_3 H_{2,0} - \frac{15}{4}\zeta_5 H_{2,0} - \zeta_2 \zeta_3 H_{2,1} + \frac{19}{4}\zeta_4 H_{2,2} + 2\zeta_3 H_{2,3} \\ & - \zeta_2 H_{2,4} + \frac{21}{8}\zeta_4 H_{2,0,0} + \frac{19}{4}\zeta_4 H_{2,1,0} + \frac{17}{2}\zeta_4 H_{2,1,1} + 5\zeta_3 H_{2,1,2} - \zeta_2 H_{2,1,3} - \frac{3}{2}\zeta_3 H_{2,2,0} \\ & + \zeta_3 H_{2,2,1} - \zeta_2 H_{2,2,2} + \frac{1}{2}\zeta_2 H_{2,3,0} - \zeta_2 H_{2,3,1} - \frac{3}{2}\zeta_3 H_{2,0,0,0} - 3\zeta_3 H_{2,1,0,0} - 3\zeta_3 H_{2,1,1,0} \\ & + 4\zeta_3 H_{2,1,1,1} + \zeta_2 H_{2,1,2,0} - 2\zeta_2 H_{2,1,2,1} + \frac{1}{2}H_{2,1,4,0} + \zeta_2 H_{2,2,1,0} + \frac{1}{2}H_{2,3,2,0} - \frac{1}{2}H_{2,4,0,0} \\ & - H_{2,4,1,0} + \frac{1}{2}\zeta_2 H_{2,1,0,0,0} + \zeta_2 H_{2,1,1,0,0} + 2\zeta_2 H_{2,1,1,1,0} + H_{2,1,1,3,0} + H_{2,1,2,2,0} - H_{2,1,3,0,0} \\ & + 2H_{2,1,1,1,2,0} - H_{2,1,3,1,0} + H_{2,2,1,2,0} - \frac{1}{2}H_{2,2,2,0,0} - H_{2,2,2,1,0} + \frac{1}{2}H_{2,3,0,0,0} - H_{2,3,1,1,0} \\ & - H_{2,1,1,2,0,0} + \frac{1}{2}H_{2,1,2,0,0,0} - H_{2,1,2,1,0,0} - 2H_{2,1,2,1,1,0} + H_{2,2,1,0,0,0} + H_{2,2,1,1,0,0} \\ & + H_{2,1,1,1,0,0,0}. \end{aligned} \quad (3.7.47)$$

Here the H functions are all implicitly evaluated at argument x .

The contribution from $f_1(x, \bar{x}) = -f_2(1/x, 1/\bar{x})$ is made single-valued by inversion on x . So we define

$$h(x) = h_2(x) - h_2(1/x). \quad (3.7.48)$$

Finally we deduce that the combination

$$\hat{f}(x, \bar{x}) = f_a(x, \bar{x}) + f_1(x, \bar{x}) + f_2(x, \bar{x}) + h(x) - h(\bar{x}) \quad (3.7.49)$$

is single-valued and obeys the differential equation (3.7.17) and hence describes the four-loop integral $I^{(4)}$ defined in equation (3.7.1). The equations (3.7.27), (3.7.47),

(3.7.48) and (3.7.49) therefore explicitly define the function \hat{f} .

3.7.4 Expression in terms of multiple polylogarithms

Now let us rewrite the integral form (3.7.27), (3.7.31) for $f_2(x, \bar{x})$ in terms of multiple polylogarithms. We use the following generalization of relation (3.7.43),

$$\begin{aligned} G\left(\frac{1}{y}, a_2, \dots, a_n; z\right) &= \left(G\left(\frac{1}{z}; y\right) - G\left(\frac{1}{a_2}; y\right)\right) G(a_2, \dots, a_n; z) \\ &\quad + \int_0^y \left(\frac{dt}{t - \frac{1}{a_2}} - \frac{dt}{t}\right) G\left(\frac{1}{t}, a_3, \dots, a_n; z\right) \end{aligned} \quad (3.7.50)$$

to recursively rewrite the $G(\frac{1}{t}, \dots)$ appearing in the $I_{w'_i}(t, \bar{x})$ in eq. (3.7.27) so that the t appears as the final argument. Note that in eq. (3.7.50), the two terms involving an explicit appearance of $1/a_2$ vanish in the case $a_2 = 0$. The recursion begins with

$$G\left(\frac{1}{y}; z\right) = \log(1 - yz) = G\left(\frac{1}{z}; y\right). \quad (3.7.51)$$

The recursion allows us to write the products $H_{w_i}(t)I_{w'_i}(t, \bar{x})$ as a sum of multiple polylogarithms of the form $G(w; t)$ where the weight vectors depend on \bar{x} . Then we can perform the final integration dt/t to obtain an expression for f_2 in terms of multiple polylogarithms.

We may relate $f_1(x, \bar{x})$ directly to $f_2(x, \bar{x})$ since

$$\begin{aligned} f_1(x, \bar{x}) &= - \int_1^x \frac{dt}{t} \int_1^{\bar{x}} \frac{d\bar{t}}{\bar{t}} \frac{E_+(t, \bar{t})}{1 - t\bar{t}} = \int_1^x \frac{dt}{t^2} \int_1^{\bar{x}} \frac{d\bar{t}}{\bar{t}(\bar{t} - 1/t)} E_+(t, \bar{t}) \\ &= \int_1^x \frac{dt}{t} \left[\int_1^{\bar{x}} \frac{d\bar{t}}{\bar{t} - 1/t} E_+(t, \bar{t}) - \int_1^{\bar{x}} \frac{d\bar{t}}{\bar{t}} E_+(t, \bar{t}) \right] \\ &= f_2(x, \bar{x}) - \sum_i [H_{0w_i}(x) - H_{0w_i}(1)] [H_{0w'_i}(\bar{x}) - H_{0w'_i}(1)]. \end{aligned} \quad (3.7.52)$$

For a practical scheme we express E_+ as a sum over $H_{w_i}(t)H_{w'_i}(\bar{t})$ and do the \bar{t} integration. In any single term of the integrand of f_2 , the recursion (3.7.50) will lead to multiple polylogarithms of the type $G(\dots, 1/\bar{x}; t)$. Next, we take the shuffle product with the second polylogarithm and integrate over t .

In this raw form our result is not manifestly antisymmetric under $x \leftrightarrow \bar{x}$. Remarkably, in the sum over all terms only $G(0, 1/\bar{x}, \dots; x)$ remain. Upon rewriting

$$G\left(0, \frac{1}{\bar{x}}, a_1, \dots, a_n; x\right) = G(0; x)G\left(\frac{1}{\bar{x}}, a_1, \dots, a_n; x\right) - \int_0^x \frac{dt}{t - \frac{1}{\bar{x}}} G(0; t)G(a_1, \dots, a_n; t) \quad (3.7.53)$$

we can use (3.7.50) to swap $G(1/\bar{x}, \dots; x)$ for (a sum over) $G(\dots, 1/x; \bar{x})$. Replacing the original two-variable polylogarithms by 1/2 themselves and 1/2 the x, \bar{x} swapped version, we can obtain a manifestly antisymmetric form. The shuffle algebra is needed to remove zeroes from the rightmost position of the weight vectors and to bring the letters $1/x, 1/\bar{x}$ to the left of all entries 1. Finally we rescale to argument 1.

In analogy to the notation introduced for the Hard integral let us write

$$G_{\hat{3},2,1} = G\left(0, 0, \frac{1}{x\bar{x}}, 0, \frac{1}{x}, \frac{1}{x}; 1\right) \quad (3.7.54)$$

etc. Collecting terms, we find

$$\begin{aligned} I_{14;23}^{(4)}(x, \bar{x}) = & \quad (3.7.55) \\ & -L_{2,2,4} + 2L_{2,3,3} - L_{2,4,2} - 2L_{2,1,1,4} + 2L_{2,1,2,3} - 2L_{2,1,3,2} + 2L_{2,1,4,1} + 2L_{2,2,1,3} - 2L_{2,2,2,2} \\ & - 2L_{2,2,3,1} + 2L_{2,3,1,2} + 2L_{2,3,2,0} + 2L_{2,3,2,1} - 2L_{2,4,1,0} - 2L_{2,4,1,1} - 2L_{3,1,3,0} + 2L_{3,3,1,0} \\ & - 4L_{2,1,1,2,2} + 4L_{2,1,2,2,1} + 4L_{2,2,1,1,2} - 4L_{2,2,2,1,0} - 4L_{2,2,2,1,1} - 4L_{3,1,1,2,0} + 2L_{3,2,1,0,0} \\ & + 4L_{3,2,1,1,0} + L_0 \left(-H_{1,2,4}^- + 2H_{1,3,3}^- - H_{1,4,2}^- - 2H_{1,1,1,4}^- + 2H_{1,1,2,3}^- - 2H_{1,1,3,2}^- + 2H_{1,1,4,1}^- \right. \\ & + 2H_{1,2,1,3}^- - 2H_{1,2,2,2}^- - 2H_{1,2,3,1}^- + 2H_{1,3,1,2}^- + 2H_{1,3,2,1}^- - 2H_{1,4,1,1}^- - 4H_{1,1,1,2,2}^- + 4H_{1,1,2,2,1}^- \\ & \left. + 4H_{1,2,1,1,2}^- - 4H_{1,2,2,1,1}^- \right) + 4H_{1,2,5}^- - 4H_{1,3,4}^- - 4H_{1,4,3}^- + 4H_{1,5,2}^- + 8H_{1,1,1,5}^- - 4H_{1,1,2,4}^- \\ & + 4H_{1,1,4,2}^- - 8H_{1,1,5,1}^- - 4H_{1,2,1,4}^- + 8H_{1,2,3,2}^- + 4H_{1,2,4,1}^- - 8H_{1,3,1,3}^- - 4H_{1,4,1,2}^- - 4H_{1,4,2,1}^- \\ & + 8H_{1,5,1,1}^- + 8H_{1,1,1,2,3}^- + 8H_{1,1,1,3,2}^- - 8H_{1,1,2,3,1}^- - 8H_{1,1,3,2,1}^- - 8H_{1,2,1,1,3}^- + 8H_{1,2,3,1,1}^- \\ & - 8H_{1,3,1,1,2}^- + 8H_{1,3,2,1,1}^- + \zeta_3 (8\bar{L}_{2,3} - 12\bar{L}_{3,2} - 12\bar{L}_{2,1,2} + 12\bar{L}_{2,2,1} - 12\bar{L}_{3,1,0} - 16\bar{L}_{3,1,1} \\ & - 12L_0 H_{1,1,2}^- + 12L_0 H_{1,2,1}^- + 16H_{1,1,3}^- - 16H_{1,3,1}^- - 16H_{1,1,1,2}^- + 16H_{1,2,1,1}^-) + 2\bar{L}_3 \zeta_5 \\ & + \zeta_3^2 (-24L_2 - 72H_2^- - 48H_{1,1}^-) + \\ & G_2^+ \left(-L_{4,2} - L_{4,0,0} - 2L_{4,1,0} - 2L_{4,1,1} - 4\bar{L}_{2,1} \zeta_3 + 4L_0 \zeta_3 H_2^- + 4L_1 \zeta_3 H_2^- \right. \end{aligned}$$

$$\begin{aligned}
& +3\bar{L}_2H_4^- + 2\bar{L}_{1,1}H_4^- - 4L_1H_5^- + 4\zeta_3H_{1,2}^- - 2\bar{L}_{0,0}H_{1,3}^- + 5L_0H_{1,4}^- - 2L_1H_{1,4}^- - 12H_{1,5}^- \\
& + 12\zeta_3H_{2,1}^- - \bar{L}_{0,0}H_{2,2}^- + 2L_0H_{2,3}^- - 2L_1H_{2,3}^- - 6H_{2,4}^- + L_0H_{3,2}^- - 2L_1H_{3,2}^- - 4L_0H_{4,1}^- \\
& - 2L_1H_{4,1}^- + 2H_{4,2}^- + 16H_{5,1}^- + 16\zeta_3H_{1,1,1}^- - 2\bar{L}_{0,0}H_{1,1,2}^- + 6L_0H_{1,1,3}^- - 12H_{1,1,4}^- - 2\bar{L}_{0,0}H_{1,2,1}^- \\
& + 6L_0H_{1,2,2}^- - 8H_{1,2,3}^- + 2L_0H_{1,3,1}^- - 8H_{1,3,2}^- + 4H_{1,4,1}^- + 2\bar{L}_{0,0}H_{2,1,1}^- + 2L_0H_{2,1,2}^- - 4H_{2,1,3}^- \\
& - 2L_0H_{2,2,1}^- - 4H_{2,2,2}^- + 4H_{2,3,1}^- - 6L_0H_{3,1,1}^- + 4H_{3,1,2}^- + 12H_{3,2,1}^- + 12H_{4,1,1}^- \\
& + 4L_0H_{1,1,1,2}^- - 8H_{1,1,1,3}^- - 8H_{1,1,2,2}^- - 4L_0H_{1,2,1,1}^- + 8H_{1,2,2,1}^- + 8H_{1,3,1,1}^- - L_2H_4^+) + \\
& G_3^+ (2\bar{L}_{3,2} + 4\bar{L}_{3,1,0} + 4\bar{L}_{3,1,1} - 8\zeta_3H_2^- - 6\bar{L}_2H_3^- - 2\bar{L}_{0,0}H_3^- - 4\bar{L}_{1,1}H_3^- + 8L_0H_4^- \\
& + 6L_1H_4^- - 20H_5^- - 8\zeta_3H_{1,1}^- + 8L_0H_{1,3}^- + 4L_1H_{1,3}^- - 20H_{1,4}^- + 6L_0H_{2,2}^- + 4L_1H_{2,2}^- \\
& - 16H_{2,3}^- + 4L_0H_{3,1}^- + 4L_1H_{3,1}^- - 16H_{3,2}^- - 8H_{4,1}^- + 4L_0H_{1,1,2}^- - 16H_{1,1,3}^- + 4L_0H_{1,2,1}^- \\
& - 16H_{1,2,2}^- - 8H_{1,3,1}^- - 4L_0H_{2,1,1}^- - 8H_{2,1,2}^- + 8H_{3,1,1}^- - 8H_{1,1,1,2}^- + 8H_{1,2,1,1}^- + 2L_2H_3^+) + \\
& G_{2,1}^+ (2\bar{L}_{3,2} - \bar{L}_{4,0} - 2\bar{L}_{4,1} + 2\bar{L}_{3,1,0} - 12L_2\zeta_3 + 16\zeta_3H_2^- - 4\bar{L}_2H_3^- \\
& - 2\bar{L}_{0,0}H_3^- + 8L_0H_4^- + 8L_1H_4^- - 20H_5^- + 16\zeta_3H_{1,1}^- + 4L_0H_{1,3}^- - 16H_{1,4}^- + 4L_0H_{2,2}^- \\
& - 12H_{2,3}^- - 12H_{3,2}^- + 4L_0H_{1,1,2}^- - 8H_{1,1,3}^- - 8H_{1,2,2}^- - 4L_0H_{2,1,1}^- + 8H_{2,2,1}^- + 8H_{3,1,1}^-) + \\
& G_4^+ (3L_0H_3^- - 12H_4^- + 3L_0H_{1,2}^- - 12H_{1,3}^- + 6L_0H_{2,1}^- - 12H_{2,2}^- - 12H_{3,1}^- + 6L_0H_{1,1,1}^- \\
& - 12H_{1,1,2}^- - 12H_{1,2,1}^-) + G_{3,1}^+ (2L_{3,0} + 4L_{3,1} - 8\zeta_3H_1^- + 2L_0H_3^- - 4L_1H_3^- - 8H_4^- \\
& + 4L_0H_{1,2}^- - 8H_{1,3}^- + 4L_0H_{2,1}^- - 8H_{2,2}^- - 8H_{1,1,2}^- + 8H_{2,1,1}^-) + G_{2,2}^+ (L_4 + L_{3,0} + 4L_{3,1} \\
& - 16\zeta_3H_1^- - 4L_1H_3^- + 4H_{1,3}^- + 4H_{2,2}^- + 8H_{3,1}^- - 4L_0H_{1,1,1}^- + 8H_{1,2,1}^- + 8H_{2,1,1}^-) + \\
& G_{2,1,1}^+ (-2L_4 + 2L_{3,0} + 16\zeta_3H_1^- + 4L_0H_{1,2}^- - 8H_{1,3}^- - 8H_{2,2}^-) + \\
& G_5^+ (-4H_3^- - 4H_{1,2}^- - 8H_{2,1}^- - 8H_{1,1,1}^-) + G_{4,1}^+ (-6\bar{L}_{2,1} + 3L_0H_2^- + 6L_1H_2^- - 12H_3^- \\
& - 12H_{1,2}^- - 12H_{2,1}^-) + G_{3,2}^+ (-2\bar{L}_3 - 8\bar{L}_{2,1} + 2L_0H_2^- + 8L_1H_2^- - 4H_3^- - 8H_{1,2}^- \\
& - 8H_{2,1}^- + 8H_{1,1,1}^-) + G_{3,1,1}^+ (4\bar{L}_3 + 4L_0H_2^- - 16H_3^- - 8H_{1,2}^-) + G_{2,3}^+ (-4\bar{L}_3 - 8\bar{L}_{2,1} \\
& + 2L_0H_2^- + 8L_1H_2^- - 4H_{1,2}^- - 8H_{2,1}^- + 8H_{1,1,1}^-) + G_{2,2,1}^+ (4\bar{L}_3 - 8H_3^- - 8H_{1,2}^-) + \\
& G_{2,1,2}^+ (4\bar{L}_3 + 4\bar{L}_{2,1} - 4L_1H_2^- - 4H_3^- + 8H_{2,1}^-) + G_{2,1,1,1}^+ (4L_0H_2^- - 8H_3^-) + \\
& (10G_{2,4}^+ + 8G_{3,3}^+ + 3G_{4,2}^+ - 8G_{2,1,3}^+ - 8G_{2,2,2}^+ - 4G_{2,3,1}^+ - 8G_{3,1,2}^+ - 8G_{3,2,1}^+ - 6G_{4,1,1}^+ \\
& + 4G_{2,1,1,2}^+ - 4G_{2,2,1,1}^+)L_2 + (-16G_{2,4}^+ - 12G_{3,3}^+ - 6G_{4,2}^+ - 4G_{5,1}^+ + 12G_{2,1,3}^+
\end{aligned}$$

$$\begin{aligned}
 & +12G_{2,2,2}^+ + 8G_{2,3,1}^+ + 8G_{3,1,2}^+ + 8G_{3,2,1}^+ - 8G_{2,1,1,2}^+ - 8G_{2,1,2,1}^+ - 8G_{3,1,1,1}^+)H_2^- + \\
 & (-16G_{2,4}^+ - 16G_{3,3}^+ - 12G_{4,2}^+ - 8G_{5,1}^+ + 8G_{2,1,3}^+ + 8G_{2,2,2}^+ + 8G_{3,1,2}^+)H_{1,1}^- + \\
 & (20G_{2,5}^+ + 20G_{3,4}^+ + 12G_{4,3}^+ + 4G_{5,2}^+ - 16G_{2,1,4}^+ - 12G_{2,2,3}^+ - 12G_{2,3,2}^+ - 16G_{3,1,3}^+ \\
 & - 16G_{3,2,2}^+ - 8G_{3,3,1}^+ - 12G_{4,1,2}^+ - 12G_{4,2,1}^+ - 8G_{5,1,1}^+ + 8G_{2,1,1,3}^+ + 8G_{2,1,2,2}^+ - 8G_{2,2,2,1}^+ \\
 & - 8G_{2,3,1,1}^+ + 8G_{3,1,1,2}^+ - 8G_{3,2,1,1}^+)H_1^- + \\
 & G_{2,1}^- (2L_{3,2} - L_{4,0} - 2L_{4,1} + L_{3,0,0} + 2L_{3,1,0} - 12\bar{L}_2\zeta_3 + 8\zeta_3H_2^+ - 4\bar{L}_2H_3^+ \\
 & + 8L_1H_4^+ - 16\zeta_3H_{1,1}^+ - 4H_{2,3}^+ + 4L_0H_{3,1}^+ - 4H_{3,2}^+ - 16H_{4,1}^+ - 4L_0H_{1,1,2}^+ + 8H_{1,1,3}^+ \\
 & + 8H_{1,2,2}^+ + 4L_0H_{2,1,1}^+ - 8H_{2,2,1}^+ - 8H_{3,1,1}^+) + \\
 & G_{3,1}^- (2\bar{L}_{3,0} + 4\bar{L}_{3,1} + 4L_1\zeta_3 - 6L_0H_3^+ - 4L_1H_3^+ + 20H_4^+ - 4L_0H_{1,2}^+ + 16H_{1,3}^+ \\
 & - 4L_0H_{2,1}^+ + 16H_{2,2}^+ + 8H_{3,1}^+ + 8H_{1,1,2}^+ - 8H_{2,1,1}^+) + G_{2,2}^- (\bar{L}_4 + \bar{L}_{3,0} + 4\bar{L}_{3,1} + 8L_1\zeta_3 \\
 & - 2L_0H_3^+ - 4L_1H_3^+ + 4H_4^+ + 4H_{1,3}^+ + 4H_{2,2}^+ + 4L_0H_{1,1,1}^+ - 8H_{1,2,1}^+ - 8H_{2,1,1}^+) + \\
 & G_{2,1,1}^- (-2\bar{L}_4 + 2\bar{L}_{3,0} - 8L_1\zeta_3 - 4L_0H_3^+ + 16H_4^+ - 4L_0H_{1,2}^+ + 8H_{1,3}^+ + 8H_{2,2}^+) + \\
 & G_{4,1}^- (-3L_{2,0} - 6L_{2,1} + 3L_0H_2^+ + 6L_1H_2^+) + G_{3,2}^- (-2L_3 - 2L_{2,0} - 8L_{2,1} + \\
 & 2L_0H_2^+ + 8L_1H_2^+ - 8H_{1,2}^+ - 8H_{2,1}^+ - 8H_{1,1,1}^+) + G_{3,1,1}^- (4L_3 - 2L_{2,0} + 8H_{1,2}^+) + \\
 & G_{2,3}^- (-4L_3 - 2L_{2,0} - 8L_{2,1} - L_{0,0,0} - 8\zeta_3 + 2L_0H_2^+ + 8L_1H_2^+ - 12H_{1,2}^+ \\
 & - 8H_{2,1}^+ - 8H_{1,1,1}^+) + G_{2,2,1}^- (4L_3 + 2L_{0,0,0} + 16\zeta_3 + 8H_{1,2}^+) + G_{2,1,2}^- (4L_3 + L_{2,0} \\
 & + 4L_{2,1} + L_{0,0,0} + 8\zeta_3 - 2L_0H_2^+ - 4L_1H_2^+ + 8H_{1,2}^+) + G_{2,1,1,1}^- (-2L_{2,0} - 2L_{0,0,0} - 16\zeta_3) + \\
 & G_{5,1}^- (4H_2^+ + 8H_{1,1}^+) + G_{4,2}^- (3\bar{L}_2 + 12H_{1,1}^+) + G_{4,1,1}^- (-6\bar{L}_2 + 12H_2^+) + G_{3,3}^- (8\bar{L}_2 + 2\bar{L}_{0,0} \\
 & - 4H_2^+ + 16H_{1,1}^+) + G_{3,2,1}^- (-8\bar{L}_2 - 4\bar{L}_{0,0} + 8H_2^+) + G_{3,1,2}^- (-8\bar{L}_2 - 2\bar{L}_{0,0} + 8H_2^+ \\
 & - 8H_{1,1}^+) + G_{3,1,1,1}^- (4\bar{L}_{0,0} + 8H_2^+) + G_{2,4}^- (10\bar{L}_2 + 4\bar{L}_{0,0} - 4H_2^+ + 16H_{1,1}^+) + \\
 & G_{2,3,1}^- (-4\bar{L}_2 - 4\bar{L}_{0,0}) + G_{2,2,2}^- (-8\bar{L}_2 - 4\bar{L}_{0,0} + 4H_2^+ - 8H_{1,1}^+) + G_{2,2,1,1}^- (-4\bar{L}_2 + 8H_2^+) + \\
 & G_{2,1,3}^- (-8\bar{L}_2 - 4\bar{L}_{0,0} + 4H_2^+ - 8H_{1,1}^+) + G_{2,1,2,1}^- (4\bar{L}_{0,0} + 8H_2^+) + G_{2,1,1,2}^- (4\bar{L}_2 + 4\bar{L}_{0,0}) + \\
 & (-10G_{2,5}^- - 8G_{3,4}^- - 3G_{4,3}^- + 10G_{2,1,4}^- + 8G_{2,2,3}^- + 8G_{2,3,2}^- + 4G_{2,4,1}^- + 8G_{3,1,3}^- \\
 & + 8G_{3,2,2}^- + 8G_{3,3,1}^- + 3G_{4,1,2}^- + 6G_{4,2,1}^- - 8G_{2,1,1,3}^- - 8G_{2,1,2,2}^- - 4G_{2,1,3,1}^- - 4G_{2,2,1,2}^-)
 \end{aligned}$$

$$\begin{aligned}
& +4G_{\hat{2},3,1,1}^- - 8G_{\hat{3},1,1,2}^- - 8G_{\hat{3},1,2,1}^- - 6G_{\hat{4},1,1,1}^- + 4G_{\hat{2},1,1,1,2}^- - 4G_{\hat{2},1,2,1,1}^-) L_0 + \\
& (-10G_{\hat{2},5}^- - 10G_{\hat{3},4}^- - 6G_{\hat{4},3}^- - 2G_{\hat{5},2}^- + 8G_{\hat{2},1,4}^- + 6G_{\hat{2},2,3}^- + 6G_{\hat{2},3,2}^- + 8G_{\hat{3},1,3}^- \\
& + 8G_{\hat{3},2,2}^- + 4G_{\hat{3},3,1}^- + 6G_{\hat{4},1,2}^- + 6G_{\hat{4},2,1}^- + 4G_{\hat{5},1,1}^- - 4G_{\hat{2},1,1,3}^- - 4G_{\hat{2},1,2,2}^- + 4G_{\hat{2},2,2,1}^- \\
& + 4G_{\hat{2},3,1,1}^- - 4G_{\hat{3},1,1,2}^- + 4G_{\hat{3},2,1,1}^-) L_1 + \\
& 20G_{\hat{2},6}^- + 20G_{\hat{3},5}^- + 12G_{\hat{4},4}^- + 4G_{\hat{5},3}^- - 20G_{\hat{2},1,5}^- - 16G_{\hat{2},2,4}^- - 12G_{\hat{2},3,3}^- - 12G_{\hat{2},4,2}^- \\
& - 20G_{\hat{3},1,4}^- - 16G_{\hat{3},2,3}^- - 16G_{\hat{3},3,2}^- - 8G_{\hat{3},4,1}^- - 12G_{\hat{4},1,3}^- - 12G_{\hat{4},2,2}^- - 12G_{\hat{4},3,1}^- - 4G_{\hat{5},1,2}^- \\
& - 8G_{\hat{5},2,1}^- + 16G_{\hat{2},1,1,4}^- + 12G_{\hat{2},1,2,3}^- + 12G_{\hat{2},1,3,2}^- + 8G_{\hat{2},2,1,3}^- + 8G_{\hat{2},2,2,2}^- - 8G_{\hat{2},3,2,1}^- - 8G_{\hat{2},4,1,1}^- \\
& + 16G_{\hat{3},1,1,3}^- + 16G_{\hat{3},1,2,2}^- + 8G_{\hat{3},1,3,1}^- + 8G_{\hat{3},2,1,2}^- - 8G_{\hat{3},3,1,1}^- + 12G_{\hat{4},1,1,2}^- + 12G_{\hat{4},1,2,1}^- + 8G_{\hat{5},1,1,1}^- \\
& - 8G_{\hat{2},1,1,1,3}^- - 8G_{\hat{2},1,1,2,2}^- + 8G_{\hat{2},1,2,2,1}^- + 8G_{\hat{2},1,3,1,1}^- - 8G_{\hat{3},1,1,1,2}^- + 8G_{\hat{3},1,2,1,1}^-
\end{aligned}$$

3.7.5 Numerical consistency tests for $I^{(4)}$

In order to check the correctness of the result from the previous section, we evaluated $I^{(4)}$ numerically and compared it to a direct numerical evaluation of the coordinate space integral using FIESTA. In detail, we evaluate the conformally-invariant function $f(u, v) = x_{13}^2 x_{24}^2 I^{(4)}(x_1, x_2, x_3, x_4)$ by first applying a conformal transformation to send x_4 to infinity, the integral takes the simplified form,

$$\lim_{x_4 \rightarrow \infty} x_{13}^2 x_{24}^2 I_{14;23}^{(4)} = \frac{1}{\pi^8} \int \frac{d^4 x_5 d^4 x_6 d^4 x_7 d^4 x_8 x_{13}^2}{x_{15}^2 x_{18}^2 x_{25}^2 x_{26}^2 x_{37}^2 x_{38}^2 x_{56}^2 x_{67}^2 x_{78}^2}, \quad (3.7.56)$$

and then using the remaining freedom to fix $x_{13}^2 = 1$ so that $u = x_{12}^2$ and $v = x_{23}^2$. In comparison with the two 3-loop integrals, the extra loop in this case yields a moderately more cumbersome numerical evaluation. As such, we modify the setup for the 3-loop examples slightly and only perform 5×10^5 integral evaluations. We nevertheless obtain about 5 digits of precision, and excellent agreement with the analytic function at 40 different points. See Table 3.4 for an illustrative sample of points.

u	v	Analytic	FIESTA	δ
0.1	0.2	156.733	156.733	4.9e-7
0.2	0.3	116.962	116.962	5.9e-8
0.3	0.1	110.366	110.366	2.8e-7
0.4	0.5	84.2632	84.2632	1.4e-7
0.5	0.6	75.2575	75.2575	1.4e-7
0.6	0.2	78.3720	78.3720	3.7e-8
0.7	0.3	70.7417	70.7417	6.8e-8
0.8	0.9	58.6362	58.6363	1.4e-7
0.9	0.5	60.1295	60.1295	1.1e-7

Table 3.4: Numerical comparison of the analytic result for $x_{13}^2 x_{24}^2 I^{(4)}(x_1, x_2, x_3, x_4)$ against FIESTA for several values of the conformal cross ratios.

3.8 Conclusions

Recent years have seen a lot of advances in the analytic computation of Feynman integrals contributing to the perturbative expansion of physical observables. In particular, a more solid understanding of the mathematics underlying the leading singularities and the classes of functions that appear at low loop orders have opened up new ways of evaluating multi-scale multi-loop Feynman integrals analytically.

In this paper we applied some of these new mathematical techniques to the computation of the two so far unknown integrals appearing in the three-loop four-point stress-tensor correlator in $\mathcal{N} = 4$ SYM, and even a first integral occurring in the planar four-loop contribution to the same function. The computation was made possible by postulating that these integrals can be written as a sum over all the leading singularities (defined as the residues at the global poles of the loop integrand), each leading singularity being multiplied by a pure transcendental function that can be written as a \mathbb{Q} -linear combination of single-valued multiple polylogarithms in one complex variable. After a suitable choice was made for the entries that can appear in the symbols of these functions, the coefficients can easily be fixed by matching to some asymptotic expansions of the integrals in the limit where one of the cross

ratios vanishes. In all cases we were able to integrate the symbols obtained from this procedure to a unique polylogarithmic function, thus completing the analytic computation of the the three-loop four-point stress-tensor correlator in $\mathcal{N} = 4$ SYM. While for the Easy integral the space of polylogarithmic function is completely classified in the mathematical literature, new classes of multiple polylogarithms appear in the analytic results for the Hard integral and the four-loop integral we considered.

One might wonder, given that the Hard integral function $H^{(a)}$ involves genuine two-variable functions, whether there could have been a similar contribution to the Easy integral, compatible with all asymptotic limits. Indeed there does exist a symbol of a single-valued function, not expressible in terms of SVHPLs alone, which evades all constraints from the asymptotic limits. In other words the function is power suppressed in all limits, possibly up to terms proportional to zeta values. However, the evidence we have presented (in particular the numerical checks) strongly suggests that such a contribution is absent and therefore the Easy integral is expressible in terms of SVHPLs only.

We emphasize that the techniques we used for the computation are not limited to the rather special setting of the $\mathcal{N} = 4$ model. First, by sending a point to infinity a conformal four-point integral becomes a near generic three-point integral. Such integrals appear as master integrals for phenomenologically relevant processes, like for example the quantum corrections to the decay of a heavy particle into two massive particles. Second, the conformal integrals we calculated have the structure $\sum R_i F_i$ (so residue times pure function) that is also observed for integrals contributing to on-shell amplitudes. However, we believe that this is in fact a common feature of large classes of Feynman integrals (if not all) and one purpose of this work is to advocate our combination of techniques as a means of solving many other diagrams.

Further increasing the loop-order or the number of points might eventually hamper our prospects of success. Indeed, beyond problems of merely combinatorial nature there are also more fundamental issues, for example to what extent multiple polylogarithms exhaust the function spaces. It is anticipated in ref. [132, 133] that elliptic integrals will eventually appear in higher-point on-shell amplitudes. Via the correlator/amplitude duality this observation will eventually carry over to our setting.

Nevertheless, some papers [133, 134] also hint at a more direct albeit related way of evaluating loop-integrals by casting them into a ‘ $d\log$ -form’, which should have a counterpart for off-shell correlators.

Part II

Functions of three variables

Chapter 4

Hexagon functions and the three-loop remainder function

4.1 Introduction

For roughly half a century we have known that many physical properties of scattering amplitudes in quantum field theories are encoded in different kinds of analytic behavior in various regions of the kinematical phase space. The idea that the amplitudes of a theory can be reconstructed (or ‘bootstrapped’) from basic physical principles such as unitarity, by exploiting the link to the analytic behavior, became known as the “Analytic S -Matrix program” (see *e.g.* ref. [135]). In the narrow resonance approximation, crossing symmetry duality led to the Veneziano formula [136] for tree-level scattering amplitudes in string theory.

In conformal field theories, there exists a different kind of bootstrap program, whereby correlation functions can be determined by imposing consistency with the operator product expansion (OPE), crossing symmetry, and unitarity [137, 138]. This program was most successful in two-dimensional conformal field theories, for which conformal symmetry actually extends to an infinite-dimensional Virasoro symmetry [139]. However, the basic idea can be applied in any dimension and recent progress has been made in applying the program to conformal field theories in three and four dimensions [140–142].

In recent years, the scattering amplitudes of the planar $\mathcal{N} = 4$ super-Yang-Mills theory have been seen to exhibit remarkable properties. In particular, the amplitudes exhibit dual conformal symmetry and a duality to light-like polygonal Wilson loops [21, 22, 24, 25, 143]. The dual description and its associated conformal symmetry mean that CFT techniques can be applied to calculating scattering amplitudes. In particular, the idea of imposing consistency with the OPE applies. However, since the dual observables are non-local Wilson loop operators, a different OPE, involving the near-collinear limit of two sides of the light-like polygon, has to be employed [38–40, 144].

Dual conformal symmetry implies that the amplitudes involving four or five particles are fixed, because there are no invariant cross ratios that can be formed from a five-sided light-like polygon [3, 26, 83]. The four- and five-point amplitudes are governed by the BDS ansatz [32]. The amplitudes not determined by dual conformal symmetry begin at six points. When the external gluons are in the maximally-helicity-violating (MHV) configuration, such amplitudes can be expressed in terms of the BDS ansatz, which contains all of the infrared divergences and transforms anomalously under dual conformal invariance, and a so-called “remainder function” [1, 2], which only depends on dual-conformally-invariant cross ratios. In the case of non-MHV amplitudes, one can define the “ratio function” [27], which depends on the cross ratios as well as dual superconformal invariants. For six external gluons, the remainder and ratio functions are described in terms of functions of three dual conformal cross ratios.

At low orders in perturbation theory, these latter functions can be expressed in terms of multiple polylogarithms. In general, multiple polylogarithms are functions of many variables that can be defined as iterated integrals over rational kernels. A particularly useful feature of such functions is that they can be classified according to their symbols [145–147], elements of the n -fold tensor product of the algebra of rational functions. The integer n is referred to as the transcendental weight or degree. The symbol can be defined iteratively in terms of the total derivative of the function, or alternatively, in terms of the maximally iterated coproduct by using the Hopf structure conjecturally satisfied by multiple polylogarithms [63, 148]. Complicated

functional identities among polylogarithms become simple algebraic relations satisfied by their symbols, making the symbol a very useful tool in the study of polylogarithmic functions. The symbol can miss terms in the function that are proportional to transcendental constants (which in the present case are all multiple zeta values), so special care must be given to account for these terms. The symbol and coproduct have been particularly useful in recent field theory applications [14, 36, 40, 64, 71]. In the case of $\mathcal{N} = 4$ super-Yang-Mills theory, all amplitudes computed to date have exhibited a uniform maximal transcendentality, in which the finite terms (such as the remainder or ratio functions) always have weight $n = 2L$ at the L loop order in perturbation theory.

Based on the simplified form of the two-loop six-point remainder function obtained in ref. [36] (which was first constructed analytically in terms of multiple polylogarithms [6, 7]), it was conjectured [14, 71] that for multi-loop six-point amplitudes, both the MHV remainder function and the next-to-MHV (NMHV) ratio function are described in terms of polylogarithmic functions whose symbols are made from an alphabet of nine letters. The nine letters are related to the nine projectively-inequivalent differences z_{ij} of projective variables z_i [36], which can also be represented in terms of momentum twistors [149]. Using this conjecture, the symbol for the three-loop six-point remainder function was obtained up to two undetermined parameters [14], which were later fixed [45] using a dual supersymmetry “anomaly” equation [44, 45]. The idea of ref. [14] was to start with an ansatz for the symbol, based on the above nine-letter conjecture, and then impose various mathematical and physical consistency conditions. For example, imposing a simple integrability condition [146, 147] guarantees that the ansatz is actually the symbol of some function, and demanding that the amplitude has physical branch cuts leads to a condition on the initial entries of the symbol.

Because of the duality between scattering amplitudes and Wilson loops, one can also impose conditions on the amplitude that are more naturally expressed in terms of the Wilson loop, such as those based on the OPE satisfied by its near-collinear limit. In refs. [38–40, 144], the leading-discontinuity terms in the OPE were computed. In

terms of the cross ratio variable that vanishes in the near-collinear limit, the leading-discontinuity terms correspond to just the maximum powers of logarithms of this variable ($L - 1$ at L loops), although they can be arbitrarily power suppressed. These terms require only the one-loop anomalous dimensions of the operators corresponding to excitations of the Wilson line, or flux tube. That is, higher-loop corrections to the anomalous dimensions and to the OPE coefficients can only generate subleading logarithmic terms. While the leading-discontinuity information is sufficient to determine all terms in the symbol at two loops, more information is necessary starting at three loops [14].

Very recently, a new approach to polygonal Wilson loops has been set forth [150, 151], which is fully nonperturbative and based on integrability. The Wilson loop is partitioned into a number of “pentagon transitions”, which are labeled by flux tube excitation states on either side of the transition. (If one edge of the pentagon coincides with an edge of the Wilson loop, then the corresponding state is the flux tube vacuum.) The pentagon transitions obey a set of bootstrap consistency conditions. Remarkably, they can be solved in terms of factorizable S matrices for two-dimensional scattering of the flux tube excitations [150, 151].

In principle, the pentagon transitions can be solved for arbitrary excitations, but it is simplest to first work out the low-lying excitations, which correspond to the leading power-suppressed terms in the near-collinear limit in the six-point case (and similar terms in multi-near-collinear limits for more than six particles). Compared with the earlier leading-discontinuity data, now *all* terms at a given power-suppressed order can be determined (to all loop orders), not just the leading logarithms. This information is very powerful. The first power-suppressed order in the six-point near-collinear limit is enough to fix the two terms in the ansatz for the symbol of the three-loop remainder function that could not be fixed using the leading discontinuity [150]. At four loops, the first power-suppressed order [150] and part of the second power-suppressed order [152] are sufficient to fix all terms in the symbol [153]. At these orders, the symbol becomes heavily over-constrained, providing strong cross checks on the assumptions about the letters of the symbol, as well as on the solutions to the pentagon transition bootstrap equations.

In short, the application of integrability to the pentagon-transition decomposition of Wilson loops provides, through the OPE, all-loop-order boundary-value information for the problem of determining Wilson loops (or scattering amplitudes) at generic nonzero (interior) values of the cross ratios. We will use this information in the six-point case to uniquely determine the three-loop remainder function, not just at symbol level, but at function level as well.

A second limit we study is the limit of multi-Regge kinematics (MRK), which has provided another important guide to the perturbative structure of the six-point remainder function [5, 8–10, 12–15], as well as higher-point remainder functions [16, 17] and NMHV amplitudes [18]. The six-point remainder function and, more generally, the hexagon functions that we define shortly have simple behavior in the multi-Regge limit. These functions depend on three dual-conformally-invariant cross ratios, but in the multi-Regge limit they collapse [19] into single-valued harmonic polylogarithms [47], which are functions of two surviving real variables, or of a complex variable and its conjugate. The multi-Regge limit factorizes [15] after taking the Fourier-Mellin transform of this complex variable. This factorization imposes strong constraints on the remainder function at high loop order [15, 19, 154].

Conversely, determining the multi-loop remainder function, or just its multi-Regge limit, allows the perturbative extraction of the two functions that enter the factorized form of the amplitude, the BFKL eigenvalue (in the adjoint representation) and a corresponding impact factor. This approach makes use of a map between the single-valued harmonic polylogarithms and their Fourier-Mellin transforms, which can be constructed from harmonic sums [19]. Using the three- and four-loop remainder-function symbols, the BFKL eigenvalue has been determined to next-to-next-to-leading-logarithmic accuracy (NNLLA), and the impact factor at NNLLA and N³LLA [19]. However, the coefficients of certain transcendental constants in these three quantities could not be fixed, due to the limitation of the symbol. Here we will use the MRK limit at three loops to fix the three undetermined constants in the NNLLA impact factor. Once the four-loop remainder function is determined, a similar analysis will fix the undetermined constants in the NNLLA BFKL eigenvalue and in the N³LLA impact factor.

In general, polylogarithmic functions are not sufficient to describe scattering amplitudes. For example, an elliptic integral, in which the kernel is not rational but contains a square root, enters the two-loop equal-mass sunrise graph [155], and it has been shown that a very similar type of integral enters a particular $N^3\text{MHV}$ 10-point scattering amplitude in planar $\mathcal{N} = 4$ super-Yang-Mills theory [132]. However, it has been argued [133], based on a novel form of the planar loop integrand, that MHV and NMHV amplitudes can all be described in terms of multiple polylogarithms alone. Similar “ $d\log$ ” representations have appeared in a recent twistor-space formulation [134, 156]. Because six-particle amplitudes are either MHV (or the parity conjugate $\overline{\text{MHV}}$) or NMHV, we expect that multiple polylogarithms and their associated symbols should suffice in this case. The nine letters that we assume for the symbol then follow naturally from the fact that the kinematics can be described in terms of dual conformally invariant combinations of six momentum twistors [149].

Having the symbol of an amplitude is not the same thing as having the function. In order to reconstruct the function one first needs a representative, well-defined function in the class of multiple polylogarithms which has the correct symbol. Before enough physical constraints are imposed, there will generally be multiple functions matching the symbol, because of the symbol-level ambiguity associated with transcendental constants multiplying well-defined functions of lower weight. Here we will develop techniques for building up the relevant class of functions for hexagon kinematics, which we call *hexagon functions*, whose symbols are as described above, but which are well-defined and have the proper branch cuts at the function level as well. We will argue that the hexagon functions form the basis for a perturbative solution to the MHV and NMHV six-point problem.

We will pursue two complementary routes toward the construction of hexagon functions. The first route is to express them explicitly in terms of multiple polylogarithms. This route has the advantage of being completely explicit in terms of functions with well-known mathematical properties, which can be evaluated numerically quite quickly, or expanded analytically in various regions. However, it also has the disadvantages that the representations are rather lengthy, and they are specific to particular regions of the full space of cross ratios.

The second route we pursue is to define each weight- n hexagon function iteratively in the weight, using the three first-order differential equations they satisfy. This information can also be codified by the $\{n-1, 1\}$ component of the coproduct of the function, whose elements contain weight- $(n-1)$ hexagon functions (the source terms for the differential equations). The differential equations can be integrated numerically along specific contours in the space of cross ratios. In some cases, they can be integrated analytically, at least up to the determination of certain integration constants.

We can carry out numerical comparisons of the two approaches in regions of overlapping validity. We have also been able to determine the near-collinear and multi-Regge limits of the functions analytically using both routes. As mentioned above, these limits are how we fix all undetermined constants in the function-level ansatz, and how we extract additional predictions for both regimes.

We have performed a complete classification of hexagon functions through weight five. Although the three-loop remainder function is a hexagon function of weight six, its construction is possible given the weight-five basis. There are other potential applications of our classification, beyond the three-loop remainder function. One example is the three-loop six-point NMHV ratio function, whose components are expected [71] to be hexagon functions of weight six. Therefore, it should be possible to construct the ratio function in an identical fashion to the remainder function.

Once we have fixed all undetermined constants in the three-loop remainder function, we can study its behavior in various regions, and compare it with the two-loop function. On several lines passing through the space of cross ratios, the remainder function collapses to simple combinations of harmonic polylogarithms of a single variable. Remarkably, over vast swathes of the space of positive cross ratios, the two- and three-loop remainder functions are strikingly similar, up to an overall constant rescaling. This similarity is in spite of the fact that they have quite different analytic behavior along various edges of this region. We can also compare the perturbative remainder function with the result for strong coupling, computed using the AdS/CFT correspondence, along the line where all three cross ratios are equal [157]. We find

that the two-loop, three-loop and strong-coupling results all have a remarkably similar shape when the common cross ratio is less than unity. Although we have not attempted any kind of interpolation formula from weak to strong coupling, it seems likely from the comparison that the nature of the interpolation will depend very weakly on the common cross ratio in this region.

The remainder of this paper is organized as follows. In section 4.2 we recall some properties of pure functions (iterated integrals) and their symbols, as well as a representation of the two-loop remainder function (and its symbol) in terms of an “extra pure” function and its cyclic images. We use this representation as motivation for an analogous decomposition of the three-loop symbol. In section 4.3 we describe the first route to constructing hexagon functions, via multiple polylogarithms. In section 4.4 we describe the second route to constructing the same set of functions, via the differential equations they satisfy. In section 4.5 we discuss how to extract the near-collinear limits, and give results for some of the basis functions and for the remainder function in this limit. In section 4.6 we carry out the analogous discussion for the Minkowski multi-Regge limit. In section 4.7 we give the final result for the three-loop remainder function, in terms of a specific integral, as well as defining it through the $\{5, 1\}$ components of its coproduct. We also present the specialization of the remainder function onto various lines in the three-dimensional space of cross ratios; along these lines its form simplifies dramatically. Finally, we plot the function on several lines and two-dimensional slices. We compare it numerically to the two-loop function in some of these regions, and to the strong-coupling result evaluated for equal cross ratios. In section 4.8 we present our conclusions and outline avenues for future research. We include three appendices. Appendix C.1 provides some background material on multiple polylogarithms. Appendix C.2 gives the complete set of independent hexagon functions through weight five in terms of the $\{n - 1, 1\}$ components of their coproducts, and in appendix C.3 we provide the same description of the extra pure weight six function R_{ep} entering the remainder function.

In attached, computer-readable files we give the basis of hexagon functions through

weight five, as well as the three-loop remainder function, expressed in terms of multiple polylogarithms in two different kinematic regions. We also provide the near-collinear and multi-Regge limits of these functions.

4.2 Extra-pure functions and the symbol of $R_6^{(3)}$

In this section, we describe the symbol of the three-loop remainder function as obtained in ref. [14], which is the starting point for our reconstruction of the full function. Motivated by an alternate representation [71] of the two-loop remainder function, we will rearrange the three-loop symbol. In the new representation, part of the answer will involve products of lower-weight (hence simpler) functions, and the rest of the answer will be expressible as the sum of an *extra-pure* function, called R_{ep} , plus its two images under cyclic permutations of the cross ratios. An extra-pure function of m variables, by definition, has a symbol with only m different final entries. For the case of hexagon kinematics, where there are three cross ratios, the symbol of an extra-pure function has only three final entries, instead of the potential nine. Related to this, the three derivatives of the full function can be written in a particularly simple form, which helps somewhat in its construction.

All the functions we consider in this paper will be *pure functions*. The definition of a pure function $f^{(n)}$ of transcendental weight (or degree) n is that its first derivative obeys,

$$df^{(n)} = \sum_r f_r^{(n-1)} d \ln \phi_r, \quad (4.2.1)$$

where ϕ_r are rational functions and the sum over r is finite. The only weight-zero functions are assumed to be rational constants. The $f_r^{(n-1)}$ and ϕ_r are not all independent of each other because the integrability condition $d^2 f^{(n)} = 0$ imposes relations among them,

$$\sum_r df_r^{(n-1)} \wedge d \ln \phi_r = 0. \quad (4.2.2)$$

Functions defined by the above conditions are iterated integrals of polylogarithmic type. Such functions have a *symbol*, defined recursively as an element of the n -fold tensor product of the algebra of rational functions, following eq. (4.2.1),

$$\mathcal{S}(f^{(n)}) = \sum_r \mathcal{S}(f_r^{(n-1)}) \otimes \phi_r. \quad (4.2.3)$$

In the case of the six-particle amplitudes of planar $\mathcal{N} = 4$ super Yang-Mills theory,

we are interested in pure functions depending on the three dual conformally invariant cross ratios,

$$u_1 = u = \frac{x_{13}^2 x_{46}^2}{x_{14}^2 x_{36}^2}, \quad u_2 = v = \frac{x_{24}^2 x_{51}^2}{x_{25}^2 x_{41}^2}, \quad u_3 = w = \frac{x_{35}^2 x_{62}^2}{x_{36}^2 x_{52}^2}. \quad (4.2.4)$$

The six particle momenta k_i^μ are differences of the dual coordinates x_i^μ : $x_i^\mu - x_{i+1}^\mu = k_i^\mu$, with indices taken mod 6.

Having specified the class of functions we are interested in, we impose further [14, 71] that the entries of the symbol are drawn from the following set of nine letters,

$$\mathcal{S}_u = \{u, v, w, 1-u, 1-v, 1-w, y_u, y_v, y_w\}. \quad (4.2.5)$$

The nine letters are related to the nine projectively-inequivalent differences of six \mathbb{CP}^1 variables z_i [36] via

$$u = \frac{(12)(45)}{(14)(25)}, \quad 1-u = \frac{(24)(15)}{(14)(25)}, \quad y_u = \frac{(26)(13)(45)}{(46)(12)(35)}, \quad (4.2.6)$$

and relations obtained by cyclically rotating the six points. The variables y_u, y_v and y_w can be expressed locally in terms of the cross ratios,

$$y_u = \frac{u - z_+}{u - z_-}, \quad y_v = \frac{v - z_+}{z - z_-}, \quad y_w = \frac{w - z_+}{w - z_-}, \quad (4.2.7)$$

where

$$z_\pm = \frac{1}{2} \left[-1 + u + v + w \pm \sqrt{\Delta} \right], \quad \Delta = (1 - u - v - w)^2 - 4uvw. \quad (4.2.8)$$

Note that under the cyclic permutation $z_i \rightarrow z_{i+1}$ we have $u \rightarrow v \rightarrow w \rightarrow u$, while the y_i variables transform as $y_u \rightarrow 1/y_v \rightarrow y_w \rightarrow 1/y_u$. A three-fold cyclic rotation amounts to a space-time parity transformation, under which the parity-even cross ratios are invariant, while the parity-odd y variables invert. Consistent with the inversion of the y variables under parity, and eq. (4.2.7), the quantity Δ must flip

sign under parity, so we have altogether,

$$\text{Parity : } u_i \rightarrow u_i, \quad y_i \rightarrow \frac{1}{y_i}, \quad \sqrt{\Delta} \rightarrow -\sqrt{\Delta}. \quad (4.2.9)$$

The transformation of $\sqrt{\Delta}$ can also be seen from its representation in terms of the z_{ij} variables,

$$\sqrt{\Delta} = \frac{(12)(34)(56) - (23)(45)(61)}{(14)(25)(36)}, \quad (4.2.10)$$

upon letting $z_i \rightarrow z_{i+3}$. It will prove very useful to classify hexagon functions by their parity. The remainder function is a parity-even function, but some of its derivatives (or more precisely coproduct components) are parity-odd, so we need to understand both the even and odd sectors.

Since the y variables invert under parity, $y_u \rightarrow 1/y_u$, *etc.*, it is often better to think of the y variables as fundamental and the cross ratios as parity-even functions of them. The cross ratios can be expressed in terms of the y variables without any square roots,

$$\begin{aligned} u &= \frac{y_u(1-y_v)(1-y_w)}{(1-y_u y_v)(1-y_u y_w)}, & 1-u &= \frac{(1-y_u)(1-y_u y_v y_w)}{(1-y_u y_v)(1-y_u y_w)}, \\ v &= \frac{y_v(1-y_w)(1-y_u)}{(1-y_v y_w)(1-y_v y_u)}, & 1-v &= \frac{(1-y_v)(1-y_u y_v y_w)}{(1-y_v y_w)(1-y_u y_v)}, \\ w &= \frac{y_w(1-y_u)(1-y_v)}{(1-y_w y_u)(1-y_w y_v)}, & 1-w &= \frac{(1-y_w)(1-y_u y_v y_w)}{(1-y_u y_w)(1-y_v y_w)}, \\ \sqrt{\Delta} &= \frac{(1-y_u)(1-y_v)(1-y_w)(1-y_u y_v y_w)}{(1-y_u y_v)(1-y_v y_w)(1-y_w y_u)}, \end{aligned} \quad (4.2.11)$$

where we have picked a particular branch of $\sqrt{\Delta}$.

Following the strategy of ref. [14], we construct all integrable symbols of the required weight, using the letters (4.2.5), subject to certain additional physical constraints. In the case of the six-point MHV remainder function at L loops, we require a weight- $2L$ parity-even function with full S_3 permutation symmetry among the cross ratios. The initial entries in the symbol can only be the cross ratios themselves, in

order to have physical branch cuts [40]:

$$\text{first entry} \in \{u, v, w\} . \quad (4.2.12)$$

In addition we require that the final entries of the symbol are taken from the following restricted set of six letters [14, 46]:

$$\text{final entry} \in \left\{ \frac{u}{1-u}, \frac{v}{1-v}, \frac{w}{1-w}, y_u, y_v, y_w \right\} . \quad (4.2.13)$$

Next one can apply constraints from the collinear OPE of Wilson loops. The leading-discontinuity constraints [38–40] can be expressed in terms of differential operators with a simple action on the symbol [14]. At two loops, the leading (single) discontinuity is the only discontinuity, and it is sufficient to determine the full remainder function $R_6^{(2)}(u, v, w)$ [39]. At three loops, the constraint on the leading (double) discontinuity leaves two free parameters in the symbol, α_1 and α_2 [14]. These parameters were determined in refs. [45, 150], but we will leave them arbitrary here to see what other information can fix them.

The two-loop remainder function $R_6^{(2)}$ can be expressed simply in terms of classical polylogarithms [36]. However, here we wish to recall the form found in ref. [71] in terms of the infrared-finite double pentagon integral $\Omega^{(2)}$, which was introduced in ref. [79] and studied further in refs. [71, 158]:

$$R_6^{(2)}(u, v, w) = \frac{1}{4} \left[\Omega^{(2)}(u, v, w) + \Omega^{(2)}(v, w, u) + \Omega^{(2)}(w, u, v) \right] + R_{6,\text{rat}}^{(2)}(u, v, w) . \quad (4.2.14)$$

The function $R_{6,\text{rat}}^{(2)}$ can be expressed in terms of single-variable classical polylogarithms,

$$R_{6,\text{rat}}^{(2)} = -\frac{1}{2} \left[\frac{1}{4} \left(\text{Li}_2(1-1/u) + \text{Li}_2(1-1/v) + \text{Li}_2(1-1/w) \right)^2 + r(u) + r(v) + r(w) - \zeta_4 \right] , \quad (4.2.15)$$

with

$$r(u) = -\text{Li}_4(u) - \text{Li}_4(1-u) + \text{Li}_4(1-1/u) - \ln u \text{Li}_3(1-1/u) - \frac{1}{6} \ln^3 u \ln(1-u)$$

$$+ \frac{1}{4} \left(\text{Li}_2(1 - 1/u) \right)^2 + \frac{1}{12} \ln^4 u + \zeta_2 \left(\text{Li}_2(1 - u) + \ln^2 u \right) + \zeta_3 \ln u. \quad (4.2.16)$$

We see that $R_{6,\text{rat}}^{(2)}$ decomposes into a product of simpler, lower-weight functions $\text{Li}_2(1 - 1/u_i)$, plus the cyclic images of the function $r(u)$, whose symbol can be written as,

$$\mathcal{S}(r(u)) = -2 \, u \otimes \frac{u}{1-u} \otimes \frac{u}{1-u} \otimes \frac{u}{1-u} + \frac{1}{2} \, u \otimes \frac{u}{1-u} \otimes u \otimes \frac{u}{1-u}. \quad (4.2.17)$$

The symbol of $\Omega^{(2)}$ can be deduced [71] from the differential equations it satisfies [158, 159]. There are only three distinct final entries of the symbol of $\Omega^{(2)}(u, v, w)$, namely

$$\left\{ \frac{u}{1-u}, \frac{v}{1-v}, y_u y_v \right\}. \quad (4.2.18)$$

Note that three is the minimum possible number of distinct final entries we could hope for, since $\Omega^{(2)}$ is genuinely dependent on all three variables. As mentioned above, we define extra-pure functions, such as $\Omega^{(2)}$, to be those functions for which the number of final entries in the symbol equals the number of variables on which they depend. Another way to state the property (which also extends it from a property of symbols to a property of functions) is that p -variable pure functions f of weight n are extra-pure if there exist p independent commuting first-order differential operators \mathcal{O}_i , such that $\mathcal{O}_i f$ are themselves all pure of weight $(n - 1)$.

More explicitly, the symbol of $\Omega^{(2)}$ can be written as [71],

$$\mathcal{S}(\Omega^{(2)}(u, v, w)) = -\frac{1}{2} \left[\mathcal{S}(Q_\phi) \otimes \phi + \mathcal{S}(Q_r) \otimes r + \mathcal{S}(\tilde{\Phi}_6) \otimes y_u y_v \right], \quad (4.2.19)$$

where

$$\phi = \frac{uv}{(1-u)(1-v)}, \quad r = \frac{u(1-v)}{v(1-u)}. \quad (4.2.20)$$

The functions Q_ϕ and Q_r will be defined below. The function $\tilde{\Phi}_6$ is the weight-three, parity-odd one-loop six-dimensional hexagon function [159, 160], whose symbol is given by [159],

$$\mathcal{S}(\tilde{\Phi}_6) = -\mathcal{S}(\Omega^{(1)}(u, v, w)) \otimes y_w + \text{cyclic}, \quad (4.2.21)$$

where $\Omega^{(1)}$ is a finite, four-dimensional one-loop hexagon integral [79, 158],

$$\Omega^{(1)}(u, v, w) = \ln u \ln v + \text{Li}_2(1 - u) + \text{Li}_2(1 - v) + \text{Li}_2(1 - w) - 2\zeta_2. \quad (4.2.22)$$

Although we have written eq. (4.2.21) as an equation for the symbol of $\tilde{\Phi}_6$, secretly it contains more information, because we have written the symbol of a full function, $\Omega^{(1)}(u, v, w)$ in the first two slots. Later we will codify this extra information as corresponding to the $\{2, 1\}$ component of the coproduct of $\tilde{\Phi}_6$. Another way of saying it is that all three derivatives of the function $\tilde{\Phi}_6$, with respect to the logarithms of the y variables, are given by $-\Omega^{(1)}(u, v, w)$ or its permutations, including the ζ_2 term in eq. (4.2.22). Any other derivative can be obtained by the chain rule. For example, to get the derivative with respect to u , we just need,

$$\frac{\partial \ln y_u}{\partial u} = \frac{1 - u - v - w}{u\sqrt{\Delta}}, \quad \frac{\partial \ln y_v}{\partial u} = \frac{1 - u - v + w}{(1 - u)\sqrt{\Delta}}, \quad \frac{\partial \ln y_w}{\partial u} = \frac{1 - u + v - w}{(1 - u)\sqrt{\Delta}}, \quad (4.2.23)$$

which leads to the differential equation found in ref. [159],

$$\begin{aligned} \partial_u \tilde{\Phi}_6 = & -\frac{1 - u - v - w}{u\sqrt{\Delta}} \Omega^{(1)}(v, w, u) - \frac{1 - u - v + w}{(1 - u)\sqrt{\Delta}} \Omega^{(1)}(w, u, v) \\ & - \frac{1 - u + v - w}{(1 - u)\sqrt{\Delta}} \Omega^{(1)}(u, v, w). \end{aligned} \quad (4.2.24)$$

Hence $\tilde{\Phi}_6$ can be fully specified, up to a possible integration constant, by promoting the first two slots of its symbol to a function in an appropriate way. In fact, the ambiguity of adding a constant of integration is actually fixed in this case, by imposing the property that the function $\tilde{\Phi}_6$ is parity odd.

Note that for the solution to the differential equation (4.2.24) and its cyclic images to have physical branch cuts, the correct coefficients of the ζ_2 terms in eq. (4.2.22) are crucial. Changing the coefficients of these terms in any of the cyclic images of $\Omega^{(1)}$ would correspond to adding a logarithm of the y variables to $\tilde{\Phi}_6$, which would have branch cuts in unphysical regions.

The other weight-three symbols in eq. (4.2.19) can similarly be promoted to full

functions. To do this we employ the harmonic polylogarithms (HPLs) in one variable [48], $H_{\vec{w}}(u)$. In our case, the weight vector \vec{w} contains only 0's and 1's. If the weight vector is a string of n 0's, $\vec{w} = 0_n$, then we have $H_{0_n}(u) = \frac{1}{n!} \log^n u$. The remaining functions are defined recursively by

$$H_{0,\vec{w}}(u) = \int_0^u \frac{dt}{t} H_{\vec{w}}(t), \quad H_{1,\vec{w}}(u) = \int_0^u \frac{dt}{1-t} H_{\vec{w}}(t). \quad (4.2.25)$$

Such functions have symbols with only two letters, $\{u, 1-u\}$. We would like the point $u = 1$ to be a regular point for the HPLs. This can be enforced by choosing the argument to be $1-u$, and restricting to weight vectors whose last entry is 1. The symbol and HPL definitions have a reversed ordering, so to find an HPL with argument $1-u$ corresponding to a symbol in $\{u, 1-u\}$, one reverses the string, replaces $u \rightarrow 1$ and $1-u \rightarrow 0$, and multiplies by (-1) for each 1 in the weight vector. We also use a compressed notation where $(k-1)$ 0's followed by a 1 is replaced by k in the weight vector, and the argument $(1-u)$ is replaced by the superscript u . For example, ignoring ζ -value ambiguities we have,

$$\begin{aligned} u \otimes (1-u) &\rightarrow -H_{0,1}(1-u) \rightarrow -H_2^u, \\ u \otimes u \otimes (1-u) &\rightarrow H_{0,1,1}(1-u) \rightarrow H_{2,1}^u, \\ v \otimes (1-v) \otimes v \otimes (1-v) &\rightarrow H_{0,1,0,1}(1-v) \rightarrow H_{2,2}^v. \end{aligned} \quad (4.2.26)$$

The combination

$$H_2^u + \frac{1}{2} \ln^2 u = -\text{Li}_2(1 - 1/u) \quad (4.2.27)$$

occurs frequently, because it is the lowest-weight extra-pure function, with symbol $u \otimes u / (1-u)$.

In terms of HPLs, the functions corresponding to the weight-three, parity-even symbols appearing in eq. (4.2.19) are given by,

$$\begin{aligned} Q_\phi &= [-H_3^u - H_{2,1}^u - H_2^v \ln u - \frac{1}{2} \ln^2 u \ln v + (H_2^u - \zeta_2) \ln w + (u \leftrightarrow v)] \\ &\quad + 2H_{2,1}^w + H_2^w \ln w + \ln u \ln v \ln w, \\ Q_r &= [-H_3^u + H_{2,1}^u + (H_2^u + H_2^w - 2\zeta_2) \ln u + \frac{1}{2} \ln^2 u \ln v - (u \leftrightarrow v)]. \end{aligned} \quad (4.2.28)$$

Here we have added some ζ_2 terms with respect to ref. [71], in order to match the $\{3, 1\}$ component of the coproduct of $\Omega^{(2)}$ that we determine later.

Note that the simple form of the symbol of $R_{6,\text{rat}}^{(2)}$ in eq. (4.2.15) means that it can be absorbed into the three cyclic images of $\Omega^{(2)}(u, v, w)$ without ruining the extra-purity of the latter functions. Hence $R_6^{(2)}$ is the cyclic sum of an extra-pure function.

With the decomposition (4.2.14) in mind, we searched for an analogous decomposition of the symbol of the three-loop remainder function [14] into extra-pure components. In other words, we looked for a representation of $\mathcal{S}(R_6^{(3)})$ in terms a function whose symbol has the same final entries (4.2.18) as $\Omega^{(2)}(u, v, w)$, plus its cyclic rotations. After removing some products of lower-weight functions we find that this is indeed possible. Specifically, we find that,

$$\mathcal{S}(R_6^{(3)}) = \mathcal{S}(R_{\text{ep}}(u, v, w) + R_{\text{ep}}(v, w, u) + R_{\text{ep}}(w, u, v)) + \mathcal{S}(P_6(u, v, w)). \quad (4.2.29)$$

Here P_6 is the piece constructed from products of lower-weight functions,

$$\begin{aligned} P_6(u, v, w) = & -\frac{1}{4} \left[\Omega^{(2)}(u, v, w) \text{Li}_2(1 - 1/w) + \text{cyclic} \right] - \frac{1}{16} (\tilde{\Phi}_6)^2 \\ & + \frac{1}{4} \text{Li}_2(1 - 1/u) \text{Li}_2(1 - 1/v) \text{Li}_2(1 - 1/w). \end{aligned} \quad (4.2.30)$$

The function R_{ep} is very analogous to $\Omega^{(2)}$ in that it has the same $(u \leftrightarrow v)$ symmetry, and its symbol has the same final entries,

$$\begin{aligned} \mathcal{S}(R_{\text{ep}}(u, v, w)) = & \mathcal{S}(R_{\text{ep}}^u(u, v, w)) \otimes \frac{u}{1-u} + \mathcal{S}(R_{\text{ep}}^u(v, u, w)) \otimes \frac{v}{1-v} \\ & + \mathcal{S}(R_{\text{ep}}^{yu}(u, v, w)) \otimes y_u y_v. \end{aligned} \quad (4.2.31)$$

In the following we will describe a systematic construction of the function R_{ep} and hence the three-loop remainder function. As in the case just described for $\tilde{\Phi}_6$, and implicitly for $\Omega^{(2)}$, the construction will involve promoting the quantities $\mathcal{S}(R_{\text{ep}}^u)$ and $\mathcal{S}(R_{\text{ep}}^{yu})$ to full functions, with the aid of the coproduct formalism. In fact, we will perform a complete classification of all well-defined functions corresponding to symbols with nine letters and obeying the first entry condition (4.2.12) (but not the final entry

condition (4.2.13)), iteratively in the weight through weight five. Knowing all such pure functions at weight 5 will then enable us to promote the weight-five quantities $\mathcal{S}(R_{\text{ep}}^u)$ and $\mathcal{S}(R_{\text{ep}}^{yu})$ to well-defined functions, subject to ζ -valued ambiguities that we will fix using physical criteria.

4.3 Hexagon functions as multiple polylogarithms

The task of the next two sections is to build up an understanding of the space of hexagon functions, using two complementary routes. In this section, we follow the route of expressing the hexagon functions explicitly in terms of multiple polylogarithms. In the next section, we will take a slightly more abstract route of defining the functions solely through the differential equations they satisfy, which leads to relatively compact integral representations for them.

4.3.1 Symbols

Our first task is to classify all integrable symbols at weight n with entries drawn from the set \mathcal{S}_u in eq. (4.2.5) that also satisfy the first entry condition (4.2.12). We do not impose the final entry condition (4.2.13) because we need to construct quantities at intermediate weight, from which the final results will be obtained by further integration; their final entries correspond to intermediate entries of R_{ep} .

The integrability of a symbol may be imposed iteratively, first as a condition on the first $n - 1$ slots, and then as a separate condition on the $\{n - 1, n\}$ pair of slots, as in eq. (4.2.2). Therefore, if \mathcal{B}_{n-1} is the basis of integrable symbols at weight $n - 1$, then a minimal ansatz for the basis at weight n takes the form,

$$\{b \otimes x \mid b \in \mathcal{B}_{n-1}, x \in \mathcal{S}_u\}, \quad (4.3.1)$$

and \mathcal{B}_n can be obtained simply by enforcing integrability in the last two slots. This method for recycling lower-weight information will also guide us toward an iterative construction of full functions, which we perform in the remainder of this section.

Integrability and the first entry condition together require the second entry to be free of the y_i . Hence the maximum number of y entries that can appear in a term in the symbol is $n - 2$. In fact, the maximum number of y 's that appear in any term in the symbol defines a natural grading for the space of functions. In table 4.1, we use this grading to tabulate the number of irreducible functions (*i.e.* those functions that cannot be written as products of lower-weight functions) through weight six. The

majority of the functions at low weight contain no y entries.

The y entries couple together u, v, w . In their absence, the symbols with letters $\{u, v, w, 1 - u, 1 - v, 1 - w\}$ can be factorized, so that the irreducible ones just have the letters $\{u, 1 - u\}$, plus cyclic permutations of them. The corresponding functions are the ordinary HPLs in one variable [48] introduced in the previous section, $H_{\vec{w}}^u$, with weight vectors \vec{w} consisting only of 0's and 1's. These functions are not all independent, owing to the existence of shuffle identities [48]. On the other hand, we may exploit Radford's theorem [161] to solve these identities in terms of a Lyndon basis,

$$\mathcal{H}_u = \{H_{l_w}^u \mid l_w \in \text{Lyndon}(0, 1) \setminus \{0\}\} , \quad (4.3.2)$$

where $H_{l_w}^u \equiv H_{l_w}(1 - u)$, and $\text{Lyndon}(0, 1)$ is the set of *Lyndon* words in the letters 0 and 1. The Lyndon words are those words w such that for every decomposition into two words $w = \{u, v\}$, the left word u is smaller¹ than the right word v , *i.e.* $u < v$. Notice that we exclude the case $l_w = 0$ because it corresponds to $\ln(1 - u)$, which has an unphysical branch cut. Further cuts of this type occur whenever l_w has a trailing zero, but such words are excluded from the Lyndon basis by construction.

The Lyndon basis of HPLs with proper branch cuts through weight six can be written explicitly as,

$$\begin{aligned} \mathcal{H}_u|_{n \leq 6} = \{ & \ln u, H_2^u, H_3^u, H_{2,1}^u, H_4^u, H_{3,1}^u, H_{2,1,1}^u, H_5^u, H_{4,1}^u, H_{3,2}^u, H_{3,1,1}^u, H_{2,2,1}^u, H_{2,1,1,1}^u, \\ & H_6^u, H_{5,1}^u, H_{4,2}^u, H_{4,1,1}^u, H_{3,2,1}^u, H_{3,1,2}^u, H_{3,1,1,1}^u, H_{2,2,1,1}^u, H_{2,1,1,1,1}^u \} . \end{aligned} \quad (4.3.3)$$

Equation (4.3.3) and its two cyclic permutations, \mathcal{H}_v and \mathcal{H}_w , account entirely for the y^0 column of table 4.1. Although the y -containing functions are not very numerous through weight five or so, describing them is considerably more involved.

In order to parametrize the full space of functions whose symbols can be written in terms of the elements in the set \mathcal{S}_u , it is useful to reexpress those elements in terms of three independent variables. The cross ratios themselves are not a convenient choice

¹We take the ordering of words to be lexicographic. The ordering of the letters is specified by the order in which they appear in the argument of “ $\text{Lyndon}(0, 1)$ ”, *i.e.* $0 < 1$. Later we will encounter words with more letters for which this specification is less trivial.

Weight	y^0	y^1	y^2	y^3	y^4
1	3	-	-	-	-
2	3	-	-	-	-
3	6	1	-	-	-
4	9	3	3	-	-
5	18	4	13	6	-
6	27	4	27	29	18

Table 4.1: The dimension of the irreducible basis of hexagon functions, graded by the maximum number of y entries in their symbols.

of variables because rewriting the y_i in terms of the u_i produces explicit square roots. A better choice is to consider the y_i as independent variables, in terms of which the u_i are given by eq. (4.2.11). In this representation, the symbol has letters drawn from the ten-element set,

$$\mathcal{S}_y = \{y_u, y_v, y_w, 1-y_u, 1-y_v, 1-y_w, 1-y_u y_v, 1-y_u y_w, 1-y_v y_w, 1-y_u y_v y_w\}. \quad (4.3.4)$$

We appear to have taken a step backward since there is an extra letter in \mathcal{S}_y relative to \mathcal{S}_u . Indeed, writing the symbol of a typical function in this way greatly increases the length of its expression. Also, the first entry condition becomes more complicated in the y variables. On the other hand, \mathcal{S}_y contains purely rational functions of the y_i , and as such it is easy to construct the space of functions that give rise to symbol entries of this type. We will discuss these functions in the next subsection.

4.3.2 Multiple polylogarithms

Multiple polylogarithms are a general class of multi-variable iterated integrals, of which logarithms, polylogarithms, harmonic polylogarithms, and various other iterated integrals are special cases. They are defined recursively by $G(z) = 1$, and,

$$G(a_1, \dots, a_n; z) = \int_0^z \frac{dt}{t - a_1} G(a_2, \dots, a_n; t), \quad G(\underbrace{0, \dots, 0}_p; z) = \frac{\ln^p z}{p!}. \quad (4.3.5)$$

Many of their properties are reviewed in appendix C.1, including an expression for their symbol, which is also defined recursively [162],

$$\mathcal{S}(G(a_{n-1}, \dots, a_1; a_n)) = \sum_{i=1}^{n-1} \left[\mathcal{S}(G(a_{n-1}, \dots, \hat{a}_i, \dots, a_1; a_n)) \otimes (a_i - a_{i+1}) - \mathcal{S}(G(a_{n-1}, \dots, \hat{a}_i, \dots, a_1; a_n)) \otimes (a_i - a_{i-1}) \right], \quad (4.3.6)$$

where $a_0 = 0$ and the hat on a_i on the right-hand side indicates that this index should be omitted.

Using eq. (4.3.6), it is straightforward to write down a set of multiple polylogarithms whose symbol entries span \mathcal{S}_y ,

$$\begin{aligned} \mathcal{G} = & \left\{ G(\vec{w}; y_u) \middle| w_i \in \{0, 1\} \right\} \cup \left\{ G(\vec{w}; y_v) \middle| w_i \in \left\{ 0, 1, \frac{1}{y_u} \right\} \right\} \\ & \cup \left\{ G(\vec{w}; y_w) \middle| w_i \in \left\{ 0, 1, \frac{1}{y_u}, \frac{1}{y_v}, \frac{1}{y_u y_v} \right\} \right\}, \end{aligned} \quad (4.3.7)$$

The set \mathcal{G} also emerges naturally from a simple procedure by which symbols are directly promoted to polylogarithmic functions. For each letter $\phi_i(y_u, y_v, y_w) \in \mathcal{S}_y$ we write $\omega_i = d \log \phi_i(t_u, t_v, t_w)$. Then following refs. [146, 163], which are in turn based on ref. [145], we use the integration map,

$$\phi_1 \otimes \dots \otimes \phi_n \mapsto \int_{\gamma} \omega_n \circ \dots \circ \omega_1. \quad (4.3.8)$$

The integration is performed iteratively along the contour γ which we choose to take from the origin $t_i = 0$ to the point $t_i = y_i$. The precise choice of path is irrelevant, provided the symbol we start from is integrable [145, 146]. So we may choose to take a path which goes sequentially along the t_u, t_v, t_w directions. Near the axes we may find some divergent integrations of the form $\int_0^y dt/t \circ \dots \circ dt/t$. We regularize these divergences in the same way as in the one-dimensional HPL case (see the text before eq. (4.2.25)) by replacing them with $\frac{1}{n!} \log^n y$. In this way we immediately obtain an expression in terms of the functions in \mathcal{G} , with the three subsets corresponding to the

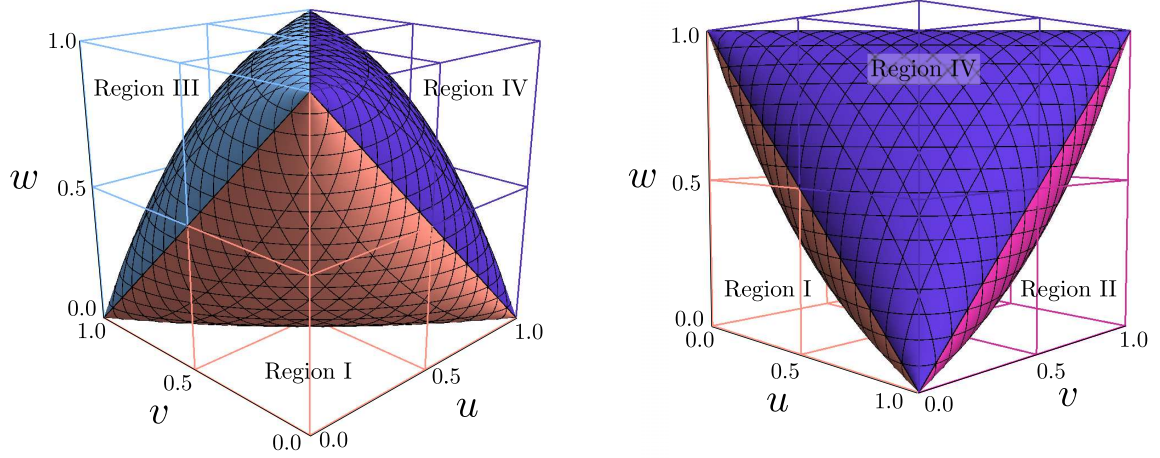


Figure 4.1: Illustration of Regions I, II, III and IV. Each region lies between the colored surface and the respective corner of the unit cube.

three segments of the contour.

The set \mathcal{G} is larger than what is required to construct the basis of hexagon functions. One reason for this is that \mathcal{G} generates unwanted symbol entries outside of the set \mathcal{S}_u , such as the differences $y_i - y_j$, as is easy to see from eq. (4.3.6); the cancellation of such terms is an additional constraint that any valid hexagon function must satisfy. Another reason is that multiple polylogarithms satisfy many identities, such as the shuffle and stuffle identities (see appendix C.1 or refs. [37, 162] for a review). While there are no relevant stuffle relations among the functions in \mathcal{G} , there are many relations resulting from shuffle identities. Just as for the single-variable case of HPLs, these shuffle relations may be resolved by constructing a Lyndon basis, $\mathcal{G}_I^L \subset \mathcal{G}$,

$$\begin{aligned} \mathcal{G}_I^L = & \left\{ G(\vec{w}; y_u) \middle| w_i \in \text{Lyndon}(0, 1) \right\} \cup \left\{ G(\vec{w}; y_v) \middle| w_i \in \text{Lyndon}\left(0, 1, \frac{1}{y_u}\right) \right\} \\ & \cup \left\{ G(\vec{w}; y_w) \middle| w_i \in \text{Lyndon}\left(0, 1, \frac{1}{y_u}, \frac{1}{y_v}, \frac{1}{y_u y_v}\right) \right\}. \end{aligned} \quad (4.3.9)$$

A multiple polylogarithm $G(w_1, \dots, w_n; z)$ admits a convergent series expansion if $|z| \leq |w_i|$ for all nonzero w_i , and it is manifestly real-valued if the nonzero w_i and z are real and positive. Therefore, the set \mathcal{G}_I^L is ideally suited for describing

configurations for which $0 < y_i < 1$. In terms of the original cross ratios, this region is characterized by,

$$\text{Region I : } \begin{cases} \Delta > 0, & 0 < u_i < 1, & \text{and} & u + v + w < 1, \\ 0 < y_i < 1. \end{cases} \quad (4.3.10)$$

We will construct the space of hexagon functions in Region I as a subspace of \mathcal{G}_I^L with good branch-cut properties.

What about other regions? As we will discuss in the next subsection, multiple polylogarithms in the y variables are poorly suited to regions where $\Delta < 0$; in these regions the y_i are complex. For such cases, we turn to certain integral representations that we will describe in section 4.4. In this section, we restrict ourselves to the subspace of the unit cube for which $\Delta > 0$. As shown in fig. 4.1, there are four disconnected regions with $\Delta > 0$, which we refer to as Regions I, II, III, and IV. They are the regions that extend respectively from the four points $(0, 0, 0)$, $(1, 1, 0)$, $(0, 1, 1)$, and $(1, 0, 1)$ to the intersection with the $\Delta = 0$ surface. Three of the regions (II, III and IV) are related to one another by permutations of the u_i , so it suffices to consider only one of them,

$$\text{Region II : } \begin{cases} \Delta > 0, & 0 < u_i < 1, & \text{and} & u + v - w > 1, \\ 0 < y_w < \frac{1}{y_u y_v} < \frac{1}{y_u}, \frac{1}{y_v} < 1. \end{cases} \quad (4.3.11)$$

In Region II, the set \mathcal{G}_I^L includes functions $G(w_1, \dots, w_n; z)$ for which $|w_i| < |z|$ for some i . As mentioned above, such functions require an analytic continuation and are not manifestly real-valued. On the other hand, it is straightforward to design an alternative basis set that does not suffer from this issue,

$$\begin{aligned} \mathcal{G}_{II}^L = & \left\{ G\left(\vec{w}; \frac{1}{y_u}\right) \middle| w_i \in \text{Lyndon}(0, 1) \right\} \cup \left\{ G\left(\vec{w}; \frac{1}{y_v}\right) \middle| w_i \in \text{Lyndon}(0, 1, y_u) \right\} \\ & \cup \left\{ G(\vec{w}; y_w) \middle| w_i \in \text{Lyndon}\left(0, 1, \frac{1}{y_u}, \frac{1}{y_v}, \frac{1}{y_u y_v}\right) \right\}. \end{aligned} \quad (4.3.12)$$

Like \mathcal{G}_I^L , \mathcal{G}_{II}^L also generates symbols with the desired entries. It is therefore a good starting point for constructing a basis of hexagon functions in Region II.

4.3.3 The coproduct bootstrap

The space of multiple polylogarithms enjoys various nice properties, many of which are reviewed in appendix C.1. For example, it can be endowed with the additional structure necessary to promote it to a Hopf algebra. For the current discussion, we make use of one element of this structure, namely the coproduct. The coproduct on multiple polylogarithms has been used in a variety of contexts [37, 64, 106, 164–166]. It serves as a powerful tool to help lift symbols to full functions and to construct functions or identities iteratively in the weight.

Let \mathcal{A} denote the Hopf algebra of multiple polylogarithms and \mathcal{A}_n the weight- n subspace, so that,

$$\mathcal{A} = \bigoplus_{n=0}^{\infty} \mathcal{A}_n. \quad (4.3.13)$$

Then, for $G_n \in \mathcal{A}_n$, the coproduct decomposes as,

$$\Delta(G_n) = \sum_{p+q=n} \Delta_{p,q}(G_n), \quad (4.3.14)$$

where $\Delta_{p,q} \in \mathcal{A}_p \otimes \mathcal{A}_q$. It is therefore sensible to discuss an individual $\{p, q\}$ component of the coproduct, $\Delta_{p,q}$. In fact, we will only need two cases, $\{p, q\} = \{n-1, 1\}$ and $\{p, q\} = \{1, n-1\}$, though the other components carry additional information that may be useful in other contexts.

A simple (albeit roundabout) procedure to extract the coproduct of a generic multiple polylogarithm, G , is reviewed in appendix C.1. One first rewrites G in the notation of a slightly more general function, usually denoted by I in the mathematical literature. Then one applies the main coproduct formula, eq. (C.1.15), and finally converts back into the G notation.

Let us discuss how the coproduct can be used to construct identities between multiple polylogarithms iteratively. Suppose we know all relevant identities up to

weight $n - 1$, and we would like to establish the validity of some potential weight- n identity, which can always be written in the form,

$$A_n = 0, \quad (4.3.15)$$

for some combination of weight- n functions, A_n . If this identity holds, then we may further conclude that each component of the coproduct of A_n should vanish. In particular,

$$\Delta_{n-1,1}(A_n) = 0. \quad (4.3.16)$$

Since this is an equation involving functions of weight less than or equal to $n - 1$, we may check it explicitly. Equation (4.3.16) does not imply eq. (4.3.15), because $\Delta_{n-1,1}$ has a nontrivial kernel. For our purposes, the only relevant elements of the kernel are multiple zeta values, zeta values, $i\pi$, and their products. Through weight six, the elements of the kernel are the transcendental constants,

$$\mathcal{K} = \{i\pi, \zeta_2, \zeta_3, i\pi^3, \zeta_4, i\pi\zeta_3, \zeta_2\zeta_3, \zeta_5, i\pi^5, \zeta_6, \zeta_3^2, i\pi\zeta_5, i\pi^3\zeta_3, \dots\}. \quad (4.3.17)$$

At weight two, for example, we may use this information to write,

$$\Delta_{1,1}(A_2) = 0 \quad \Rightarrow \quad A_2 = c\zeta_2, \quad (4.3.18)$$

for some undetermined rational number c , which we can fix numerically or by looking at special limits. Consider the following example for some real positive $x \leq 1$,

$$\begin{aligned} A_2 &= -G(0, x; 1) - G\left(0, \frac{1}{x}; 1\right) + \frac{1}{2}G(0; x)^2 - i\pi G(0; x) \\ &= \text{Li}_2\left(\frac{1}{x}\right) + \text{Li}_2(x) + \frac{1}{2}\ln^2 x - i\pi \ln x. \end{aligned} \quad (4.3.19)$$

Using eq. (4.3.19) and simple identities among logarithms, it is easy to check that

$$\Delta_{1,1}(A_2) = 0, \quad (4.3.20)$$

so we conclude that $A_2 = c\zeta_2$. Specializing to $x = 1$, we find $c = 2$ and therefore $A_2 = 2\zeta_2$. Indeed, this confirms the standard inversion relation for dilogarithms.

The above procedure may be applied systematically to generate all identities within a given ring of multiple polylogarithms and multiple zeta values. Denote this ring by \mathcal{C} and its weight- n subspace by \mathcal{C}_n . Assume that we have found all identities through weight $n - 1$. To find the identities at weight n , we simply look for all solutions to the equation,

$$\Delta_{n-1,1} \left(\sum_i c_i G_i \right) = \sum_i c_i \left(\Delta_{n-1,1}(G_i) \right) = 0, \quad (4.3.21)$$

where $G_i \in \mathcal{C}_n$ and the c_i are rational numbers. Because we know all identities through weight $n - 1$, we can write each $\Delta_{n-1,1}(G_i)$ as a combination of linearly-independent functions of weight $n - 1$. The problem is then reduced to one of linear algebra. The nullspace encodes the set of new identities, modulo elements of the kernel \mathcal{K} . The latter transcendental constants can be fixed numerically, or perhaps analytically with the aid of an integer-relation algorithm like PSLQ [167].

For the appropriate definition of \mathcal{C} , the above procedure can generate a variety of interesting relations. For example, we can choose $\mathcal{C} = \mathcal{G}_I^L$ or $\mathcal{C} = \mathcal{G}_{II}^L$ and confirm that there are no remaining identities within these sets.

We may also use this method to express all harmonic polylogarithms with argument u_i or $1 - u_i$ in terms of multiple polylogarithms in the set \mathcal{G}_I^L or the set \mathcal{G}_{II}^L . The only trick is to rewrite the HPLs as multiple polylogarithms. For example, using the uncompressed notation for the HPLs,

$$H_{a_1, \dots, a_n}(u) = (-1)^{w_1} G(a_1, \dots, a_n; u) = (-1)^{w_1} G \left(a_1, \dots, a_n; \frac{y_u(1-y_v)(1-y_w)}{(1-y_u y_v)(1-y_u y_w)} \right), \quad (4.3.22)$$

where w_1 is the number of a_i equal to one. With this understanding, we can simply take,

$$\mathcal{C} = \{H_{\vec{w}}(u_i)\} \cup \mathcal{G}_I^L \quad \text{or} \quad \mathcal{C} = \{H_{\vec{w}}(u_i)\} \cup \mathcal{G}_{II}^L, \quad (4.3.23)$$

and then proceed as above to generate all identities within this expanded ring.

In all cases, the starting point for the iterative procedure for generating identities is the set of identities at weight one, *i.e.* the set of identities among logarithms. All identities among logarithms are of course known, but in some cases they become rather cumbersome, and one must take care to properly track various terms that depend on the ordering of the y_i . For example, consider the following identity, which is valid for all complex y_i ,

$$\begin{aligned}
\ln u &= \ln \left(\frac{y_u(1-y_v)(1-y_w)}{(1-y_u y_v)(1-y_u y_w)} \right) \\
&= \ln y_u + \ln(1-y_v) + \ln(1-y_w) - \ln(1-y_u y_v) - \ln(1-y_u y_w) \\
&\quad + i \left[\operatorname{Arg} \left(\frac{y_u(1-y_v)(1-y_w)}{(1-y_u y_v)(1-y_u y_w)} \right) - \operatorname{Arg}(y_u) - \operatorname{Arg}(1-y_v) - \operatorname{Arg}(1-y_w) \right. \\
&\quad \left. + \operatorname{Arg}(1-y_u y_v) + \operatorname{Arg}(1-y_u y_w) \right],
\end{aligned} \tag{4.3.24}$$

where Arg denotes the principal value of the complex argument. In principle, this identity can be used to seed the iterative procedure for constructing higher-weight identities, which would also be valid for all complex y_i . Unfortunately, the bookkeeping quickly becomes unwieldy and it is not feasible to track the proliferation of Arg 's for high weight.

To avoid this issue, we will choose to focus on Regions I and II, defined by eqs. (4.3.10) and (4.3.11). In both regions, $\Delta > 0$, so the y variables are real, and the Arg 's take on specific values. In Region I, for example, we may write,

$$\begin{aligned}
\ln u &\stackrel{\text{Region I}}{=} \ln y_u + \ln(1-y_v) + \ln(1-y_w) - \ln(1-y_u y_v) - \ln(1-y_u y_w) \\
&= G(0; y_u) + G(1; y_v) + G(1; y_w) - G\left(\frac{1}{y_u}; y_v\right) - G\left(\frac{1}{y_u}; y_w\right).
\end{aligned} \tag{4.3.25}$$

In the last line, we have rewritten the logarithms in terms of multiple polylogarithms in the set \mathcal{G}_I^L , which, as we argued in the previous subsection, is the appropriate basis

for this region. In Region II, the expression for $\ln u$ looks a bit different,

$$\begin{aligned} \ln u &\stackrel{\text{Region II}}{=} \ln \left(1 - \frac{1}{y_v}\right) + \ln(1 - y_w) - \ln \left(1 - \frac{1}{y_u y_v}\right) - \ln(1 - y_u y_w) \\ &= G \left(1; \frac{1}{y_v}\right) + G(1; y_w) - G \left(y_u; \frac{1}{y_v}\right) - G \left(\frac{1}{y_u}; y_w\right). \end{aligned} \quad (4.3.26)$$

In this case, we have rewritten the logarithms as multiple polylogarithms belonging to the set \mathcal{G}_{II}^L .

We now show how to use these relations and the coproduct to deduce relations at weight two. In particular, we will derive an expression for $H_2^u = H_2(1 - u)$ in terms of multiple polylogarithms in the basis \mathcal{G}_I^L in Region I. A similar result holds in Region II. First, we need one more weight-one identity,

$$\ln(1 - u) \stackrel{\text{Region I}}{=} G(1; y_u) - G \left(\frac{1}{y_u}; y_v\right) - G \left(\frac{1}{y_u}; y_w\right) + G \left(\frac{1}{y_u y_v}; y_w\right). \quad (4.3.27)$$

Next, we take the $\{1, 1\}$ component of the coproduct,

$$\Delta_{1,1}(H_2^u) = -\ln u \otimes \ln(1 - u), \quad (4.3.28)$$

and substitute eqs. (4.3.25) and (4.3.27),

$$\begin{aligned} \Delta_{1,1}(H_2^u) &= - \left[G(0; y_u) + G(1; y_v) + G(1; y_w) - G \left(\frac{1}{y_u}; y_v\right) - G \left(\frac{1}{y_u}; y_w\right) \right] \\ &\quad \otimes \left[G(1; y_u) - G \left(\frac{1}{y_u}; y_v\right) - G \left(\frac{1}{y_u}; y_w\right) + G \left(\frac{1}{y_u y_v}; y_w\right) \right]. \end{aligned} \quad (4.3.29)$$

Finally, we ask which combination of weight-two functions in \mathcal{G}_I^L has the $\{1, 1\}$ component of its coproduct given by eq. (4.3.29). There is a unique answer, modulo

elements in \mathcal{K} ,

$$\begin{aligned}
H_2^u \stackrel{\text{Region I}}{=} & -G\left(\frac{1}{y_u}, \frac{1}{y_u y_v}; y_w\right) + G\left(1, \frac{1}{y_u y_v}; y_w\right) - G\left(1, \frac{1}{y_u}; y_w\right) - G\left(1, \frac{1}{y_u}; y_v\right) \\
& + G(0, 1; y_u) + G\left(\frac{1}{y_u y_v}; y_w\right) G\left(\frac{1}{y_u}; y_w\right) + G\left(\frac{1}{y_u}; y_v\right) G\left(\frac{1}{y_u y_v}; y_w\right) \\
& - G(1; y_w) G\left(\frac{1}{y_u y_v}; y_w\right) - G(1; y_v) G\left(\frac{1}{y_u y_v}; y_w\right) - G(0; y_u) G\left(\frac{1}{y_u y_v}; y_w\right) \\
& - \frac{1}{2} G\left(\frac{1}{y_u}; y_w\right)^2 - G\left(\frac{1}{y_u}; y_v\right) G\left(\frac{1}{y_u}; y_w\right) + G(1; y_w) G\left(\frac{1}{y_u}; y_w\right) \\
& + G(1; y_v) G\left(\frac{1}{y_u}; y_w\right) + G(0; y_u) G\left(\frac{1}{y_u}; y_w\right) - \frac{1}{2} G\left(\frac{1}{y_u}; y_v\right)^2 \\
& + G(1; y_v) G\left(\frac{1}{y_u}; y_v\right) + G(0; y_u) G\left(\frac{1}{y_u}; y_v\right) - G(0; y_u) G(1; y_u) + \zeta_2.
\end{aligned} \tag{4.3.30}$$

We have written a specific value for the coefficient of ζ_2 , though at this stage it is completely arbitrary since $\Delta_{1,1}(\zeta_2) = 0$. To verify that we have chosen the correct value, we specialize to the surface $y_u = 1$, on which $u = 1$ and $H_2^u = 0$. It is straightforward to check that the right-hand side of eq. (4.3.30) does indeed vanish in this limit.

An alternative way to translate expressions made from HPLs of arguments u_i into expressions in terms of the y variables is as follows. Any expression in terms of HPLs of arguments u, v, w may be thought of as the result of applying the integration map to words made from the letters u_i and $1 - u_i$ only. For example,

$$H_2^u = H_2(1 - u) = H_{10}(u) + \zeta_2 \tag{4.3.31}$$

$$= - \int_{\gamma} d \log(1 - s_1) \circ d \log s_1 + \zeta_2, \tag{4.3.32}$$

where, to verify the final equality straightforwardly, we may choose the contour γ to run from $s_i = 0$ to $(s_1 = u, s_2 = v, s_3 = w)$ sequentially along the s_1, s_2, s_3 axes. In the above simple example the second and third parts of the contour are irrelevant since the form to be integrated only depends on s_1 anyway. Then we can change

variables from u, v, w to y_u, y_v, y_w by defining

$$s_1 = \frac{t_1(1-t_2)(1-t_3)}{(1-t_1t_2)(1-t_1t_3)}, \quad (4.3.33)$$

and similarly for s_2, s_3 . Since the result obtained depends only on the end points of the contour, and not the precise path taken, we may instead choose the contour as the one which goes from the origin $t_i = 0$ to the point $t_1 = y_u, t_2 = y_v, t_3 = y_w$ sequentially along the t_1, t_2, t_3 axes, as in the discussion around eq. (4.3.8). Then expression (4.3.32) yields an expression equivalent to eq. (4.3.30).

Continuing this procedure on to higher weights is straightforward, although the expressions become increasingly complicated. For example, the expression for $H_{4,2}^w$ has 9439 terms. It is clear that \mathcal{G}_I^L is not an efficient basis, at least for representing harmonic polylogarithms with argument u_i . Despite this inefficiency, \mathcal{G}_I^L and \mathcal{G}_{II}^L have the virtue of spanning the space of hexagon functions, although they still contain many more functions than desired. In the next subsection, we describe how we can iteratively impose constraints in order to construct a basis for just the hexagon functions.

4.3.4 Constructing the hexagon functions

Unitarity requires the branch cuts of physical quantities to appear in physical channels. For dual conformally-invariant functions corresponding to the scattering of massless particles, the only permissible branching points are when a cross ratio vanishes or approaches infinity. The location of branch points in an iterated integral is controlled by the first entry of the symbol; hence the first entry should be one of the cross ratios, as discussed previously. However, it is not necessary to restrict our attention to the symbol: it was argued in ref. [64] that the condition of only having physical branch points can be promoted to the coproduct. Then the monodromy operator $\mathcal{M}_{z_k=z_0}$ (which gives the phase in analytically continuing the variable z_k around the point z_0) acts on the first component of the coproduct Δ (see appendix C.1.2),

$$\Delta \circ \mathcal{M}_{z_k=z_0} = (\mathcal{M}_{z_k=z_0} \otimes \text{id}) \circ \Delta. \quad (4.3.34)$$

We conclude that if F_n is a weight- n function with the proper branch-cut locations, and

$$\Delta_{n-1,1}(F_n) = \sum_r F_{n-1}^r \otimes d \ln \phi_r, \quad (4.3.35)$$

then F_{n-1}^r must also be a weight- $(n-1)$ function with the proper branch-cut locations, for every r (which labels the possible letters in the symbol). Working in the other direction, suppose we know the basis of hexagon functions through weight $n-1$. We may then use eq. (4.3.35) and the coproduct bootstrap of section 4.3.3 to build the basis at weight n .

There are a few subtleties that must be taken into account before applying this method directly. To begin with, the condition that all the F_{n-1}^r belong to the basis of hexagon functions guarantees that they have symbol entries drawn from \mathcal{S}_u . However, it does not guarantee that F_n has this property since the ϕ_r are drawn from the set \mathcal{S}_y , which is larger than \mathcal{S}_u . This issue is easily remedied by simply disregarding those functions whose symbols have final entries outside of the set \mathcal{S}_u .

In pushing to higher weights, it becomes necessary to pursue a more efficient construction. For this purpose, it is useful to decompose the space of hexagon functions, which we denote by \mathcal{H} , into its parity-even and parity-odd components,

$$\mathcal{H} = \mathcal{H}^+ \oplus \mathcal{H}^-. \quad (4.3.36)$$

The coproduct can be taken separately on each component,

$$\begin{aligned} \Delta_{n-1,1}(\mathcal{H}_n^+) &\subseteq (\mathcal{H}_{n-1}^+ \otimes \mathcal{L}_1^+) \oplus (\mathcal{H}_{n-1}^- \otimes \mathcal{L}_1^-), \\ \Delta_{n-1,1}(\mathcal{H}_n^-) &\subseteq (\mathcal{H}_{n-1}^+ \otimes \mathcal{L}_1^-) \oplus (\mathcal{H}_{n-1}^- \otimes \mathcal{L}_1^+), \end{aligned} \quad (4.3.37)$$

where \mathcal{L}_1^+ and \mathcal{L}_1^- are the parity-even and parity-odd functions of weight one,

$$\begin{aligned} \mathcal{L}_1^+ &= \{\ln u, \ln(1-u), \ln v, \ln(1-v), \ln w, \ln(1-w)\}, \\ \mathcal{L}_1^- &= \{\ln y_u, \ln y_v, \ln y_w\}. \end{aligned} \quad (4.3.38)$$

To construct \mathcal{H}_n^\pm , we simply write down the most general ansatz for both the

left-hand side and the right-hand side of eq. (4.3.37) and solve the linear system. The ansatz for \mathcal{H}_n^\pm will be constructed from the either \mathcal{G}_I^L or \mathcal{G}_{II}^L , supplemented by multiple zeta values, while a parametrization of the right-hand side is known by assumption. For high weights, the linear system becomes prohibitively large, which is one reason why it is useful to construct the even and odd sectors separately, since it effectively halves the computational burden. We note that not every element on the right hand side of eq. (4.3.37) is actually in the image of $\Delta_{n-1,1}$. For such cases, we will simply find no solution to the linear equations. Finally, this parametrization of the $\{n-1, 1\}$ component of the coproduct guarantees that the symbol of any function in \mathcal{H}_n will have symbol entries drawn from \mathcal{S}_u .

Unfortunately, the procedure we just have outlined does not actually guarantee proper branch cuts in all cases. The obstruction is related to the presence of weight- $(n-1)$ multiple zeta values in the space \mathcal{H}_{n-1}^+ . Such terms may become problematic when used as in eq. (4.3.37) to build the weight- n space, because they get multiplied by logarithms, which may contribute improper branch cuts. For example,

$$\zeta_{n-1} \otimes \ln(1-u) \in \mathcal{H}_{n-1}^+ \otimes \mathcal{L}_1^+, \quad (4.3.39)$$

but the function $\zeta_{n-1} \ln(1-u)$ has a spurious branch point at $u=1$. Naively, one might think such terms must be excluded from our ansatz, but this turns out to be incorrect. In some cases, they are needed to cancel off the bad behavior of other, more complicated functions.

We can exhibit this bad behavior in a simple one-variable function,

$$f_2(u) = \text{Li}_2(u) + \ln u \ln(1-u) \in \mathcal{H}_2^+. \quad (4.3.40)$$

It is easy to write down a weight-three function $f_3(u)$ that satisfies,

$$\Delta_{2,1}(f_3(u)) = f_2(u) \otimes \ln(1-u). \quad (4.3.41)$$

Indeed, one may easily check that

$$f_3(u) = H_{2,1}(u) + \text{Li}_2(u) \ln(1-u) + \frac{1}{2} \ln^2(1-u) \ln u \quad (4.3.42)$$

does the job. The problem is that $f_3(u) \notin \mathcal{H}_3^+$ because it has a logarithmic branch cut starting at $u = 1$. In fact, the presence of this cut is indicated by a simple pole at $u = 1$ in its first derivative,

$$f'_3(u) \Big|_{u \rightarrow 1} \rightarrow -\frac{\zeta_2}{1-u}. \quad (4.3.43)$$

The residue of the pole is just $f_2(1)$ and can be read directly from eq. (4.3.40) without ever writing down $f_3(u)$. This suggests that the problem can be remedied by subtracting ζ_2 from $f_2(u)$. Indeed, for

$$\tilde{f}_2(u) = f_2(u) - \zeta_2 = -\text{Li}_2(1-u), \quad (4.3.44)$$

there does exist a function,

$$\tilde{f}_3(u) = -\text{Li}_3(1-u) \in \mathcal{H}_3^+, \quad (4.3.45)$$

for which,

$$\Delta_{2,1}(\tilde{f}_3(u)) = \tilde{f}_2(u) \otimes \ln(1-u). \quad (4.3.46)$$

More generally, any function whose first derivative yields a simple pole has a logarithmic branch cut starting at the location of that pole. Therefore, the only allowed poles in the u_i -derivative are at $u_i = 0$. In particular, the absence of poles at $u_i = 1$ provides additional constraints on the space \mathcal{H}_n^\pm .

These constraints were particularly simple to impose in the above single-variable example, because the residue of the pole at $u = 1$ could be directly read off from a single term in the coproduct, namely the one with $\ln(1-u)$ in the last slot. In the full multiple-variable case, the situation is slightly more complicated. The coproduct

of any hexagon function will generically have nine terms,

$$\Delta_{n-1,1}(F) \equiv \sum_{i=1}^3 \left[F^{u_i} \otimes \ln u_i + F^{1-u_i} \otimes \ln(1-u_i) + F^{y_i} \otimes \ln y_i \right], \quad (4.3.47)$$

where F is a function of weight n and the nine functions $\{F^{u_i}, F^{1-u_i}, F^{y_i}\}$ are of weight $(n-1)$ and completely specify the $\{n-1, 1\}$ component of the coproduct. The derivative with respect to u can be evaluated using eqs. (4.2.23) and (4.3.47) and the chain rule,

$$\left. \frac{\partial F}{\partial u} \right|_{v,w} = \frac{F^u}{u} - \frac{F^{1-u}}{1-u} + \frac{1-u-v-w}{u\sqrt{\Delta}} F^{y_u} + \frac{1-u-v+w}{(1-u)\sqrt{\Delta}} F^{y_v} + \frac{1-u+v-w}{(1-u)\sqrt{\Delta}} F^{y_w}. \quad (4.3.48)$$

Clearly, a pole at $u = 1$ can arise from F^{1-u} , F^{y_v} or F^{y_w} , or it can cancel between these terms.

The condition that eq. (4.3.48) has no pole at $u = 1$ is a strong one, because it must hold for any values of v and w . In fact, this condition mainly provides consistency checks, because a much weaker set of constraints turns out to be sufficient to fix all undetermined constants in our ansatz.

It is useful to consider the constraints in the even and odd subspaces separately. Referring to eq. (4.2.9), parity sends $\sqrt{\Delta} \rightarrow -\sqrt{\Delta}$, and, therefore, any parity-odd function must vanish when $\Delta = 0$. Furthermore, recalling eq. (4.2.11),

$$\sqrt{\Delta} = \frac{(1-y_u)(1-y_v)(1-y_w)(1-y_u y_v y_w)}{(1-y_u y_v)(1-y_v y_w)(1-y_w y_u)}, \quad (4.3.49)$$

we see that any odd function must vanish when $y_i \rightarrow 1$ or when $y_u y_v y_w \rightarrow 1$. It turns out that these conditions are sufficient to fix all undetermined constants in the odd sector. One may then verify that there are no spurious poles in the u_i -derivatives.

There are no such vanishing conditions in the even sector, and to fix all undetermined constants we need to derive specific constraints from eq. (4.3.48). We found it convenient to enforce the constraint for the particular values of v and w such that the $u \rightarrow 1$ limit coincides with the limit of Euclidean multi-Regge kinematics (EMRK).

In this limit, v and w vanish at the same rate that u approaches 1,

$$\text{EMRK: } u \rightarrow 1, v \rightarrow 0, w \rightarrow 0; \quad \frac{v}{1-u} \equiv x, \quad \frac{w}{1-u} \equiv y, \quad (4.3.50)$$

where x and y are fixed. In the y variables, the EMRK limit takes $y_u \rightarrow 1$, while y_v and y_w are held fixed, and can be related to x and y by,

$$x = \frac{y_v(1-y_w)^2}{(1-y_v y_w)^2}, \quad y = \frac{y_w(1-y_v)^2}{(1-y_v y_w)^2}. \quad (4.3.51)$$

This limit can also be called the (Euclidean) soft limit, in which one particle gets soft. The final point, $(u, v, w) = (1, 0, 0)$, also lies at the intersection of two lines representing different collinear limits: $(u, v, w) = (x, 1-x, 0)$ and $(u, v, w) = (x, 0, 1-x)$, where $x \in [0, 1]$.

In the case at hand, F is an even function and so the coproduct components F^{y_i} are odd functions of weight $n-1$, and as such have already been constrained to vanish when $y_i \rightarrow 1$. (Although the coefficients of F^{y_v} and F^{y_w} in eq. (4.3.48) contain factors of $1/\sqrt{\Delta}$, which diverge in the limit $y_u \rightarrow 1$, the numerator factors $1-u \mp (v-w)$ can be seen from eq. (4.3.50) to vanish in this limit, canceling the $1/\sqrt{\Delta}$ divergence.) Therefore, the constraint that eq. (4.3.48) have no pole at $u=1$ simplifies considerably:

$$F^{1-u}(y_u=1, y_v, y_w) = 0. \quad (4.3.52)$$

Of course, two additional constraints can be obtained by taking cyclic images. These narrower constraints turn out to be sufficient to completely fix all free coefficients in our ansatz in the even sector.

Finally, we are in a position to construct the functions of the hexagon basis. At weight one, the basis simply consists of the three logarithms, $\ln u_i$. Before proceeding to weight two, we must rewrite these functions in terms of multiple polylogarithms. This necessitates a choice between Regions I and II, or between the bases \mathcal{G}_I^L and \mathcal{G}_{II}^L . We construct the basis for both cases, but for definiteness let us work in Region I.

Our ansatz for $\Delta_{1,1}(\mathcal{H}_2^+)$ consists of the 18 tensor products,

$$\{\ln u_i \otimes x \mid x \in \mathcal{L}_1^+\}, \quad (4.3.53)$$

which we rewrite in terms of multiple polylogarithms in \mathcal{G}_I^L . Explicit linear algebra shows that only a nine-dimensional subspace of these tensor products can be written as $\Delta_{1,1}(G_2)$ for $G_2 \in \mathcal{G}_I^L$. Six of these weight-two functions can be written as products of logarithms. The other three may be identified with $H_2(1-u_i)$ by using the methods of section 4.3.3. (See *e.g.* eq. (4.3.30).)

Our ansatz for $\Delta_{1,1}(\mathcal{H}_2^-)$ consists of the nine tensor products,

$$\{\ln u_i \otimes x \mid x \in \mathcal{L}_1^-\}, \quad (4.3.54)$$

which we again rewrite in terms of multiple polylogarithms in \mathcal{G}_I^L . In this case, it turns out that there is no linear combination of these tensor products that can be written as $\Delta_{1,1}(G_2)$ for $G_2 \in \mathcal{G}_I^L$. This confirms the analysis at symbol level as summarized in table 4.1, which shows three parity-even irreducible functions of weight two (which are identified as HPLs), and no parity-odd functions.

A similar situation unfolds in the parity-even sector at weight three, namely that the space is spanned by HPLs of a single variable. However, the parity-odd sector reveals a new function. To find it, we write an ansatz for $\Delta_{2,1}(\mathcal{H}_3^-)$ consisting of the 39 objects,

$$\{f_2 \otimes x \mid f_2 \in \mathcal{H}_2^+, x \in \mathcal{L}_1^-\} \quad (4.3.55)$$

(where $\mathcal{H}_2^+ = \{\zeta_2, \ln u_i \ln u_j, H_2^{u_i}\}$), and then look for a linear combination that can be written as $\Delta_{2,1}(G_3)$ for $G_3 \in \mathcal{G}_I^L$. After imposing the constraints that the function

vanish when $y_i \rightarrow 1$ and when $y_u y_v y_w \rightarrow 1$, there is a unique solution,

$$\begin{aligned}
\tilde{\Phi}_6 \stackrel{\text{Region I}}{=} & -G(0; y_u) G(0; y_v) G(0; y_w) + G(0, 1; y_u) G(0; y_u) - G(0, 1; y_u) G(0; y_v) \\
& - G(0, 1; y_u) G(0; y_w) - G(0, 1; y_v) G(0; y_u) + G(0, 1; y_v) G(0; y_v) \\
& - G(0, 1; y_v) G(0; y_w) - G\left(0, \frac{1}{y_u}; y_v\right) G(0; y_u) - G\left(0, \frac{1}{y_u}; y_v\right) G(0; y_v) \\
& + G\left(0, \frac{1}{y_u}; y_v\right) G(0; y_w) - G(0, 1; y_w) G(0; y_u) - G(0, 1; y_w) G(0; y_v) \\
& + G(0, 1; y_w) G(0; y_w) + 2G(0, 1; y_w) G\left(\frac{1}{y_u}; y_v\right) - G\left(0, \frac{1}{y_u}; y_w\right) G(0; y_u) \\
& + G\left(0, \frac{1}{y_u}; y_w\right) G(0; y_v) - G\left(0, \frac{1}{y_u}; y_w\right) G(0; y_w) - 2G(0, 0, 1; y_u) \\
& - 2G\left(0, \frac{1}{y_u}; y_w\right) G(1; y_v) + G\left(0, \frac{1}{y_v}; y_w\right) G(0; y_u) - 2G(0, 0, 1; y_v) \\
& - G\left(0, \frac{1}{y_v}; y_w\right) G(0; y_v) - G\left(0, \frac{1}{y_v}; y_w\right) G(0; y_w) - 2G(0, 0, 1; y_w) \\
& - 2G\left(0, \frac{1}{y_v}; y_w\right) G(1; y_u) + G\left(0, \frac{1}{y_u y_v}; y_w\right) G(0; y_u) - 2G(0, 1, 1; y_u) \\
& + G\left(0, \frac{1}{y_u y_v}; y_w\right) G(0; y_v) + G\left(0, \frac{1}{y_u y_v}; y_w\right) G(0; y_w) - 2G(0, 1, 1; y_v) \\
& + 2G\left(0, \frac{1}{y_u y_v}; y_w\right) G(1; y_u) + 2G\left(0, \frac{1}{y_u y_v}; y_w\right) G(1; y_v) - 2G(0, 1, 1; y_w) \\
& - 2G\left(0, \frac{1}{y_u y_v}; y_w\right) G\left(\frac{1}{y_u}; y_v\right) - 2G\left(0, 0, \frac{1}{y_u y_v}; y_w\right) \\
& + 2G\left(0, 0, \frac{1}{y_u}; y_v\right) + 2G\left(0, 0, \frac{1}{y_u}; y_w\right) + 2G\left(0, 0, \frac{1}{y_v}; y_w\right) \\
& + 2G\left(0, \frac{1}{y_u}, \frac{1}{y_u}; y_v\right) + 2G\left(0, \frac{1}{y_u}, \frac{1}{y_u}; y_w\right) + 2G\left(0, \frac{1}{y_v}, \frac{1}{y_v}; y_w\right) \\
& + 2G\left(0, \frac{1}{y_u y_v}, 1; y_w\right) - 2G\left(0, \frac{1}{y_u y_v}, \frac{1}{y_u}; y_w\right) - 2G\left(0, \frac{1}{y_u y_v}, \frac{1}{y_v}; y_w\right) \\
& - \zeta_2 G(0; y_u) - \zeta_2 G(0; y_v) - \zeta_2 G(0; y_w) .
\end{aligned} \tag{4.3.56}$$

The normalization can be fixed by comparing to the differential equation for $\tilde{\Phi}_6$,

Weight	y^0	y^1	y^2	y^3	y^4
1	3 HPLs	-	-	-	-
2	3 HPLs	-	-	-	-
3	6 HPLs	$\tilde{\Phi}_6$	-	-	-
4	9 HPLs	$3 \times F_1$	$3 \times \Omega^{(2)}$	-	-
5	18 HPLs	$G, 3 \times K_1$	$5 \times M_1, N, O, 6 \times Q_{\text{ep}}$	$3 \times H_1, 3 \times J_1$	-
6	27 HPLs	4	27	29	$3 \times R_{\text{ep}} + 15$

Table 4.2: Irreducible basis of hexagon functions, graded by the maximum number of y entries in the symbol. The indicated multiplicities specify the number of independent functions obtained by applying the S_3 permutations of the cross ratios.

eq. (4.2.24). This solution is totally symmetric under the S_3 permutation group of the three cross ratios $\{u, v, w\}$, or equivalently of the three variables $\{y_u, y_v, y_w\}$. However, owing to our choice of basis \mathcal{G}_I^L , this symmetry is broken in the representation (4.3.56).

In principle, this procedure may be continued and used to construct a basis for the space \mathcal{H}_n any value of n . In practice, it becomes computationally challenging to proceed beyond moderate weight, say $n = 5$. The three-loop remainder function is a weight-six function, but, as we will see shortly, to find its full functional form we do not need to know anything about the other weight-six functions. On the other hand, we do need a complete basis for all functions of weight five or less. We have constructed all such functions using the methods just described. Referring to table 4.1, there are 69 functions with weight less than or equal to five. However, any function with no y 's in its symbol can be written in terms of ordinary HPLs, so there are only 30 genuinely new functions. The expressions for these functions in terms of multiple polylogarithms are quite lengthy, so we present them in computer-readable format in the attached files.

The 30 new functions can be obtained from the permutations of 11 basic functions which we call $\tilde{\Phi}_6$, F_1 , $\Omega^{(2)}$, G , H_1 , J_1 , K_1 , M_1 , N , O , and Q_{ep} . Two of these functions, $\tilde{\Phi}_6$ and $\Omega^{(2)}$, have appeared in other contexts, as mentioned in section 4.2. Also, a linear combination of F_1 and its cyclic image can be identified with the odd part of the two-loop ratio function, denoted by \tilde{V} [71]. (The precise relation is given

in eq. (C.2.20).) We believe that the remaining functions are new. In table 4.2, we organize these functions by their weight and y -grading. We also indicate how many independent functions are generated by permuting the cross ratios. For example, $\tilde{\Phi}_6$ is totally symmetric, so it generates a unique entry, while F_1 and $\Omega^{(2)}$ are symmetric under exchange of two variables, so they sweep out a triplet of independent functions under cyclic permutations. The function Q_{ep} has no symmetries, so under S_3 permutations it sweeps out six independent functions. The same would be true of M_1 , except that a totally antisymmetric linear combination of its S_3 images and those of Q_{ep} are related, up to products of lower-weight functions and ordinary HPLs (see eq. (C.2.51)). Therefore we count only five independent functions arising from the S_3 permutations of M_1 .

We present the $\{n-1, 1\}$ components of the coproduct of these 11 basis functions in appendix C.2. This information, together with the value of the function at the point $(1, 1, 1)$ (which we take to be zero in all but one case), is sufficient to uniquely define the basis of hexagon functions. We will elaborate on these ideas in the next section.

4.4 Integral Representations

In the previous section, we described an iterative procedure to construct the basis of hexagon functions in terms of multiple polylogarithms in the y variables. The result is a fully analytic, numerically efficient representation of any given basis function. While convenient for many purposes, this representation is not without some drawbacks. Because \mathcal{S}_y has one more element than \mathcal{S}_u , and because the first entry condition is fairly opaque in the y variables, the multiple polylogarithm representation is often quite lengthy, which in turn sometimes obscures interesting properties. Furthermore, the iterative construction and the numerical evaluation of multiple polylogarithms are best performed when the y_i are real-valued, limiting the kinematic regions in which these methods are practically useful.

For these reasons, it is useful to develop a parallel representation of the hexagon functions, based directly on the system of first-order differential equations they satisfy. These differential equations can be solved in terms of (iterated) integrals over lower-weight functions. Since most of the low weight functions are HPLs, which are easy to evaluate, one can obtain numerical representations for the hexagon functions, even in the kinematic regions where the y_i are complex. The differential equations can also be solved in terms of simpler functions in various limits, which will be the subject of subsequent sections.

4.4.1 General setup

One benefit of the construction of the basis of hexagon functions in terms of multiple polylogarithms is that we can explicitly calculate the coproduct of the basis functions. We tabulate the $\{n-1, 1\}$ component of the coproduct for each of these functions in appendix C.2. This data exposes how the various functions are related to one another, and, moreover, this web of relations can be used to define a system of differential equations that the functions obey. These differential equations, together with the appropriate boundary conditions, provide an alternative definition of the hexagon functions. In fact, as we will soon argue, it is actually possible to derive these differential equations iteratively, without starting from an explicit expression

in terms of multiple polylogarithms. It is also possible to express the differential equations compactly in terms of a Knizhnik-Zamolodchikov equation along the lines studied in ref. [146]. Nevertheless, the coproduct on multiple polylogarithms, in particular the $\{n-1, 1\}$ component as given in eq. (4.3.47), is useful to frame the discussion of the differential equations and helps make contact with section 4.3.

It will be convenient to consider not just derivatives with respect to a cross ratio, as in eq. (4.3.48), but also derivatives with respect to the y variables. For that purpose, we need the following derivatives, which we perform holding y_v and y_w constant,

$$\begin{aligned} \frac{\partial \ln u}{\partial y_u} &= \frac{(1-u)(1-v-w)}{y_u \sqrt{\Delta}}, & \frac{\partial \ln v}{\partial y_u} &= -\frac{u(1-v)}{y_u \sqrt{\Delta}}, \\ \frac{\partial \ln(1-u)}{\partial y_u} &= -\frac{u(1-v-w)}{y_u \sqrt{\Delta}}, & \frac{\partial \ln(1-v)}{\partial y_u} &= \frac{uv}{y_u \sqrt{\Delta}}. \end{aligned} \quad (4.4.1)$$

We also consider the following linear combination,

$$\frac{\partial}{\partial \ln(y_u/y_w)} \equiv y_u \frac{\partial}{\partial y_u} \Big|_{y_v, y_w} - y_w \frac{\partial}{\partial y_w} \Big|_{y_v, y_u}. \quad (4.4.2)$$

Using eqs. (4.2.23) and (4.4.1), as well as the definition (4.4.2), we obtain three differential equations (plus their cyclic images) relating a function F to its various coproduct components,

$$\begin{aligned} \frac{\partial F}{\partial u} \Big|_{v, w} &= \frac{F^u}{u} - \frac{F^{1-u}}{1-u} + \frac{1-u-v-w}{u \sqrt{\Delta}} F^{y_u} + \frac{1-u-v+w}{(1-u) \sqrt{\Delta}} F^{y_v} \\ &\quad + \frac{1-u+v-w}{(1-u) \sqrt{\Delta}} F^{y_w}, \end{aligned} \quad (4.4.3)$$

$$\begin{aligned} \sqrt{\Delta} y_u \frac{\partial F}{\partial y_u} \Big|_{y_v, y_w} &= (1-u)(1-v-w) F^u - u(1-v) F^v - u(1-w) F^w \\ &\quad - u(1-v-w) F^{1-u} + uv F^{1-v} + uw F^{1-w} + \sqrt{\Delta} F^{y_u}, \end{aligned} \quad (4.4.4)$$

$$\begin{aligned} \sqrt{\Delta} \frac{\partial F}{\partial \ln(y_u/y_w)} &= (1-u)(1-v) F^u - (u-w)(1-v) F^v \\ &\quad - (1-v)(1-w) F^w - u(1-v) F^{1-u} + (u-w)v F^{1-v} \\ &\quad + w(1-v) F^{1-w} + \sqrt{\Delta} F^{y_u} - \sqrt{\Delta} F^{y_w}. \end{aligned} \quad (4.4.5)$$

Let us assume that we somehow know the coproduct components of F , either from the explicit representations given in appendix C.2, or from the iterative approach that we will discuss in the next subsection. We then know the right-hand sides of eqs. (4.4.3)-(4.4.5), and we can integrate any of these equations along the appropriate contour to obtain an integral representation for the function F . While eq. (4.4.3) integrates along a very simple contour, namely a line that is constant in v and w , this also means that the boundary condition, or initial data, must be specified over a two-dimensional plane, as a function of v and w for some value of u . In contrast, we will see that the other two differential equations have the convenient property that the initial data can be specified on a single point.

Let us begin with the differential equation (4.4.4) and its cyclic images. For definiteness, we consider the differential equation in y_v . To integrate it, we must find the contour in (u, v, w) that corresponds to varying y_v , while holding y_u and y_w constant. Following ref. [71], we define the three ratios,

$$\begin{aligned} r &= \frac{w(1-u)}{u(1-w)} = \frac{y_w(1-y_u)^2}{y_u(1-y_w)^2}, \\ s &= \frac{w(1-w)u(1-u)}{(1-v)^2} = \frac{y_w(1-y_w)^2 y_u(1-y_u)^2}{(1-y_w y_u)^4}, \\ t &= \frac{1-v}{uw} = \frac{(1-y_w y_u)^2 (1-y_u y_v y_w)}{y_w(1-y_w) y_u(1-y_u)(1-y_v)}. \end{aligned} \quad (4.4.6)$$

Two of these ratios, r and s , are actually independent of y_v , while the third, t , varies. Therefore, we can let t parameterize the contour, and denote by (u_t, v_t, w_t) the values of the cross ratios along this contour at generic values of t . Since r and s are constants, we have two constraints,

$$\begin{aligned} \frac{w_t(1-u_t)}{u_t(1-w_t)} &= \frac{w(1-u)}{u(1-w)}, \\ \frac{w_t(1-w_t)u_t(1-u_t)}{(1-v_t)^2} &= \frac{w(1-w)u(1-u)}{(1-v)^2}. \end{aligned} \quad (4.4.7)$$

We can solve these equations for v_t and w_t , giving,

$$v_t = 1 - \frac{(1-v)u_t(1-u_t)}{u(1-w) + (w-u)u_t}, \quad w_t = \frac{(1-u)wu_t}{u(1-w) + (w-u)u_t}. \quad (4.4.8)$$

Finally, we can change variables so that u_t becomes the integration variable. Calculating the Jacobian, we find,

$$\frac{d \ln y_v}{du_t} = \frac{d \ln y_v}{d \ln t} \frac{d \ln t}{du_t} = \frac{(1-y_v)(1-y_u y_v y_w)}{y_v(1-y_w y_u)} \frac{1}{u_t(u_t-1)} = \frac{\sqrt{\Delta_t}}{v_t u_t(u_t-1)}, \quad (4.4.9)$$

where $\Delta_t \equiv \Delta(u_t, v_t, w_t)$. There are two natural basepoints for the integration: $u_t = 0$, for which $y_v = 1$ and $(u, v, w) = (0, 1, 0)$; and $u_t = 1$, for which $y_v = 1/(y_u y_w)$ and $(u, v, w) = (1, 1, 1)$. Both choices have the convenient property that they correspond to a surface in terms the variables (y_u, y_v, y_w) but only to a single point in terms of the variables (u, v, w) . This latter fact allows for the simple specification of boundary data.

For most purposes, we choose to integrate off of the point $u_t = 1$, in which case we find the following solution to the differential equation,

$$\begin{aligned} F(u, v, w) &= F(1, 1, 1) + \int_{\frac{1}{y_u y_w}}^{y_v} d \ln \hat{y}_v \frac{\partial F}{\partial \ln y_v}(y_u, \hat{y}_v, y_w) \\ &= F(1, 1, 1) + \int_1^u \frac{du_t}{u_t(u_t-1)} \frac{\sqrt{\Delta_t}}{v_t} \frac{\partial F}{\partial \ln y_v}(u_t, v_t, w_t) \\ &= F(1, 1, 1) - \sqrt{\Delta} \int_1^u \frac{du_t}{v_t[u(1-w) + (w-u)u_t]} \frac{\partial F}{\partial \ln y_v}(u_t, v_t, w_t). \end{aligned} \quad (4.4.10)$$

The last step follows from the observation that $\sqrt{\Delta}/(1-v)$ is independent of y_v , which implies

$$\frac{\sqrt{\Delta_t}}{1-v_t} = \frac{\sqrt{\Delta}}{1-v}. \quad (4.4.11)$$

The integral representation (4.4.10) for F may be ill-defined if the integrand diverges at the lower endpoint of integration, $u_t = 1$ or $(u, v, w) = (1, 1, 1)$. On the other hand, for F to be a valid hexagon function, it must be regular near this point,

and therefore no such divergence can occur. In fact, this condition is closely related to the constraint of good branch-cut behavior near $u = 1$ discussed in section 4.3.4. As we build up integral representations for hexagon functions, we will use this condition to help fix various undetermined constants.

Furthermore, if F is a parity-odd function, we may immediately conclude that $F(1, 1, 1) = 0$, since this point corresponds to the surface $y_u y_v y_w = 1$. If F is parity-even, we are free to define the function by the condition that $F(1, 1, 1) = 0$. We use this definition for all basis functions, except for $\Omega^{(2)}(u, v, w)$, whose value at $(1, 1, 1)$ is specified by its correspondence to a particular Feynman integral.

While eq. (4.4.10) gives a representation that can be evaluated numerically for most points in the unit cube of cross ratios $0 \leq u_i \leq 1$, it is poorly suited for Region I. The problem is that the integration contour leaves the unit cube, requiring a cumbersome analytic continuation of the integrand. One may avoid this issue by integrating along the same contour, but instead starting at the point $u_t = 0$ or $(u, v, w) = (0, 1, 0)$. The resulting representation is,

$$F(u, v, w) = F(0, 1, 0) - \sqrt{\Delta} \int_0^u \frac{du_t}{v_t[u(1-w) + (w-u)u_t]} \frac{\partial F}{\partial \ln y_v}(u_t, v_t, w_t). \quad (4.4.12)$$

If F is a parity-odd function, then the boundary value $F(0, 1, 0)$ must vanish, since this point corresponds to the EMRK limit $y_v \rightarrow 1$. In the parity-even case, there is no such condition, and in many cases this limit is in fact divergent. Therefore, in contrast to eq. (4.4.10), this expression may require some regularization near the $u_t = 0$ endpoint in the parity-even case.

It is also possible to integrate the differential equation (4.4.5). In this case, we look for a contour where y_v and $y_u y_w$ are held constant, while the ratio y_u/y_w is allowed to vary. The result is a contour (u_t, v_t, w_t) defined by,

$$v_t = \frac{vu_t(1-u_t)}{uw + (1-u-w)u_t}, \quad w_t = \frac{uw(1-u_t)}{uw + (1-u-w)u_t}. \quad (4.4.13)$$

Again, there are two choices for specifying the boundary data: either we set $y_u/y_w = y_u y_w$ for which we may take $u_t = 0$ and $(u, v, w) = (0, 0, 1)$; or $y_u/y_w = 1/(y_u y_w)$, for

which we may take $u_t = 1$ and $(u, v, w) = (1, 0, 0)$. We therefore obtain two different integral representations,

$$\begin{aligned} F(u, v, w) &= F(0, 0, 1) + \int_0^u \frac{du_t \sqrt{\Delta_t}}{u_t(1-u_t)(1-v_t)} \frac{\partial F}{\partial \ln(y_u/y_w)}(u_t, v_t, w_t) \\ &= F(0, 0, 1) + \sqrt{\Delta} \int_0^u \frac{du_t}{(1-v_t)[uw + (1-u-w)u_t]} \frac{\partial F}{\partial \ln(y_u/y_w)}(u_t, v_t, w_t), \end{aligned} \quad (4.4.14)$$

and,

$$F(u, v, w) = F(1, 0, 0) + \sqrt{\Delta} \int_1^u \frac{du_t}{(1-v_t)[uw + (1-u-w)u_t]} \frac{\partial F}{\partial \ln(y_u/y_w)}(u_t, v_t, w_t). \quad (4.4.15)$$

Here we used the relation,

$$\frac{\sqrt{\Delta_t}}{v_t} = \frac{\sqrt{\Delta}}{v}, \quad (4.4.16)$$

which follows from the observation that $\sqrt{\Delta}/v$ is constant along either integration contour. Finally, we remark that the boundary values $F(1, 0, 0)$ and $F(0, 0, 1)$ must vanish for parity-odd functions, since the points $(1, 0, 0)$ and $(0, 0, 1)$ lie on the $\Delta = 0$ surface. In the parity-even case, there may be issues of regularization near the endpoints, just as discussed for eq. (4.4.12).

Altogether, there are six different contours, corresponding to the three cyclic images of the two types of contours just described. They may be labeled by the y -variables or their ratios that are allowed to vary along the contour: $y_u, y_v, y_w, y_u/y_w, y_v/y_u$, and y_w/y_v . The base points for these contours together encompass $(1, 1, 1)$, $(0, 1, 0)$, $(1, 0, 0)$ and $(0, 0, 1)$, the four corners of a tetrahedron whose edges lie on the intersection of the surface $\Delta = 0$ with the unit cube. See fig. 4.2 for an illustration of the contours passing through the point $(u, v, w) = (\frac{3}{4}, \frac{1}{4}, \frac{1}{2})$.

4.4.2 Constructing the hexagon functions

In this subsection, we describe how to construct differential equations and integral representations for the basis of hexagon functions. We suppose that we do not have

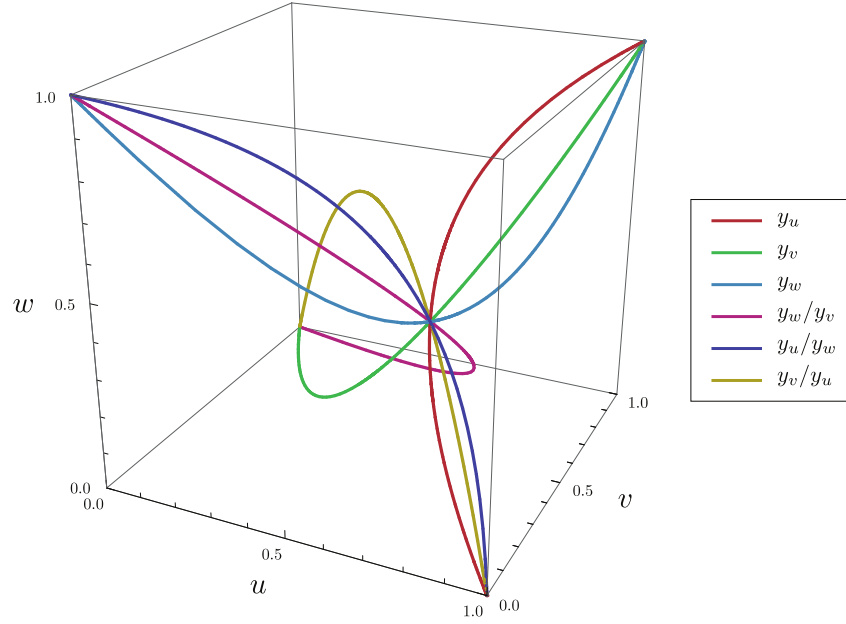


Figure 4.2: The six different integration contours for the point $(u, v, w) = (\frac{3}{4}, \frac{1}{4}, \frac{1}{2})$, labeled by the y -variables (or their ratios) that vary along the contour.

any of the function-level data that we obtained from the analysis of section 4.3; instead, we will develop a completely independent alternative method starting from the symbol. The two approaches are complementary and provide important cross-checks of one another.

In section 4.3.1, we presented the construction of the basis of hexagon functions at symbol level. Here we will promote these symbols to functions in a three-step iterative process:

1. Use the symbol of a given weight- n function to write down an ansatz for the $\{n-1, 1\}$ component of its coproduct in terms of a function-level basis at weight $n-1$ that we assume to be known.
2. Fix the undetermined parameters in this ansatz by imposing various function-level consistency conditions. These conditions are:
 - (a) Symmetry. The symmetries exhibited by the symbol should carry over to the function.

- (b) Integrability. The ansatz should be in the image of $\Delta_{n-1,1}$. This condition is equivalent to the consistency of mixed partial derivatives.
 - (c) Branch cuts. The only allowed branch cuts start when a cross ratio vanishes or approaches infinity.
3. Integrate the resulting coproduct using the methods of the previous subsection, specifying the boundary value and thereby obtaining a well-defined function-level member of the hexagon basis.

Let us demonstrate this procedure with some examples. Recalling the discussion in section 4.3.1, any function whose symbol contains no y variables can be written as products of single-variable HPLs. Therefore, the first nontrivial example occurs at weight three. As previously mentioned, this function corresponds to the one-loop six-dimensional hexagon integral, $\tilde{\Phi}_6$. Its symbol is given by,

$$\mathcal{S}(\tilde{\Phi}_6) = \left[-u \otimes v - v \otimes u + u \otimes (1-u) + v \otimes (1-v) + w \otimes (1-w) \right] \otimes y_w + \text{cyclic} . \quad (4.4.17)$$

It is straightforward to identify the object in brackets as the symbol of a linear combination of weight-two hexagon functions (which are just HPLs), allowing us to write an ansatz for the $\{2, 1\}$ component of the coproduct,

$$\Delta_{2,1}(\tilde{\Phi}_6) = - \left[\ln u \ln v + \text{Li}_2(1-u) + \text{Li}_2(1-v) + \text{Li}_2(1-w) + a\zeta_2 \right] \otimes \ln y_w + \text{cyclic} , \quad (4.4.18)$$

for some undetermined rational number a .

The single constant, a , can be fixed by requiring that $\tilde{\Phi}_6$ have the same symmetries as its symbol. In particular, we demand that $\tilde{\Phi}_6$ be odd under parity. As discussed in the previous section, this implies that it must vanish in the limit that one of the y_i goes to unity. In this EMRK limit (4.3.50), the corresponding u_i goes to unity while the other two cross ratios go to zero. The right-hand side of eq. (4.4.18) vanishes in this limit only for the choice $a = -2$. So we can write,

$$\Delta_{2,1}(\tilde{\Phi}_6) = -\Omega^{(1)}(u, v, w) \otimes \ln y_w + \text{cyclic} , \quad (4.4.19)$$

where,

$$\begin{aligned}\Omega^{(1)}(u, v, w) &= \ln u \ln v + \text{Li}_2(1 - u) + \text{Li}_2(1 - v) + \text{Li}_2(1 - w) - 2\zeta_2 \\ &= H_2^u + H_2^v + H_2^w + \ln u \ln v - 2\zeta_2,\end{aligned}\tag{4.4.20}$$

confirming the expression given in eq. (4.2.21). It is also straightforward to verify that eq. (4.4.18) is integrable and that it does not encode improper branch cuts. We will not say more about these conditions here, but we will elaborate on them shortly, in the context of our next example.

Now that we have the coproduct, we can use eqs. (4.4.4) and (4.4.5) to immediately write down the differential equations,

$$\frac{\partial \tilde{\Phi}_6}{\partial \ln y_v} = -\Omega^{(1)}(w, u, v),\tag{4.4.21}$$

$$\frac{\partial \tilde{\Phi}_6}{\partial \ln(y_u/y_w)} = -\Omega^{(1)}(v, w, u) + \Omega^{(1)}(u, v, w) = \ln(u/w) \ln v.\tag{4.4.22}$$

These derivatives lead, via eqs. (4.4.10) and (4.4.14), to the following integral representations:

$$\tilde{\Phi}_6 = \sqrt{\Delta(u, v, w)} \int_1^u \frac{du_t \Omega^{(1)}(w_t, u_t, v_t)}{v_t[u(1 - w) + (w - u)u_t]},\tag{4.4.23}$$

with (u_t, v_t, w_t) as in eq. (4.4.8), or

$$\tilde{\Phi}_6 = \sqrt{\Delta(u, v, w)} \int_0^u \frac{du_t \ln(u_t/w_t) \ln v_t}{(1 - v_t)[uw + (1 - u - w)u_t]},\tag{4.4.24}$$

with (u_t, v_t, w_t) as in eq. (4.4.13). We have set the integration constants to zero because $\tilde{\Phi}_6$ is a parity-odd function.

We have now completed the construction of the hexagon basis through weight three. Moving on to weight four, the symbol-level classification reveals one new parity-even function, $\Omega^{(2)}(u, v, w)$, and one new parity-odd function, $F_1(u, v, w)$, as well as their cyclic images. We will discuss the parity-even function $\Omega^{(2)}(u, v, w)$ since it exhibits a variety of features that the parity-odd functions lack.

As discussed in section 4.2, $\Omega^{(2)}(u, v, w)$ is an extra-pure function, and as such its

symbol has only three distinct final entries, which were given in eq. (4.2.18),

$$\text{final entry} \in \left\{ \frac{u}{1-u}, \frac{v}{1-v}, y_u y_v \right\}. \quad (4.4.25)$$

Furthermore, the symbol is symmetric under the exchange of u with v . Taken together, these symmetry properties dictate the form of the $\{3, 1\}$ component of the coproduct,

$$\Delta_{3,1}(\Omega^{(2)}(u, v, w)) = \Omega^{(2),u} \otimes \ln\left(\frac{u}{1-u}\right) + \Omega^{(2),u} \Big|_{u \leftrightarrow v} \otimes \ln\left(\frac{v}{1-v}\right) + \Omega^{(2),y_u} \otimes \ln y_u y_v. \quad (4.4.26)$$

There are two independent functions in eq. (4.4.26), $\Omega^{(2),u}$ and $\Omega^{(2),y_u}$. The symbols of these functions can be read off from the symbol of $\Omega^{(2)}(u, v, w)$. Both functions must be valid hexagon functions of weight three. The symbol indicates that $\Omega^{(2),u}$ is parity-even and $\Omega^{(2),y_u}$ is parity-odd.

The most general linear combination of parity-even hexagon functions of weight three whose symbol is consistent with that of $\Omega^{(2),u}$ is

$$\begin{aligned} \Omega^{(2),u} = & H_3^u + H_{2,1}^v - H_{2,1}^w - \frac{1}{2} \ln(uw/v) (H_2^u + H_2^w) + \frac{1}{2} \ln(uv/w) H_2^v \\ & + \frac{1}{2} \ln u \ln v \ln(v/w) + a_1 \zeta_2 \ln u + a_2 \zeta_2 \ln v + a_3 \zeta_2 \ln w + a_4 \zeta_3, \end{aligned} \quad (4.4.27)$$

for four arbitrary rational numbers a_i . There is only a single parity-odd hexagon function of weight three, so $\Omega^{(2),y_u}$ is uniquely determined from its symbol,

$$\Omega^{(2),y_u} = -\frac{1}{2} \tilde{\Phi}_6. \quad (4.4.28)$$

It is not necessarily the case that the right hand side of eq. (4.4.26) is actually the $\{3, 1\}$ component of the coproduct of a well-defined function for arbitrary values of the parameters a_i . This integrability condition can be formalized by the requirement that the operator

$$(\text{id} \otimes d \wedge d)(\Delta_{2,1} \otimes \text{id}) \quad (4.4.29)$$

annihilate the right hand side of eq. (4.4.26). To see this, note that $(\Delta_{2,1} \otimes \text{id}) \circ$

$\Delta_{3,1} = \Delta_{2,1,1}$, and therefore $d \wedge d$ acts on the the last two slots, which are just weight-one functions (logarithms). This can be recognized as the familiar symbol-level integrability condition, eq. (4.2.2), promoted to function-level.

Another way of thinking about the integrability condition is that it guarantees the consistency of mixed partial derivatives. Since there are three variables, there are three pairs of derivatives to check. To illustrate the procedure, we will examine one pair of derivatives by verifying the equation,

$$\sqrt{\Delta} \frac{\partial}{\partial \ln y_w} \left[\frac{\partial \Omega^{(2)}(u, v, w)}{\partial \ln(y_v/y_u)} \right] = \sqrt{\Delta} \frac{\partial}{\partial \ln(y_v/y_u)} \left[\frac{\partial \Omega^{(2)}(u, v, w)}{\partial \ln y_w} \right]. \quad (4.4.30)$$

We have multiplied by an overall factor of $\sqrt{\Delta}$ for convenience. To simplify the notation, let us define,

$$U \equiv \Omega^{(2),u} \quad \text{and} \quad V \equiv \Omega^{(2),u}|_{u \leftrightarrow v}. \quad (4.4.31)$$

Then, using eqs. (4.4.4) and (4.4.5), we can immediately write down an expression for the left-hand side of eq. (4.4.30),

$$\begin{aligned} \sqrt{\Delta} \frac{\partial}{\partial \ln y_w} \left[\frac{\partial \Omega^{(2)}(u, v, w)}{\partial \ln(y_v/y_u)} \right] &= \sqrt{\Delta} \frac{\partial}{\partial \ln y_w} \left[-\frac{1-w}{\sqrt{\Delta}}(U - V) \right] \\ &= (1-w)^2(1-u-v)(V^w - U^w) \\ &\quad + w(1-w)(U^u + U^v + U^{1-w} - V^u - V^v - V^{1-w}) \\ &\quad - uw(1-w)(U^u + U^{1-u} + U^{1-w} - V^u - V^{1-u} - V^{1-w}) \\ &\quad - vw(1-w)(U^v + U^{1-v} + U^{1-w} - V^v - V^{1-v} - V^{1-w}). \end{aligned} \quad (4.4.32)$$

The algebra leading to the second line may be simplified by using the fact that $(1-w)/\sqrt{\Delta}$ is independent of y_w . Similarly, it is straightforward to write down an

expression for the right-hand side of eq. (4.4.30),

$$\begin{aligned}
\sqrt{\Delta} \frac{\partial}{\partial \ln(y_v/y_u)} \left[\frac{\partial \Omega^{(2)}(u, v, w)}{\partial \ln y_w} \right] &= \sqrt{\Delta} \frac{\partial}{\partial \ln(y_v/y_u)} \left[-\frac{w}{\sqrt{\Delta}} (U + V) \right] \\
&= -w(1-w)(U^v - U^u + V^v - V^u) \\
&\quad - uw(1-w)(U^w + U^u + U^{1-u} + V^w + V^u + V^{1-u}) \\
&\quad + vw(1-w)(U^w + U^v + U^{1-v} + V^w + V^v + V^{1-v}) \\
&\quad + w^2(u-v)(U^{1-w} + V^{1-w}),
\end{aligned} \tag{4.4.33}$$

where we have used the fact that $w/\sqrt{\Delta}$ is annihilated by $\partial/\partial \ln(y_v/y_u)$.

As usual, the superscripts indicate the various coproduct components. A special feature of this example is that the functions U and V are built entirely from single-variable HPLs, so it is straightforward to extract these coproduct components using the definitions in appendix C.1. More generally, the functions may contain non-HPL elements of the hexagon basis. For these cases, the coproduct components are already known from previous steps in the iterative construction of the basis.

The nonzero coproduct components of U are,

$$\begin{aligned}
U^u &= -\frac{1}{2} \left(H_2^u - H_2^v + H_2^w - \ln v \ln(v/w) \right) + a_1 \zeta_2, \\
U^v &= \frac{1}{2} \left(H_2^u + H_2^v + H_2^w + 2 \ln u \ln v - \ln u \ln w \right) + a_2 \zeta_2, \\
U^w &= -\frac{1}{2} \left(H_2^u + H_2^v + H_2^w + \ln u \ln v \right) + a_3 \zeta_2, \\
U^{1-u} &= H_2^u + \frac{1}{2} \ln u \ln(uw/v), \\
U^{1-v} &= -\frac{1}{2} \ln v \ln(u/w), \\
U^{1-w} &= \frac{1}{2} \ln w \ln(u/v),
\end{aligned} \tag{4.4.34}$$

while those of V are related by symmetry,

$$\begin{aligned} V^u &= U^v, & V^v &= U^u, & V^w &= U^w|_{u \leftrightarrow v}, \\ V^{1-u} &= U^{1-v}, & V^{1-v} &= U^{1-u}, & V^{1-w} &= U^{1-w}|_{u \leftrightarrow v}. \end{aligned} \quad (4.4.35)$$

Using eqs. (4.4.33), (4.4.34), and (4.4.35), it is straightforward to check that the equality of mixed-partial derivatives, eq. (4.4.30), is satisfied if and only if $a_2 = -a_3$.

Continuing in this way, we can derive similar constraints from the remaining two mixed partial derivative consistency conditions. The result is that

$$a_2 = -1, \quad \text{and} \quad a_3 = 1. \quad (4.4.36)$$

Finally, we must impose good branch-cut behavior. As discussed in section 4.3.4, this constraint can be implemented by imposing eq. (4.3.52), or, in this case,

$$U(1, 0, 0) = 0, \quad (4.4.37)$$

which implies that $a_4 = 0$.

The one remaining parameter, a_1 , corresponds to an ambiguity that cannot be fixed by considering mathematical consistency conditions. Indeed, it arises from a well-defined weight-four function with all the appropriate symmetries and mathematical properties. In particular, it is the product of ζ_2 with an extra-pure weight-two hexagon function that is symmetric under $u \leftrightarrow v$,

$$-\zeta_2 \left[\text{Li}_2(1 - 1/u) + \text{Li}_2(1 - 1/v) \right]. \quad (4.4.38)$$

In general, we would resolve such an ambiguity by making an arbitrary (though perhaps convenient) choice in order to define the new hexagon function. But because $\Omega^{(2)}(u, v, w)$ corresponds to a particular Feynman integral, the value of a_1 is not arbitrary, and the only way to fix it is to bring in specific data about that integral. We are not interested in determining the value of a_1 directly from the Feynman integral since this integral has been evaluated previously [71]. Instead, we will be

satisfied simply to verify that a consistent value of a_1 exists.

From eq. (4.4.33) we have,

$$\sqrt{\Delta} \frac{\partial \Omega^{(2)}(u, v, w)}{\partial \ln y_w} = -w (U + V) , \quad (4.4.39)$$

$$\sqrt{\Delta} \frac{\partial \Omega^{(2)}(u, v, w)}{\partial \ln(y_v/y_u)} = -(1 - w) (U - V) . \quad (4.4.40)$$

Equation (4.4.39) is consistent with the differential equations of section 4 of ref. [71] only if the function Q_ϕ from that reference (and eq. (4.2.28)) is related to U and V by,

$$Q_\phi = -(U + V) . \quad (4.4.41)$$

This equation is satisfied, provided that $a_1 = 1$. Having fixed all a_i , we have uniquely determined the $\{3, 1\}$ component of the coproduct of $\Omega^{(2)}(u, v, w)$. Indeed, eq. (4.4.26) is consistent with the expressions in eqs. (4.2.19) and (4.2.28), as of course it must be.

We remark that the antisymmetric combination appearing in eq. (4.4.40) is related to another function defined in ref. [71],

$$\tilde{Z}(v, w, u) = -2(U - V) , \quad (4.4.42)$$

where \tilde{Z} appears in a derivative of the odd part of the NMHV ratio function (see eq. (C.2.19)).

Following the discussion in section 4.4.1, the differential equation eq. (4.4.39) gives rise to the integral representation,

$$\Omega^{(2)}(u, v, w) = -6\zeta_4 + \int_1^u du_t \frac{Q_\phi(u_t, v_t, w_t)}{u_t(u_t - 1)} , \quad (4.4.43)$$

where,

$$v_t = \frac{(1 - u)vu_t}{u(1 - v) + (v - u)u_t} , \quad w_t = 1 - \frac{(1 - w)u_t(1 - u_t)}{u(1 - v) + (v - u)u_t} . \quad (4.4.44)$$

While our conventions for generic hexagon functions require the functions to vanish at the boundary value $(1, 1, 1)$, in this specific case we must specify a nonzero value $\Omega^{(2)}(1, 1, 1) = -6\zeta_4$ in order to match a prior definition of the function.

The differential equation (4.4.40) gives rise to another integral representation for $\Omega^{(2)}$,

$$\Omega^{(2)}(u, v, w) = \frac{1}{2} \int_0^v \frac{dv_t \tilde{Z}(v_t, w_t, u_t)}{v_t(1-v_t)}, \quad (4.4.45)$$

where,

$$u_t = \frac{uv(1-v_t)}{uv + (1-u-v)v_t}, \quad w_t = \frac{wv_t(1-v_t)}{uv + (1-u-v)v_t}. \quad (4.4.46)$$

There is no constant of integration in eq. (4.4.45) because in this case $\Omega^{(2)}$ vanishes at the lower endpoint, $\Omega^{(2)}(1, 0, 0) = 0$ [71, 158].

Continuing onward, we construct the remaining functions of the hexagon basis in an iterative fashion, using the above methods. We collect the results through weight five in appendix C.2. We present the data by the $\{n-1, 1\}$ component of the coproduct, plus the constraint that the functions vanish at $(u, v, w) = (1, 1, 1)$ (except for the special case of $\Omega^{(2)}$). With this information, we can build an ansatz for the three-loop remainder function, as we discuss in the next subsection.

4.4.3 Constructing the three-loop remainder function

In this subsection, we complete the construction of an ansatz for the three-loop remainder function. We use the decomposition (4.2.29) of the symbol of $R_6^{(3)}$ as a template, and extend it to a definition of the function using the same steps as in section 4.4.2:

1. From the symbol of the extra-pure function $R_{\text{ep}}(u, v, w)$, which depends on α_1 and α_2 , we expand the $\{5, 1\}$ components of its coproduct in terms of our weight-five basis functions. These functions can be given as multiple polylogarithms, as in section 4.3.4, or as integral representations, as in section 4.4.2. We also allow for the addition of zeta values multiplying lower-weight basis functions.

2. We fix as many undetermined parameters in this ansatz as possible by enforcing various mathematical consistency conditions. In particular,
 - (a) We impose extra-purity and symmetry in the exchange of u and v as function-level conditions on the coproduct entries, since these conditions are satisfied at symbol level:

$$\begin{aligned} R_{\text{ep}}^v &= -R_{\text{ep}}^{1-v} = -R_{\text{ep}}^{1-u}(u \leftrightarrow v) = R_{\text{ep}}^u(u \leftrightarrow v), \\ R_{\text{ep}}^{yv} &= R_{\text{ep}}^{yu}, \quad R_{\text{ep}}^w = R_{\text{ep}}^{1-w} = R_{\text{ep}}^{yw} = 0. \end{aligned} \tag{4.4.47}$$

In principle, beyond-the-symbol terms do not need to obey the extra-purity relations. At the end of section 4.5, we will relax this assumption and use the near-collinear limits to show that the potential additional terms vanish.

- (b) We demand that the ansatz be integrable. For the multiple polylogarithm approach, this amounts to verifying that there is a weight-six function with our ansatz as the $\{5, 1\}$ component of its coproduct. For the approach based on integral representations, we check that there are consistent mixed partial derivatives.
 - (c) We require that the resulting function have the proper branch-cut structure. We impose this constraint by verifying that there are no spurious poles in the first derivatives, just as we did in the construction of the hexagon basis.

After imposing these constraints, there are still nine undetermined beyond-the-symbol parameters. They correspond to well-defined extra-pure hexagon functions of weight six, and cannot be fixed by mathematical consistency conditions.

3. We integrate the resulting coproduct. This result is a weight-six function, $R_{\text{ep}}^{(\alpha_1, \alpha_2)}$, which depends on the symbol-level constants, α_1 and α_2 , and nine lower-weight functions r_1, \dots, r_9 , which come multiplied by zeta values. The r_i may be expressed in terms of previously-determined hexagon functions, while

$R_{\text{ep}}^{(\alpha_1, \alpha_2)}$ may be given as an integral representation or explicitly in terms of multiple polylogarithms.

This procedure leaves us with the following ansatz for $R_6^{(3)}$:

$$R_6^{(3)}(u, v, w) = \left[\left(R_{\text{ep}}^{(\alpha_1, \alpha_2)}(u, v, w) + \sum_{i=1}^9 c_i r_i(u, v) \right) + \text{cyclic} \right] + P_6(u, v, w) \quad (4.4.48)$$

$$+ c_{10} \zeta_6 + c_{11} (\zeta_3)^2.$$

where the c_i are undetermined rational numbers, and

$$\begin{aligned} r_1 &= \zeta_4 \left[H_2^u + \frac{1}{2} \ln^2 u + (u \leftrightarrow v) \right], \\ r_2 &= \zeta_3 \left[H_{2,1}^u - \frac{1}{6} \ln^3 u + (u \leftrightarrow v) \right], \\ r_3 &= \zeta_3 \left[H_3^u - 2H_{2,1}^u + H_1^u H_2^u + (u \leftrightarrow v) \right], \\ r_4 &= \zeta_2 \left[H_4^u + H_1^u H_3^u - \frac{1}{2} (H_2^u)^2 + (u \leftrightarrow v) \right], \\ r_5 &= \zeta_2 \left[H_4^u - 3H_{2,1,1}^u + H_1^u H_3^u + \frac{1}{2} (H_1^u)^2 H_2^u + (u \leftrightarrow v) \right], \\ r_6 &= \zeta_2 \left[H_{3,1}^u - 3H_{2,1,1}^u + H_1^u H_{2,1}^u + (u \leftrightarrow v) \right], \\ r_7 &= \zeta_2 \left[H_{2,1,1}^u + \frac{1}{24} (H_1^u)^4 + (u \leftrightarrow v) \right], \\ r_8 &= \zeta_2 \left(H_2^u + \frac{1}{2} \ln^2 u \right) \left(H_2^v + \frac{1}{2} \ln^2 v \right), \\ r_9 &= \zeta_2 \Omega^{(2)}(u, v, w). \end{aligned} \quad (4.4.49)$$

In the following section we will use the collinear limits of this expression to fix α_1 , α_2 and the c_i . After fixing these parameters, we can absorb all but the constant terms into a redefinition of R_{ep} . The $\{5, 1\}$ component of its coproduct is given in appendix C.3. The final integral representation for $R_6^{(3)}$, having fixed also c_{10} and c_{11} , is given in section 4.7, eq. (4.7.1). The final expression in terms of multiple polylogarithms is quite lengthy, but it is provided in a computer-readable format in the attached files.

4.5 Collinear limits

In the previous section, we constructed a 13-parameter ansatz for the three-loop remainder function. It has the correct symbol, proper branch structure, and total S_3 symmetry in the cross ratios. In other words, the ansatz obeys all relevant mathematical consistency conditions. So in order to fix the undetermined constants, we need to bring in some specific physical data.

Some of the most useful data available comes from the study of the collinear limit. In the strict collinear limit in which two gluons are exactly collinear, the remainder function must vanish to all loop orders. This condition fixes many, but not all, of the parameters in our ansatz. To constrain the remaining constants, we expand in the near-collinear limit, keeping track of the power-suppressed terms. These terms are predicted by the OPE for flux tube excitations. In fact, the information about the leading discontinuity terms in the OPE [38–40] was already incorporated at symbol level and used to constrain the symbol for the three-loop remainder function up to two undetermined parameters [14].

Here we take the same limit at function level, and compare to the recent work of Basso, Sever and Vieira (BSV) [150], which allows us to uniquely constrain all of the beyond-the-symbol ambiguities, as well as the two symbol-level parameters. The two symbol-level parameters were previously fixed by using dual supersymmetry [45], and also by studying the near-collinear limit at symbol level [150], and we agree with both of these determinations.

4.5.1 Expanding in the near-collinear limit

In the (Euclidean) limit that two gluons become collinear, one of the cross ratios goes to zero and the sum of the other cross ratios goes to one. For example, if we let k_2 and k_3 become parallel, then $x_{24}^2 \equiv (k_2 + k_3)^2 \rightarrow 0$, corresponding to $v \rightarrow 0$, and $u + w \rightarrow 1$. BSV [150] provide a convenient set of variables (τ, σ, ϕ) with which one

can approach this collinear limit. They are related to the (u_i, y_i) variables by [152]:

$$\begin{aligned}
u &= \frac{FS^2}{(1+T^2)(F+FS^2+ST+F^2ST+FT^2)}, \\
v &= \frac{T^2}{1+T^2}, \\
w &= \frac{F}{F+FS^2+ST+F^2ST+FT^2}, \\
y_u &= \frac{FS+T}{F(S+FT)}, \\
y_v &= \frac{(S+FT)(1+FST+T^2)}{(FS+T)(F+ST+FT^2)}, \\
y_w &= \frac{F+ST+FT^2}{F(1+FST+T^2)}.
\end{aligned} \tag{4.5.1}$$

where $T = e^{-\tau}$, $S = e^\sigma$, and $F = e^{i\phi}$.

As $T \rightarrow 0$ ($\tau \rightarrow \infty$) we approach the collinear limit. The parameter S controls the partitioning of the momentum between the two collinear gluons, according to $k_2/k_3 \sim S^2$, or $k_2/(k_2+k_3) \sim S^2/(1+S^2)$. The parameter F controls the azimuthal dependence as the two gluons are rotated around their common axis with respect to the rest of the scattering process. This dependence is related to the angular momentum of flux-tube excitations in the OPE interpretation.

By expanding an expression in T we can probe its behavior in the near-collinear limit, order by order in T . Each order in T also contains a polynomial in $\ln T$. In general, the expansions of parity even and odd hexagon functions f^{even} and f^{odd} have the form,

$$f^{\text{even}}(T, F, S) = \sum_{m=0}^{\infty} \sum_{n=0}^N \sum_{p=0}^m T^m (-\ln T)^n \cos^p \phi f_{m,n,p}^{\text{even}}(S), \tag{4.5.2}$$

$$f^{\text{odd}}(T, F, S) = 2i \sin \phi \sum_{m=1}^{\infty} \sum_{n=0}^N \sum_{p=0}^{m-1} T^m (-\ln T)^n \cos^p \phi f_{m,n,p}^{\text{odd}}(S). \tag{4.5.3}$$

Odd parity necessitates an extra overall factor of $\sin \phi$. The maximum degree of the polynomial in $e^{\pm i\phi}$ is m , the number of powers in the T expansion, which is related

to the twist of a flux tube excitation in the final answer. The maximum degree N of the polynomial in $\tau \equiv -\ln T$ satisfies $N = w - 2$ for the non-HPL hexagon functions with weight w in appendix C.3, although in principle it could be as large as $N = w$ for the $m = 0$ term (but only from the function $\ln^w v$), and as large as $N = w - 1$ when $m > 0$. For the final remainder function at L loops, with weight $w = 2L$, the leading discontinuity terms in the OPE imply a relatively small value of N compared to the maximum possible, namely $N = L - 1 = 2L - (L + 1)$ for $R_6^{(L)}$, or $N = 2$ for $R_6^{(3)}$.

BSV predict the full order T^1 behavior of the remainder function [150]. The part of the T^2 behavior that is simplest for them to predict (because it is purely gluonic) contains azimuthal variation proportional to $\cos^2 \phi$, *i.e.* the $T^2 F^2$ or $T^2 F^{-2}$ terms; however, they can also extract the $T^2 F^0$ behavior, which depends upon the scalar and fermionic excitations as well [152]. To compare with this data, we must expand our expression for $R_6^{(3)}$ to this order.

The expansion of an expression is relatively straightforward when its full analytic form is known, for example when the expression is given in terms of multiple polylogarithms. In this case, one merely needs to know how to take a derivative with respect to T and how to evaluate the functions at $T = 0$. The derivative of a generic multiple polylogarithm can be read off from its coproduct, which is given in appendix C.1. Evaluating the functions at $T = 0$ is more involved because it requires taking $y_u \rightarrow 1$ and $y_w \rightarrow 1$ simultaneously. However, the limit of all relevant multiple polylogarithms can be built up iteratively using the coproduct bootstrap of section 4.3.3.

If the expression is instead represented in integral form, or is defined through differential equations, then it becomes necessary to integrate up the differential equations, iteratively in the transcendental weight, and order by order in the T expansion. Recall that for any function in our basis we have a complete set of differential equations whose inhomogeneous terms are lower weight hexagon functions. The change of variables (4.5.1), and its Jacobian, allows us to go from differential equations in the u_i or y variables to differential equations in (F, S, T) .

The structure of the $T \rightarrow 0$ expansion makes most terms very straightforward to integrate. In eqs. (4.5.2) and (4.5.3), T only appears as powers of T , whose coefficients

are polynomials of fixed order in $\ln T$. The variable F only appears as a polynomial in $\cos \phi$ and $\sin \phi$, *i.e.* as powers of F and F^{-1} . Hence any T or F derivative can be integrated easily, up to a constant of integration, which can depend on S . The S derivatives require a bit of extra work. However, the differential equation in S is only required for the T and F independent term arising in the parity-even case, $f_{0,0,0}^{\text{even}}(S)$. This coefficient is always a pure function of the same transcendental weight as f itself, and it can be constructed from a complete set of HPLs in the argument $-S^2$. Thus we can integrate the one required differential equation in S by using a simple ansatz built out of HPLs.

There is still one overall constant of integration to determine for each parity-even function, a term that is completely independent of T , F and S . It is a linear combination of zeta values. (The parity-odd functions all vanish as $T \rightarrow 0$, so they do not have this problem.) The constant of integration can be determined at the endpoint $S = 0$ or $S = \infty$, with the aid of a second limiting line, $(u, v, w) = (u, u, 1)$. On this line, all the hexagon functions are very simple, collapsing to HPLs with argument $(1 - u)$. In the limit $u \rightarrow 0$ this line approaches the point $(0, 0, 1)$, which can be identified with the $S \rightarrow 0$ “soft-collinear” corner of the $T \rightarrow 0$ collinear limit in the parametrization (4.5.1). Similarly, the $S \rightarrow \infty$ corner of the $T \rightarrow 0$ limit intersects the line $(1, v, v)$ at $v = 0$. Both lines $(u, u, 1)$ and $(1, v, v)$ pass through the point $(1, 1, 1)$. At this point, (most of) the hexagon functions are defined to vanish, which fixes the integration constants on the $(u, u, 1)$ and $(1, v, v)$ lines. HPL identities then give the desired values of the functions in the soft-collinear corner, which is enough to fix the integration constant for the near-collinear limit. We will illustrate this method with an example below.

The coefficients of the power-suppressed terms that also depend on T and F , namely $f_{m,n,p}(S)$ in eqs. (4.5.2) and (4.5.3) for $m > 0$, are functions of S that involve HPLs with the same argument $-S^2$, but they also can include prefactors to the HPLs that are rational functions of S . The $f_{m,n,p}(S)$ for $m > 0$ generally have a mixed transcendental weight. Mixed transcendentality is common when series expanding generic HPLs around particular points. For example, expanding $\text{Li}_2(1 - x)$ around

$x = 0$ gives

$$\text{Li}_2(1-x) \sim \frac{\pi^2}{6} + x(\ln x - 1) + x^2\left(\frac{\ln x}{2} - \frac{1}{4}\right) + x^3\left(\frac{\ln x}{3} - \frac{1}{9}\right) + \mathcal{O}(x^4). \quad (4.5.4)$$

Using an HPL ansatz for the pure S -dependent terms, we use the differential equations to fix any unfixed parameters and cross-check the ansatz. Repeating this process order by order we build up the near-collinear limiting behavior of each element of the basis of hexagon functions as a series expansion.

4.5.2 Examples

In order to illustrate the collinear expansion, it is worthwhile to present a few low-weight examples. We begin with the simplest nontrivial example, the weight-three parity-odd function $\tilde{\Phi}_6$. Since $\tilde{\Phi}_6$ is fully symmetric in the u_i and vanishes in the collinear limit (like any parity-odd function), its expansion is particularly simple. To conserve space in later formulas, we adopt the notation,

$$s = S^2, \quad L = \ln S^2, \quad H_{\vec{w}} = H_{\vec{w}}(-S^2). \quad (4.5.5)$$

The expansion of $\tilde{\Phi}_6$ is then

$$\begin{aligned} \tilde{\Phi}_6 = & \frac{2iT \sin \phi}{S} \left[2 \ln T \left((1+s)H_1 + sL \right) - (1+s) \left(H_1^2 + (L+2)H_1 \right) - 2sL \right] \\ & + \frac{2iT^2 \cos \phi \sin \phi}{S^2} \left[-2 \ln T \left((1+s^2)H_1 + s(sL+1) \right) + (1+s^2)(H_1^2 + LH_1) \right. \\ & \quad \left. + (1+s)^2H_1 + s((1+s)L+1) \right] + \mathcal{O}(T^3). \end{aligned} \quad (4.5.6)$$

The sign of eq. (4.5.6), and of the collinear expansions of all of the parity-odd functions, depend on the values of the y variables used. This sign is appropriate to approaching the collinear limit from Region I, with $0 < y_i < 1$.

Because $\Omega^{(2)}$ lacks the symmetries of $\tilde{\Phi}_6$, its expansion must be evaluated in multiple channels, and it is substantially lengthier. Through order T^2 , we find,

$$\begin{aligned}
\Omega^{(2)}(u, v, w) = & \ln^2 T \left(2(H_2 + \zeta_2) + L^2 \right) + 2 \ln T \left(H_3 - 2(H_{2,1} - \zeta_3) - LH_2 \right) + H_4 - 4H_{3,1} \\
& + 4H_{2,1,1} + \frac{1}{2} \left(H_2^2 + L^2(H_2 + \zeta_2) \right) - L \left(H_3 - 2(H_{2,1} + \zeta_3) \right) + 2\zeta_2 H_2 + \frac{5}{2} \zeta_4 \\
& + \frac{T \cos \phi}{S} \left[-4 \ln^2 T \ s(H_1 + L) + 4 \ln T \left((1+s)H_1 + s(H_1^2 + L(H_1 + 1)) \right) \right. \\
& \quad + s \left(4(H_{2,1} - \zeta_3) - \frac{4}{3} H_1^3 - H_1(2H_2 + L^2) - 2L(H_1^2 + 2) - 2\zeta_2(2H_1 + L) \right) \\
& \quad \left. - 2(1+s)(H_1^2 + H_1(L + 2)) \right] \\
& + \frac{T^2}{S^2} \left\{ \cos^2 \phi \left[4 \ln^2 T \ s^2 \left(H_1 + L + \frac{1}{1+s} \right) \right. \right. \\
& \quad - 2 \ln T \left(2s^2 H_1(H_1 + L) + H_1 + s + \frac{s^2}{1+s} \left((5+s)H_1 + (3+s)L \right) \right) \\
& \quad + s^2 \left(-4(H_{2,1} - \zeta_3) + H_1(2H_2 + L^2 + 4\zeta_2) + \frac{4}{3} H_1^3 + 2L(H_1^2 + \zeta_2) \right) \\
& \quad + H_1(H_1 + L) + (1+3s) \left((1+s)H_1 + sL \right) + s \\
& \quad \left. + \frac{s^2}{1+s} \left((5+s)H_1(H_1 + L) - s(2H_2 + L^2) \right) + 2\zeta_2 \frac{s^2(1-s)}{1+s} \right] \\
& \quad - 2 \ln^2 T \ s((2+s)(H_1 + L) + 1) \\
& \quad + \ln T \left(s^2(2H_1(H_1 + L) + 3(H_1 + L)) + s(4H_1(H_1 + L + 1) + 2L + 3) + H_1 \right) \\
& \quad + s(2+s) \left(2H_{2,1} - H_1 H_2 - LH_1^2 - \frac{2}{3} H_1^3 - \frac{1}{2} L^2 H_1 - \zeta_2(2H_1 + L) - 2\zeta_3 \right) \\
& \quad - s \left(H_2 + \frac{1}{2} L^2 + 2\zeta_2 + \frac{3}{2} \right) - \frac{1}{2} \left((1+s)(1+3s)H_1(H_1 + L) + (1+5s)H_1 \right. \\
& \quad \left. \left. + s(3+7s)(H_1 + L) \right) \right\} + \mathcal{O}(T^3).
\end{aligned} \tag{4.5.7}$$

The integral $\Omega^{(2)}(u, v, w)$ is symmetric under the exchange of u and v . This

implies that the limiting behavior of $\Omega^{(2)}(v, w, u)$ can be determined from that of $\Omega^{(2)}(u, v, w)$ by exchanging the roles of u and w in the collinear limit. At leading order in T , this symmetry corresponds to letting $S \leftrightarrow 1/S$. This symmetry is broken by the parametrization (4.5.1) at order T^2 ; nevertheless, the correction at order T^2 is relatively simple,

$$\begin{aligned} \Omega^{(2)}(v, w, u) = \Omega^{(2)}(u, v, w) \Big|_{S \rightarrow \frac{1}{S}} + 4T^2 \Bigg[\ln^2 T H_1 - \ln T H_1(H_1 + L) - H_3 + H_{2,1} \\ - \frac{1}{2} \left(H_1(H_2 - \zeta_2) - L(H_2 + H_1^2) \right) + \frac{1}{3} H_1^3 \Bigg] + \mathcal{O}(T^3). \end{aligned} \quad (4.5.8)$$

The last independent permutation is $\Omega^{(2)}(w, u, v)$. It is symmetric under $u \leftrightarrow w$ and vanishes at order T^0 , which together imply that its near-collinear expansion is symmetric under $S \leftrightarrow 1/S$ through order T^2 , although that symmetry is not manifest in the HPL representation,

$$\begin{aligned} \Omega^{(2)}(w, u, v) = \frac{T \cos \phi}{S} (1 + s) \Big(2LH_2 - H_1(L^2 + 2\zeta_2) \Big) \\ + \frac{T^2}{S^2} \Big\{ \cos^2 \phi \Big[(1 + s^2) \Big(-2LH_2 + H_1(L^2 + 2\zeta_2) \Big) + 2(1 - s^2)H_2 \\ + s(1 - s)(L^2 + 2\zeta_2) - 2(1 + s)((1 + s)H_1 + sL) \Big] \\ - 2 \ln T (1 + s)((1 + s)H_1 + sL) \\ + (1 + s)^2 \Big[LH_2 - H_1 \Big(\frac{1}{2} L^2 + \zeta_2 - L - 3 \Big) + H_1^2 \Big] + 3s(1 + s)L \Big\} \\ + \mathcal{O}(T^3). \end{aligned} \quad (4.5.9)$$

We determine these expansions by integrating the differential equations in F , S , and T , as described in the previous subsection. For parity even functions, it is necessary to fix the constants of integration. Here we present one technique for doing so. Suppose we set $S = T$ in eq. (4.5.1). Then the limit $T \rightarrow 0$ corresponds to the EMRK limit, $u = v \rightarrow 0$, $w \rightarrow 1$, approached along the line $(u, u, 1)$. As an example, let us consider

applying this limit to the expansion of $\Omega^{(2)}(u, v, w)$, eq. (4.5.7). We only need to keep the T^0 terms, and among them we find that the $H_{\vec{w}}$ terms vanish, $L \rightarrow \ln u$, and $\ln T \rightarrow \frac{1}{2} \ln u$ (since $u \sim T^2$). Therefore, as $u \rightarrow 0$ we obtain,

$$\Omega^{(2)}(u, u, 1) = \frac{1}{4} \ln^4 u + \zeta_2 \ln^2 u + 4\zeta_3 \ln u + \frac{5}{2} \zeta_4 + \mathcal{O}(u). \quad (4.5.10)$$

The constant of integration, $\frac{5}{2} \zeta_4$, clearly survives in this limit. So, assuming we did not know its value, it could be fixed if we had an independent way of examining this limit.

This independent method comes from the line $(u, u, 1)$, on which all the hexagon function have simple representations. This can be seen from the form of the integration contour parametrized by v_t and w_t in eq. (4.4.8). Setting $v = u$ and $w = 1$, it collapses to

$$v_t = u_t, \quad w_t = 1. \quad (4.5.11)$$

The integral (4.4.43) then becomes

$$\Omega^{(2)}(u, u, 1) = -6\zeta_4 - \int_1^u \frac{du_t \omega^u(u_t, u_t, 1)}{u_t(u_t - 1)}, \quad (4.5.12)$$

where

$$\omega^u(u, u, 1) = [\Omega^{(2),u} + (u \leftrightarrow v)](u, u, 1) = 2 \left[H_3^u + H_{2,1}^u + \ln u H_2^u + \frac{1}{2} \ln^3 u \right]. \quad (4.5.13)$$

Such integrals can be computed directly using the definition (4.2.25) after a partial fraction decomposition of the factor $1/[u_t(u_t - 1)]$. Expressing the result in terms of the Lyndon basis (4.3.3) gives,

$$\begin{aligned} \Omega^{(2)}(u, u, 1) = & -2H_4^u - 2H_{3,1}^u + 6H_{2,1,1}^u + 2(H_2^u)^2 + 2 \ln u (H_3^u + H_{2,1}^u) \\ & + \ln^2 u H_2^u + \frac{1}{4} \ln^4 u - 6\zeta_4. \end{aligned} \quad (4.5.14)$$

At the point $u = 1$, all the $H_{\vec{w}}^u = H_{\vec{w}}(1 - u)$ vanish, as does $\ln u = -H_1^u$, so we see

that eq. (4.5.14) becomes

$$\Omega^{(2)}(1, 1, 1) = -6\zeta_4, \quad (4.5.15)$$

in agreement with the explicit $-6\zeta_4$ in eq. (4.5.12). In order to take the limit $u \rightarrow 0$, we use HPL identities to reexpress the function in terms of HPLs with argument u instead of $(1 - u)$:

$$\begin{aligned} \Omega^{(2)}(u, u, 1) = & \frac{1}{4} \ln^4 u + H_1(u) \ln^3 u + \left(-2H_2(u) + \frac{1}{2}(H_1(u))^2 + \zeta_2 \right) \ln^2 u \\ & + \left(4(H_3(u) - H_{2,1}(u) + \zeta_3) - \frac{1}{3}(H_1(u))^3 + 2\zeta_2 H_1(u) \right) \ln u \\ & - 6H_4(u) + 2H_{3,1}(u) + 2H_{2,1,1}(u) + 2(H_2(u))^2 + H_2(u)(H_1(u))^2 \\ & - 2(H_3(u) + H_{2,1}(u) - 2\zeta_3)H_1(u) - \zeta_2(4H_2(u) + (H_1(u))^2) + \frac{5}{2}\zeta_4. \end{aligned} \quad (4.5.16)$$

In the limit $u \rightarrow 0$, the $H_{\vec{w}}(u)$ vanish, leaving only the zeta values and powers of $\ln u$, which are in complete agreement with eq. (4.5.10). In particular, the coefficient of ζ_4 agrees, and this provides a generic method to determine such constants.

In this example, we inspected the $(u, u, 1)$ line, whose $u \rightarrow 0$ limit matches the $S \rightarrow 0$ limit of the $T \rightarrow 0$ expansion. One can also use the $(1, v, v)$ line in exactly the same way; its $v \rightarrow 0$ limit matches the $S \rightarrow \infty$ limit of the $T \rightarrow 0$ expansion.

Continuing on in this fashion, we build up the near-collinear expansions through order T^2 for all of the functions in the hexagon basis and ultimately of $R_6^{(3)}$ itself. The expansions are rather lengthy, but we present them in a computer-readable file attached to this document.

4.5.3 Fixing most of the parameters

In section 4.4.3 we constructed an ansatz (4.4.48) for $R_6^{(3)}$ that contains 13 undetermined rational parameters, after imposing mathematical consistency and extra-purity of R_{ep} . Two of the parameters affect the symbol: α_1 and α_2 . (They could have been fixed using a dual supersymmetry anomaly equation [45].) The remaining 11 parameters c_i we refer to as “beyond-the-symbol” because they accompany functions (or

constants) with Riemann ζ value prefactors. Even before we compare to the OPE expansion, the requirement that $R_6^{(3)}$ vanish at order T^0 in the collinear limit is already a powerful constraint. It represents 11 separate conditions when it is organized according to powers of $\ln T$, $\ln S^2$ and $H_{\vec{w}}(-S^2)$, as well as the Riemann ζ values. (There is no dependence on F at the leading power-law order.) The 11 conditions lead to two surviving free parameters. They can be chosen as α_2 and c_9 .

Within R_{ep} , the coefficient c_9 multiplies $\zeta_2 \Omega^{(2)}(u, v, w)$, as seen from eq. (4.4.49). However, after summing over permutations, imposing vanishing in the collinear limit, and using eq. (4.2.14), c_9 is found to multiply $\zeta_2 R_6^{(2)}$. It is clear that c_9 cannot be fixed at this stage (vanishing at order T^0) because the two-loop remainder function vanishes in all collinear limits. Furthermore, its leading discontinuity is of the form $T^m(\ln T)$, which is subleading with respect to the three-loop leading discontinuity, terms of the form $T^m(\ln T)^2$. It is rather remarkable that there is only one other ambiguity, α_2 , at this stage.

The fact that α_1 can be fixed at the order T^0 stage was anticipated in ref. [14]. There the symbol multiplying α_1 was extended to a full function, called f_1 . It was observed that the collinear limit of f_1 , while vanishing at symbol level, did not vanish at function level, and the limit contained a divergence proportional to $\zeta_2 \ln T$ times a particular function of S^2 . It was argued that this divergence should cancel against contributions from completing the α_i -independent terms in the symbol into a function. Now that we have performed this step, we can fix the value of α_1 . Indeed when we examine the $\zeta_2 \ln T$ terms in the collinear limit of the full $R_6^{(3)}$ ansatz, we obtain $\alpha_1 = -3/8$, in agreement with refs. [45, 150].

4.5.4 Comparison to flux tube OPE results

In order to fix α_2 and c_9 , as well as obtain many additional consistency checks, we examine the expansion of $R_6^{(3)}$ to order T and T^2 , and compare with the flux tube OPE results of BSV.

BSV formulate scattering amplitudes in planar $\mathcal{N} = 4$ super-Yang-Mills theory, or rather the associated polygonal Wilson loops, in terms of pentagon transitions. The

pentagon transitions map flux tube excitations on one edge of a light-like pentagon, to excitations on another, non-adjacent edge. They have found that the consistency conditions obeyed by the pentagon transitions can be solved in terms of factorizable S matrices for two-dimensional scattering of the flux tube excitations. These S matrices can in turn be determined nonperturbatively for any value of the coupling, as well as expanded in perturbation theory in order to compare with perturbative results [150, 151]. The lowest twist excitations dominate the near-collinear or OPE limit $\tau \rightarrow \infty$ or $T \rightarrow 0$. The twist n excitations first appear at $\mathcal{O}(T^n)$. In particular, the $\mathcal{O}(T^1)$ term comes only from a gluonic twist-one excitation, whereas at $\mathcal{O}(T^2)$ there can be contributions of pairs of gluons, gluonic bound states, and pairs of scalar or fermionic excitations. As mentioned above, BSV have determined the full order T^1 behavior [150], and an unpublished analysis gives the $T^2 F^2$ or $T^2 F^{-2}$ terms, plus the expansion of the $T^2 F^0$ terms around $S = 0$ through S^{10} [152].

BSV consider a particular ratio of Wilson loops, the basic hexagon Wilson loop, divided by two pentagons, and then multiplied back by a box (square). The pentagons and box combine to cancel off all of the cusp divergences of the hexagon, leading to a finite, dual conformally invariant ratio. We compute the remainder function, which can be expressed as the hexagon Wilson loop divided by the BDS ansatz [32] for Wilson loops. To relate the two formulations, we need to evaluate the logarithm of the BDS ansatz for the hexagon configuration, subtract the analogous evaluation for the two pentagons, and add back the one for the box. The pentagon and box kinematics are determined from the hexagon by intersecting a light-like line from a hexagon vertex with an edge on the opposite side of the hexagon [150]. For example, if we have lightlike momenta k_i , $i = 1, 2, \dots, 6$ for the hexagon, then one pentagon is found by replacing three of the momenta, say k_4, k_5, k_6 , with two light-like momenta, say k'_4 and k'_5 , having the same sum. Also, one of the new momenta has to be parallel to one of the three replaced momenta:

$$k'_4 + k'_5 = k_4 + k_5 + k_6, \quad k'_4 = \xi' k_4. \quad (4.5.17)$$

The requirement that k'_5 is a null vector implies that $\xi' = s_{123}/(s_{123} - s_{56})$, where

$s_{ij} = (k_i + k_j)^2$, $s_{ijm} = (k_i + k_j + k_m)^2$. The five (primed) kinematic variables of the pentagon are then given in terms of the (unprimed) hexagon variables by

$$s'_{12} = s_{12}, \quad s'_{23} = s_{23}, \quad s'_{34} = \frac{s_{34}s_{123}}{s_{123} - s_{56}}, \quad s'_{45} = s_{123}, \quad s'_{51} = \frac{s_{123}s_{234} - s_{23}s_{56}}{s_{123} - s_{56}}. \quad (4.5.18)$$

The other pentagon replaces k_1, k_2, k_3 with k''_1 and k''_2 and has k'_1 parallel to k_1 , which leads to its kinematic variables being given by

$$s''_{12} = s_{123}, \quad s''_{23} = \frac{s_{123}s_{234} - s_{23}s_{56}}{s_{123} - s_{23}}, \quad s''_{34} = s_{45}, \quad s''_{45} = s_{56}, \quad s''_{51} = \frac{s_{61}s_{123}}{s_{123} - s_{23}}. \quad (4.5.19)$$

Finally, for the box Wilson loop one makes both replacements simultaneously; as a result, its kinematic invariants are given by

$$s'''_{12} = s_{123}, \quad s'''_{23} = \frac{s_{123}(s_{123}s_{234} - s_{23}s_{56})}{(s_{123} - s_{23})(s_{123} - s_{56})}. \quad (4.5.20)$$

The correction term to go between the logarithm of the BSV Wilson loop and the six-point remainder function requires the combination of one-loop normalized amplitudes V_n (from the BDS formula [32]),

$$V_6 - V'_5 - V''_5 + V'''_4, \quad (4.5.21)$$

which is finite and dual conformal invariant. There is also a prefactor proportional to the cusp anomalous dimension, whose expansion is known to all orders [168],

$$\gamma_K(a) = 4a - 4\zeta_2 a^2 + 22\zeta_4 a^3 - 4\left(\frac{219}{8}\zeta_6 + (\zeta_3)^2\right)a^4 + \dots, \quad (4.5.22)$$

where $a = g_{YM}^2 N_c / (32\pi^2) = \lambda / (32\pi^2)$. Including the proper prefactor, we obtain the following relation between the two observables,

$$\ln \left[1 + \mathcal{W}_{\text{hex}}(a/2) \right] = R_6(a) + \frac{\gamma_K(a)}{8} X(u, v, w), \quad (4.5.23)$$

where

$$X(u, v, w) = -H_2^u - H_2^v - H_2^w - \ln\left(\frac{uv}{w(1-v)}\right) \ln(1-v) - \ln u \ln w + 2\zeta_2. \quad (4.5.24)$$

Here \mathcal{W}_{hex} is BSV's observable (they use the expansion parameter $g^2 = \lambda/(16\pi^2) = a/2$) and R_6 is the remainder function.

In the near-collinear limit, the correction function $X(u, v, w)$ becomes,

$$\begin{aligned} X(u, v, w) = & 2T \cos \phi \left(\frac{H_1}{S} + S(H_1 + L) \right) \\ & + T^2 \left[(1 - 2 \cos^2 \phi) \left(\frac{H_1}{S^2} + S^2(H_1 + L) \right) + 2(H_1 + L) \right] + \mathcal{O}(T^3). \end{aligned} \quad (4.5.25)$$

Next we apply this relation in the near-collinear limit, first at order T^1 . We find that the $T^1 \ln^2 T$ terms from BSV's formula match perfectly the ones we obtain from our expression from $R_6^{(3)}$. The $T^1 \ln T$ terms also match, given one linear relation between α_2 and the coefficient of $\zeta_2 R_6^{(2)}$. Finally, the $T^1 \ln^0 T$ terms match if we fix $\alpha_2 = 7/32$, which is the last constant to be fixed. The value of α_2 is in agreement with refs. [45, 150]. The agreement with ref. [150] (BSV) is no surprise, because both are based on comparing the near-collinear limit of $R_6^{(3)}$ with the same OPE results, BSV at symbol level and here at function level.

Here we give the formula for the leading, order T term in the near-collinear limit

of $R_6^{(3)}$, after fixing all parameters as just described:

$$\begin{aligned}
R_6^{(3)} = \frac{T}{S} \cos \phi \Bigg\{ & \ln^2 T \left[\frac{2}{3} H_1^3 + H_1^2 (L + 2) + H_1 \left(\frac{1}{4} L^2 + 2L + \frac{1}{2} \zeta_2 + 3 \right) - H_3 + \frac{1}{2} H_2 (L - 1) \right] \\
& - \ln T \left[\frac{1}{2} H_1^4 + H_1^3 (L + 2) + H_1^2 \left(\frac{1}{4} L^2 + 3L + \frac{3}{2} \zeta_2 + 5 \right) \right. \\
& \quad + H_1 \left(\frac{1}{2} L^2 + (H_2 + 2\zeta_2 + 5)L - \zeta_3 + 3\zeta_2 + 9 \right) \\
& \quad \left. + \frac{1}{2} (H_3 - 2H_{2,1})(L + 1) + \frac{1}{2} H_2 (L - 1) \right] \\
& + \frac{1}{10} H_1^5 + \frac{1}{4} H_1^4 (L + 2) + \frac{1}{12} H_1^3 (L^2 + 12L + 6\zeta_2 + 20) \\
& + \frac{1}{4} H_1^2 \left(L^2 + 2(H_2 + 2\zeta_2 + 5)L - 2\zeta_3 + 6\zeta_2 + 18 \right) \\
& + \frac{1}{8} H_1 \left[8(H_4 - H_{3,1}) + 2H_2^2 + (H_2 + \zeta_2 + 3)L^2 + \left(8(H_2 - H_{2,1}) + 4\zeta_3 \right. \right. \\
& \quad \left. \left. + 16\zeta_2 + 36 \right) L + 2\zeta_2 (H_2 + 9) - 39\zeta_4 - 8\zeta_3 + 72 \right] \\
& - \frac{1}{4} H_{2,1} L^2 + \frac{1}{8} \left(-6H_4 + 8H_{2,1,1} + H_2^2 + 2H_3 - 12H_{2,1} + 2(\zeta_2 + 2)H_2 \right) L \\
& + \frac{1}{8} H_2^2 - \frac{1}{4} H_2 (2H_3 + 4H_{2,1} + 2\zeta_3 + \zeta_2) - \frac{1}{4} (2\zeta_2 - 3)H_3 - \frac{1}{2} (\zeta_2 + 1)H_{2,1} \\
& + \frac{9}{2} H_5 + H_{4,1} + H_{3,2} + 6H_{3,1,1} + 2H_{2,2,1} + \frac{3}{4} H_4 - H_{2,1,1} \Bigg\} + \left(S \rightarrow \frac{1}{S} \right) \\
& + \mathcal{O}(T^2).
\end{aligned} \tag{4.5.26}$$

The T^2 terms are presented in an attached, computer-readable file. The T^2 terms match perfectly with OPE results provided to us by BSV [152], and at this order there are no free parameters in the comparison. This provides a very nice consistency check on two very different approaches.

Recall that we imposed an extra-pure condition on the terms in eq. (4.4.49) that we added to the ansatz for $R_6^{(3)}$. We can ask what would happen if we relaxed this assumption. To do so we consider adding to the solution that we found a complete set

of beyond-the-symbol terms. Imposing total symmetry, there are 2 weight-6 constants (ζ_6 and $(\zeta_3)^2$), and 2 weight-5 constants (ζ_5 and $\zeta_2\zeta_3$) multiplying $\ln uvw$. Multiplying the zeta values ζ_4 , ζ_3 and ζ_2 there are respectively 3, 7 and 18 symmetric functions, for a total of 32 free parameters. Imposing vanishing of these additional terms at order T^0 fixes all but 5 of the 32 parameters to be zero. We used constraints from the multi-Regge limit (see the next section) to remove 4 of the 5 remaining parameters. Finally, the order T^1 term in the near-collinear limit fixes the last parameter to zero. We conclude that there are no additional ambiguities in $R_6^{(3)}$ associated with relaxing the extra-purity assumption.

4.6 Multi-Regge limits

The multi-Regge or MRK limit of n -gluon scattering is a $2 \rightarrow (n - 2)$ scattering process in which the $(n - 2)$ outgoing gluons are strongly ordered in rapidity. It generalizes the Regge limit of $2 \rightarrow 2$ scattering with large center-of-mass energy at fixed momentum transfer $s \gg t$. Here we are interested in the case of $2 \rightarrow 4$ gluon scattering, for which the MRK limit means that two of the outgoing gluons are emitted at high energy, almost parallel to the incoming gluons. The other two gluons are also typically emitted at small angles, but they are well-separated in rapidity from each other and from the leading two gluons, giving them smaller energies.

The strong ordering in rapidity for the $2 \rightarrow 4$ process leads to the following strong ordering of momentum invariants:

$$s_{12} \gg s_{345}, s_{123} \gg s_{34}, s_{45}, s_{56} \gg s_{23}, s_{61}, s_{234}. \quad (4.6.1)$$

In this limit, the cross ratio $u = s_{12}s_{45}/(s_{123}s_{345})$ approaches one. The other two cross ratios vanish,

$$u \rightarrow 1, \quad v \rightarrow 0, \quad \hat{w} \rightarrow 0. \quad (4.6.2)$$

In this section, we denote the original cross ratio w by \hat{w} , in order to avoid confusion with another variable which we are about to introduce. The cross ratios v and \hat{w} vanish at the same rate that $u \rightarrow 1$, so that the ratios x and y , defined by

$$x \equiv \frac{v}{1-u}, \quad y \equiv \frac{\hat{w}}{1-u}, \quad (4.6.3)$$

remain fixed. The variable y in eq. (4.6.3) should not be confused with the variables y_i . In the y variables, the multi-Regge limit consists of taking $y_u \rightarrow 1$, while y_v and y_w are left arbitrary. (Their values in this limit are related to x and y by eq. (4.3.51).)

It is very convenient [12] to change variables from x and y to the complex-conjugate pair (w, w^*) defined by,

$$x = \frac{1}{(1+w)(1+w^*)}, \quad y = \frac{ww^*}{(1+w)(1+w^*)}. \quad (4.6.4)$$

(Again, this variable w should not be confused with the original cross ratio called \hat{w} in this section.) This change of variables rationalizes the y variables in the MRK limit, so that

$$y_u \rightarrow 1, \quad y_v \rightarrow \frac{1+w^*}{1+w}, \quad y_w \rightarrow \frac{(1+w)w^*}{w(1+w^*)}. \quad (4.6.5)$$

As an aside, we remark here that the variables T, S, F in eq. (4.5.1), used by BSV to describe the near-collinear limit, are closely related to the variables w, w^* introduced for the MRK limit. To establish this correspondence, we consider (in this paragraph only) the MRK limit $u \rightarrow 0, v \rightarrow 0, \hat{w} \rightarrow 1$, which is related to eq. (4.6.2) by a cyclic permutation $u_i \rightarrow u_{i-1}, y_i \rightarrow y_{i-1}$. This limit corresponds to the $T \rightarrow 0$ limit in eq. (4.5.1) if we also send $S \rightarrow 0$ at the same rate, so that T/S is fixed. Let's rewrite y_u from eq. (4.5.1) as

$$y_u = \frac{1 + \frac{T}{SF}}{1 + \frac{TF}{S}} \quad (4.6.6)$$

and compare it with the limiting behavior of y_v in eq. (4.6.5). (Comparing y_u with y_v is required by the cyclic permutation of the u_i and y_i variables which we need for the two limits to correspond.) If we let

$$w = \frac{T}{S}F, \quad w^* = \frac{T}{S}\frac{1}{F}, \quad (4.6.7)$$

then y_v in eq. (4.6.5) correctly matches eq. (4.6.6). If we start with the variables T, S, F in eq. (4.5.1), insert the inverse relations to eq. (4.6.7),

$$T = S\sqrt{ww^*}, \quad F = \sqrt{\frac{w}{w^*}}, \quad (4.6.8)$$

and then let $S \rightarrow 0$ with w, w^* fixed, we can check that all variables approach the values appropriate for the multi-Regge limit $u \rightarrow 0, v \rightarrow 0, \hat{w} \rightarrow 1$. The cross-ratio \hat{w} approaches unity as S vanishes, through the relation $\hat{w} = (1 + S^2|1+w|^2)^{-1}$. Finally, we note that the MRK limit interpolates between three different limits: the collinear limit $v \rightarrow 0$, corresponding to $|w| \rightarrow 0$; the endpoint of the line $(u, u, 1)$ with $u \rightarrow 0$, corresponding to $w \rightarrow -1$; and a second collinear limit $u \rightarrow 0$, corresponding to $|w| \rightarrow \infty$.

Now we return to the $u \rightarrow 1$ version of the MRK limit in eq. (4.6.2). If this limiting behavior of the cross ratios is approached directly from the Euclidean region in which all cross ratios are positive, we call it the EMRK limit (see also eq. (4.3.50)). In this limit, the remainder function vanishes, as it does in the Euclidean collinear limit discussed in the previous section. However, the physical region for $2 \rightarrow 4$ scattering is obtained by first analytically continuing $u \rightarrow e^{-2\pi i}u$, then taking $u \rightarrow 1$, $v, \hat{w} \rightarrow 0$ as above. The analytic continuation generates imaginary terms corresponding to the discontinuity of the function in the u channel, which survive into the MRK limit; in fact they can be multiplied by logarithmic singularities as $u \rightarrow 1$.

The general form of the remainder function at L loops in the MRK limit is

$$R_6^{(L)}(1-u, w, w^*) = (2\pi i) \sum_{r=0}^{L-1} \ln^r(1-u) [g_r^{(L)}(w, w^*) + 2\pi i h_r^{(L)}(w, w^*)] + \mathcal{O}(1-u), \quad (4.6.9)$$

where the coefficient functions $g_r^{(L)}(w, w^*)$ are referred to as the leading-log approximation (LLA) for $r = L - 1$, next-to-LLA (NLLA) for $r = L - 2$, and so on. The coefficient functions $h_r^{(L)}(w, w^*)$ can be determined simply from the $g_r^{(L)}$, by using a crossing relation from the $3 \rightarrow 3$ channel [13, 19].

The coefficient functions in this limit are built out of HPLs with arguments $-w$ and $-w^*$. Only special combinations of such HPLs are allowed, with good branch-cut behavior in the (w, w^*) plane, corresponding to symbols whose first entries are limited to x and y [19]. Such functions may be called single-valued harmonic polylogarithms (SVHPLs), and were constructed by Brown [47].

Using a Fourier-Mellin transformation, Fadin, Lipatov, and Prygarin wrote an all-loop expression for the MRK limit in a factorized form depending on two quantities, the BFKL eigenvalue $\omega(\nu, n)$ and the impact factor $\Phi_{\text{Reg}}(\nu, n)$ [15]:

$$e^{R+i\pi\delta}|_{\text{MRK}} = \cos \pi \omega_{ab} + i \frac{a}{2} \sum_{n=-\infty}^{\infty} (-1)^n \left(\frac{w}{w^*}\right)^{\frac{n}{2}} \int_{-\infty}^{+\infty} \frac{d\nu}{\nu^2 + \frac{n^2}{4}} |w|^{2i\nu} \Phi_{\text{Reg}}(\nu, n) \times \left(-\frac{1}{1-u} \frac{|1+w|^2}{|w|} \right)^{\omega(\nu, n)}. \quad (4.6.10)$$

Here

$$\omega_{ab} = \frac{1}{8} \gamma_K(a) \log |w|^2, \quad (4.6.11)$$

$$\delta = \frac{1}{8} \gamma_K(a) \log \frac{|w|^2}{|1+w|^4}, \quad (4.6.12)$$

where the cusp anomalous dimension $\gamma_K(a)$ is given in eq. (4.5.22).

By taking the MRK limit of the symbol of the three-loop remainder function, it was possible to determine all of the coefficient functions $g_r^{(l)}$ and $h_r^{(l)}$ through three loops, up to four undetermined rational numbers, d_1 , d_2 , γ' and γ'' , representing beyond-the-symbol ambiguities [14]. (Two other parameters, c and γ''' , could be fixed using consistency between the MRK limits in $2 \rightarrow 4$ kinematics and in $3 \rightarrow 3$ kinematics.) One of these four constants was fixed by Fadin and Lipatov [15], using a direct calculation of the NLLA BFKL eigenvalue: $\gamma' = -9/2$. The remaining three undetermined constants, d_1 , d_2 and γ'' , all appear in the NNLLA coefficient $g_0^{(3)}(w, w^*)$.

In ref. [19], the coefficient functions $g_r^{(3)}(w, w^*)$ and $h_r^{(3)}(w, w^*)$ that appear in the MRK limit (4.6.9) of $R_6^{(3)}$ were expressed in terms of the SVHPLs defined in ref. [47]. More specifically, they were rewritten in terms of particular linear combinations of SVHPLs, denoted by L_w^\pm , that have definite eigenvalues under inversion of w and under its complex conjugation. The coefficient function $g_0^{(3)}(w, w^*)$ then becomes [19]:

$$\begin{aligned} g_0^{(3)}(w, w^*) = & \frac{27}{8} L_5^+ + \frac{3}{4} L_{3,1,1}^+ - \frac{1}{2} L_3^+ [L_1^+]^2 - \frac{15}{32} L_3^+ [L_0^-]^2 - \frac{1}{8} L_1^+ L_{2,1}^- L_0^- \\ & + \frac{3}{32} [L_0^-]^2 [L_1^+]^3 + \frac{19}{384} L_1^+ [L_0^-]^4 + \frac{3}{8} [L_1^+]^2 \zeta_3 - \frac{5}{32} [L_0^-]^2 \zeta_3 + \frac{\pi^2}{96} [L_1^+]^3 \\ & - \frac{\pi^2}{384} L_1^+ [L_0^-]^2 - \frac{3}{4} \zeta_5 - \frac{\pi^2}{6} \gamma'' \left\{ L_3^+ - \frac{1}{6} [L_1^+]^3 - \frac{1}{8} [L_0^-]^2 L_1^+ \right\} \\ & + \frac{1}{4} d_1 \zeta_3 \left\{ [L_1^+]^2 - \frac{1}{4} [L_0^-]^2 \right\} - \frac{\pi^2}{3} d_2 L_1^+ \left\{ [L_1^+]^2 - \frac{1}{4} [L_0^-]^2 \right\} + \frac{1}{30} [L_1^+]^5. \end{aligned} \quad (4.6.13)$$

In the remainder of this section we will describe how to extract the MRK limit of the three-loop remainder function at the full function level. Comparing this limit

with eq. (4.6.13) (as well as the other $g_r^{(3)}$ and $h_r^{(3)}$ coefficient functions) will serve as a check of our construction of $R_6^{(3)}$, and it will also provide for us the remaining three-loop MRK constants, d_1 , d_2 and γ'' .

4.6.1 Method for taking the MRK limit

Let us begin by discussing a method for taking the multi-Regge limit of hexagon functions in general, or of $R_6^{(3)}$ in particular, starting from an expression in terms of multiple polylogarithms. The first step is to send $u \rightarrow e^{-2\pi i}u$, *i.e.* to extract the monodromy around $u = 0$. Owing to the non-linear relationship between the u_i and the y_i , eq. (4.2.11), it is not immediately clear what the discontinuity looks like in the y variables. The correct prescription turns out simply to be to take y_u around 0. To see this, consider the $\Delta_{1,n-1}$ component of the coproduct, which can be written as,

$$\Delta_{1,n-1}(F) \equiv \ln u \otimes {}^uF + \ln v \otimes {}^vF + \ln w \otimes {}^wF. \quad (4.6.14)$$

There are only three terms, corresponding to the three possible first entries of the symbol.

Using the coproduct formulas in appendix C.1, it is straightforward to extract the functions uF , vF , and wF for any given hexagon function. These functions capture information about the discontinuities as each of the cross ratios is taken around zero. In particular, since the monodromy operator acts on the first component of the coproduct, we have (*c.f.* eq. (4.3.34)),

$$\begin{aligned} \Delta_{1,n-1}[\mathcal{M}_{u=0}(F)] &= [\mathcal{M}_{u=0}(\ln u)] \otimes {}^uF \\ &= (\ln u - 2\pi i) \otimes {}^uF. \end{aligned} \quad (4.6.15)$$

Equation (4.6.15) is not quite sufficient to deduce $\mathcal{M}_{u=0}(F)$. The obstruction comes from the fact that all higher powers of $(2\pi i)$ live in the kernel of $\Delta_{1,n-1}$. On the other hand, these terms can be extracted from the other components of the coproduct: the $(2\pi i)^k$ terms come from the piece of $\Delta_{k,n-k}(F)$ with $\ln^k u$ in the first slot.

If we write eq. (4.6.14) in terms of the y_i variables, we find,

$$\begin{aligned} \Delta_{1,n-1}(F) = & \left[G(0; y_u) + G(1; y_v) + G(1; y_w) - G\left(\frac{1}{y_u}; y_v\right) - G\left(\frac{1}{y_u}; y_w\right) \right] \otimes {}^u F \\ & + \left[G(0; y_v) + G(1; y_u) + G(1; y_w) - G\left(\frac{1}{y_u}; y_v\right) - G\left(\frac{1}{y_v}; y_w\right) \right] \otimes {}^v F \\ & + \left[G(0; y_w) + G(1; y_u) + G(1; y_v) - G\left(\frac{1}{y_u}; y_w\right) - G\left(\frac{1}{y_v}; y_w\right) \right] \otimes {}^w F, \end{aligned} \quad (4.6.16)$$

where we have now assumed that we are working in Region I. Equation (4.6.16) indicates that ${}^u F$ can be extracted uniquely from the terms with $G(0; y_u)$ in the first slot. Similarly, the elements of the full coproduct with $\ln^k u$ in the first slot are given exactly by the terms with $G(0; y_u)^k$ in the first slot. Therefore the discontinuity around $u = 0$ is the same as the discontinuity around $y_u = 0$. Furthermore, because our basis \mathcal{G}_I^L exposes all logarithms $G(0; y_u)$ (by exploiting the shuffle algebra), the only sources of such discontinuities are powers of $G(0; y_u)$. As a result, we have a simple shortcut to obtain the monodromy around $u = 0$,

$$\mathcal{M}_{u=0}(F) = F|_{G(0; y_u) \rightarrow G(0; y_u) - 2\pi i}. \quad (4.6.17)$$

The final step in obtaining the MRK limit is to take $y_u \rightarrow 1$. This limit is trivially realized on functions in the basis \mathcal{G}_I^L because the only source of singularities is $G(1; y_u)$; all other functions are finite as $y_u \rightarrow 1$. Writing the divergence in terms of $\xi \equiv 1 - u$, which approaches 0 in this limit, we take

$$G(1; y_u) \xrightarrow{y_u \rightarrow 1} \ln \xi + G(1; y_v) + G(1; y_w) - G\left(\frac{1}{y_v}; y_w\right), \quad (4.6.18)$$

and then set $y_u = 1$ in all other terms.

The result of this procedure will be a polynomial in $\ln \xi$ whose coefficients are multiple polylogarithms in the variables y_v and y_w . On the other hand, we know from general considerations that the coefficient functions should be SVHPLs. To translate the multiple polylogarithms into SVHPLs, we use the coproduct bootstrap

of section 4.3.3, seeded by the weight-one identities which follow from eq. (4.6.5) and from combining eqs. (4.3.51), (4.6.4) and (4.6.5),

$$\frac{1}{|1+w|^2} = \frac{y_v(1-y_w)^2}{(1-y_v y_w)^2}, \quad \frac{|w|^2}{|1+w|^2} = \frac{y_w(1-y_v)^2}{(1-y_v y_w)^2}. \quad (4.6.19)$$

We obtain,

$$\begin{aligned} L_0^- &= \ln |w|^2 = -G(0; y_v) + G(0; y_w) + 2G(1; y_v) - 2G(1; y_w), \\ L_1^+ &= \ln \frac{|w|}{|1+w|^2} = \frac{1}{2}G(0; y_v) + \frac{1}{2}G(0; y_w) + G(1; y_v) + G(1; y_w) - 2G\left(\frac{1}{y_v}; y_w\right), \end{aligned} \quad (4.6.20)$$

and,

$$\ln \left(\frac{1+w}{1+w^*} \right) = -G(0; y_v) \quad \text{and} \quad \ln \left(\frac{w}{w^*} \right) = -G(0; y_v) - G(0; y_w). \quad (4.6.21)$$

Alternatively, we can extract the MRK limits of the hexagon functions iteratively in the weight, by using their definitions in terms of differential equations. This procedure is similar to that used in section 4.5 to find the collinear limits of the hexagon functions, in that we expand the differential equations around the limiting region of $u \rightarrow 1$.

However, first we have to compute the discontinuities from letting $u \rightarrow e^{-2\pi i}u$ in the inhomogeneous (source) terms for the differential equations. For the lowest weight non-HPL function, $\tilde{\Phi}_6$, the source terms are pure HPLs. For pure HPL functions we use standard HPL identities to exchange the HPL argument $(1-u)$ for argument u , and again use the Lyndon basis so that the trailing index in the weight vector \vec{w} in each $H_{\vec{w}}(u)$ is 1. In this new representation, the only discontinuities come from explicit factors of $\ln u$, which are simply replaced by $\ln u - 2\pi i$ under the analytic continuation. After performing the analytic continuation, we take the MRK limit of the pure HPL functions.

Once these limits are known, we can integrate up the differential equations for the non-HPL functions in much the same fashion that we did for the collinear limits, by

using a restricted ansatz built from powers of $\ln \xi$ and SVHPLs. The Jacobian factors needed to transform from differential equations in (u, v, \hat{w}) to differential equations in the MRK variables (ξ, w, w^*) , are easily found to be:

$$\begin{aligned}\frac{\partial F}{\partial \xi} &= -\frac{\partial F}{\partial u} + x \frac{\partial F}{\partial v} + y \frac{\partial F}{\partial w}, \\ \frac{\partial F}{\partial w} &= \frac{\xi}{w(1+w)} \left[-wx \frac{\partial F}{\partial v} + y \frac{\partial F}{\partial w} \right], \\ \frac{\partial F}{\partial w^*} &= \frac{\xi}{w^*(1+w^*)} \left[-w^*x \frac{\partial F}{\partial v} + y \frac{\partial F}{\partial w} \right].\end{aligned}\tag{4.6.22}$$

We compute the derivatives on the right-hand side of these relations using the formula for $\partial F / \partial u_i$ in terms of the coproduct components, eq. (4.4.3). We also implement the transformation $u \rightarrow e^{-2\pi i} u$ on the coproduct components, as described above for the HPLs, and iteratively in the weight for the non-HPL hexagon functions. When we expand as $\xi \rightarrow 0$, we drop all power-suppressed terms in ξ , keeping only polynomials in $\ln \xi$. (In $\partial F / \partial \xi$, we keep the derivatives of such expressions, *i.e.* terms of the form $1/\xi \times \ln^k \xi$.)

In our definition of the MRK limit, we include any surviving terms from the EMRK limit. This does not matter for the remainder function, whose EMRK limit vanishes, but the individual parity-even hexagon functions can have nonzero, and even singular, EMRK limits.

4.6.2 Examples

We first consider the simplest non-HPL function, $\tilde{\Phi}_6$. Starting with the expression for $\tilde{\Phi}_6$ in Region I, eq. (4.3.56), we take the monodromy around $u = 0$, utilizing eq. (4.6.17),

$$\begin{aligned}\mathcal{M}_{u=0}(\tilde{\Phi}_6) &= 2\pi i \left[-G\left(0, \frac{1}{y_u y_v}; y_w\right) - G\left(0, \frac{1}{y_v}; y_w\right) + G\left(0, \frac{1}{y_u}; y_w\right) + G\left(0, \frac{1}{y_u}; y_v\right) \right. \\ &\quad \left. + G(0, 1; y_w) + G(0, 1; y_v) - G(0, 1; y_u) + G(0; y_v) G(0; y_w) + \zeta_2 \right].\end{aligned}\tag{4.6.23}$$

Next, we take the limit $y_u \rightarrow 1$. There are no divergent factors, so we are free to set $y_u = 1$ without first applying eq. (4.6.18). The result is,

$$\tilde{\Phi}_6|_{\text{MRK}} = 2\pi i \left[-2G\left(0, \frac{1}{y_v}; y_w\right) + 2G(0, 1; y_w) + 2G(0, 1; y_v) + G(0; y_v) G(0; y_w) + 2\zeta_2 \right]. \quad (4.6.24)$$

To transform this expression into the SVHPL notation of ref. [19], we use the coproduct bootstrap to derive an expression for the single independent SVHPL of weight two, the Bloch-Wigner dilogarithm, L_2^- ,

$$\begin{aligned} \Delta_{1,1}(L_2^-) &= \Delta_{1,1} \left(\text{Li}_2(-w) - \text{Li}_2(-w^*) + \frac{1}{2} \ln |w|^2 \ln \frac{1+w}{1+w^*} \right) \\ &= \frac{1}{2} L_0^- \otimes \left[\ln \left(\frac{1+w}{1+w^*} \right) - \frac{1}{2} \ln \left(\frac{w}{w^*} \right) \right] + \frac{1}{2} L_1^+ \otimes \ln \left(\frac{w}{w^*} \right) \\ &= \Delta_{1,1} \left(G\left(0, \frac{1}{y_v}; y_w\right) - G(0, 1; y_w) - G(0, 1; y_v) - \frac{1}{2} G(0; y_v) G(0; y_w) \right). \end{aligned} \quad (4.6.25)$$

In the last line we used eqs. (4.6.20) and (4.6.21). Lifting eq. (4.6.25) from coproducts to functions introduces one undetermined rational-number constant, proportional to ζ_2 . It is easily fixed by specializing to the point $y_v = y_w = 1$, yielding,

$$L_2^- = G\left(0, \frac{1}{y_v}; y_w\right) - G(0, 1; y_w) - G(0, 1; y_v) - \frac{1}{2} G(0; y_v) G(0; y_w) - \zeta_2, \quad (4.6.26)$$

which, when compared to eq. (4.6.24), gives,

$$\tilde{\Phi}_6|_{\text{MRK}} = -4\pi i L_2^-. \quad (4.6.27)$$

Let us derive this result in a different way, using the method based on differential equations. Like all parity-odd functions, $\tilde{\Phi}_6$ vanishes in the Euclidean MRK limit; however, it survives in the MRK limit due to discontinuities in the function $\Omega^{(1)}$ given in eq. (4.2.22), which appears on the right-hand side of the $\tilde{\Phi}_6$ differential equation (4.2.24). The MRK limits of the three cyclic permutations of $\Omega^{(1)}$ are given

by

$$\begin{aligned}\Omega^{(1)}(u, v, \hat{w})\Big|_{\text{MRK}} &= 2\pi i \ln |1 + w|^2, \\ \Omega^{(1)}(v, \hat{w}, u)\Big|_{\text{MRK}} &= 2\pi i \ln \xi, \\ \Omega^{(1)}(\hat{w}, u, v)\Big|_{\text{MRK}} &= 2\pi i \ln \frac{|1 + w|^2}{|w|^2}.\end{aligned}\tag{4.6.28}$$

Inserting these values into eq. (4.2.24) for $\partial\tilde{\Phi}_6/\partial u$ and its cyclic permutations, and then inserting those results into eq. (4.6.22), we find that

$$\begin{aligned}\frac{\partial\tilde{\Phi}_6}{\partial\xi}\Big|_{\xi^{-1}} &= 0, \\ \frac{\partial\tilde{\Phi}_6}{\partial w}\Big|_{\xi^0} &= 2\pi i \left[-\frac{\ln |w|^2}{1 + w} + \frac{\ln |1 + w|^2}{w} \right], \\ \frac{\partial\tilde{\Phi}_6}{\partial w^*}\Big|_{\xi^0} &= 2\pi i \left[\frac{\ln |w|^2}{1 + w^*} - \frac{\ln |1 + w|^2}{w^*} \right].\end{aligned}\tag{4.6.29}$$

The first differential equation implies that there is no $\ln \xi$ term in the MRK limit of $\tilde{\Phi}_6$. The second two differential equations imply that the MRK limit is proportional to the Bloch-Wigner dilogarithm,

$$\begin{aligned}\tilde{\Phi}_6\Big|_{\text{MRK}} &= -4\pi i \left[\text{Li}_2(-w) - \text{Li}_2(-w^*) + \frac{1}{2} \ln |w|^2 \ln \frac{1 + w}{1 + w^*} \right] \\ &= -4\pi i L_2^-.\end{aligned}\tag{4.6.30}$$

Now that we have the MRK limit of $\tilde{\Phi}_6$, we can find the limiting behavior of all the coproduct components of $\Omega^{(2)}$ appearing in eq. (4.4.26), and perform the analogous

expansion of the differential equations in the MRK limit. For $\Omega^{(2)}(u, v, \hat{w})$ we obtain,

$$\begin{aligned} \left. \frac{\partial \Omega^{(2)}(u, v, \hat{w})}{\partial \xi} \right|_{\xi^{-1}} &= \frac{2\pi i}{\xi} \ln |1 + w|^2 \left[-\ln \xi + \frac{1}{2} \ln |1 + w|^2 - \pi i \right], \\ \left. \frac{\partial \Omega^{(2)}(u, v, \hat{w})}{\partial w} \right|_{\xi^0} &= \frac{2\pi i}{1 + w} \left[-\frac{1}{2} \ln^2 \left(\frac{\xi}{|1 + w|^2} \right) + \frac{1}{2} \ln |w|^2 \ln |1 + w|^2 - L_2^- + \zeta_2 \right. \\ &\quad \left. - \pi i \ln \left(\frac{\xi}{|1 + w|^2} \right) \right], \end{aligned} \quad (4.6.31)$$

plus the complex conjugate equation for $\partial \Omega^{(2)}(u, v, \hat{w}) / \partial w^*$.

The solution to these differential equations can be expressed in terms of SVHPLs. One can write an ansatz for the result as a linear combination of SVHPLs, and fix the coefficients using the differential equations. One can also take the limit first at the level of the symbol, matching to the symbols of the SVHPLs; then one only has to fix the smaller set of beyond-the-symbol terms using the differential equations. The result is

$$\begin{aligned} \Omega^{(2)}(u, v, \hat{w})|_{\text{MRK}} &= 2\pi i \left[\frac{1}{4} \ln^2 \xi (2 L_1^+ - L_0^-) + \frac{1}{8} \ln \xi (2 L_1^+ - L_0^-)^2 + \frac{5}{48} [L_0^-]^3 \right. \\ &\quad \left. + \frac{1}{8} [L_0^-]^2 L_1^+ + \frac{1}{4} L_0^- [L_1^+]^2 + \frac{1}{6} [L_1^+]^3 - L_3^+ - 2 L_{2,1}^- \right. \\ &\quad \left. - \frac{\zeta_2}{2} (2 L_1^+ - L_0^-) - 2 \zeta_3 \right] \\ &\quad - (4\pi)^2 \left[\frac{1}{4} \ln \xi (2 L_1^+ - L_0^-) + \frac{1}{16} (2 L_1^+ - L_0^-)^2 \right]. \end{aligned} \quad (4.6.32)$$

In this case the constant term, proportional to ζ_3 , can be fixed by requiring vanishing in the collinear-MRK corner where $|w|^2 \rightarrow 0$. The last set of terms, multiplying $(4\pi)^2$, come from a double discontinuity.

The MRK limit of $\Omega^{(2)}(\hat{w}, u, v)$ is related by symmetry to that of $\Omega^{(2)}(u, v, \hat{w})$:

$$\Omega^{(2)}(\hat{w}, u, v)|_{\text{MRK}} = \Omega^{(2)}(u, v, \hat{w})|_{\text{MRK}}(w \rightarrow 1/w, w^* \rightarrow 1/w^*). \quad (4.6.33)$$

The final MRK limit of $\Omega^{(2)}$ is,

$$\begin{aligned} \Omega^{(2)}(v, \hat{w}, u)|_{\text{MRK}} = & \frac{1}{4} L_X^4 - \left(\frac{1}{8} [L_0^-]^2 - \zeta_2 \right) L_X^2 + 4 \zeta_3 L_X + \frac{1}{64} [L_0^-]^4 + \frac{1}{4} \zeta_2 [L_0^-]^2 + \frac{5}{2} \zeta_4 \\ & + 2\pi i \left[\frac{1}{3} L_X^3 - 2 \left(\frac{1}{8} [L_0^-]^2 - \zeta_2 \right) L_X + \frac{1}{2} [L_0^-]^2 L_1^+ - 2(L_3^+ - \zeta_3) \right], \end{aligned} \quad (4.6.34)$$

where $L_X = \ln \xi + L_1^+$. Note that this orientation of $\Omega^{(2)}$ has a nonvanishing (indeed, singular) EMRK limit, *i.e.* even before analytically continuing into the Minkowski region to pick up the imaginary part. On the other hand, there is no surviving double discontinuity for this ordering of the arguments.

As our final (simple) example, we give the MRK limit of the totally symmetric, weight five, parity-odd function $G(u, v, \hat{w})$. As was the case for $\tilde{\Phi}_6$, the limit of G is again proportional to the Bloch-Wigner dilogarithm, but with an extra factor of ζ_2 to account for the higher transcendental weight of G :

$$G(u, v, \hat{w})|_{\text{MRK}} = 16\pi i \zeta_2 L_2^-. \quad (4.6.35)$$

As usual for parity-odd functions, the EMRK limit vanishes. In this case the double discontinuity also vanishes. In general the MRK limits of the parity-odd functions must be odd under $w \leftrightarrow w^*$, which forbids any nontrivial constants of integration.

Continuing onward, we build up the MRK limits for all the remaining hexagon functions. The results are attached to this document in a computer-readable format.

4.6.3 Fixing d_1 , d_2 , and γ''

Using the MRK limit of all the hexagon functions appearing in eq. (4.4.48), we obtain the MRK limit of $R_6^{(3)}$. This is a powerful check of the function, although as mentioned above, much of it is guaranteed by the limiting behavior of the symbol. In fact, there are only three rational parameters to fix, d_1 , d_2 and γ'' , and they all enter the coefficient of the NNLLA imaginary part, $g_0^{(3)}(w, w^*)$, given in eq. (4.6.13). Inspecting the MRK limit of $R_6^{(3)}$, we find first of all perfect agreement with the functions

$h_r^{(L)}(w, w^*)$ entering the real part. (These can be determined on general grounds using consistency between the $2 \rightarrow 4$ and $3 \rightarrow 3$ MRK limits.) We also agree perfectly with the imaginary part coefficients $g_2^{(3)}$ at LLA and $g_1^{(3)}$ at NLLA.

Finally, we find for the NNLLA coefficient $g_0^{(3)}$,

$$\begin{aligned} g_0^{(3)}(w, w^*) = & \frac{27}{8} L_5^+ + \frac{3}{4} L_{3,1,1}^+ - \frac{1}{2} L_3^+ [L_1^+]^2 - \frac{15}{32} L_3^+ [L_0^-]^2 - \frac{1}{8} L_1^+ L_{2,1}^- L_0^- \\ & + \frac{3}{32} [L_0^-]^2 [L_1^+]^3 + \frac{19}{384} L_1^+ [L_0^-]^4 + \frac{1}{30} [L_1^+]^5 + \frac{1}{2} [L_1^+]^2 \zeta_3 - \frac{3}{16} [L_0^-]^2 \zeta_3 \\ & + \frac{5\pi^2}{24} L_3^+ - \frac{\pi^2}{48} L_1^+ [L_0^-]^2 - \frac{\pi^2}{18} [L_1^+]^3 - \frac{3}{4} \zeta_5. \end{aligned} \quad (4.6.36)$$

Comparing this result with eq. (4.6.13) fixes the three previously undetermined rational parameters, d_1 , d_2 , and γ'' . We find

$$d_1 = \frac{1}{2}, \quad d_2 = \frac{3}{32}, \quad \gamma'' = -\frac{5}{4}. \quad (4.6.37)$$

These three parameters were also the only ambiguities in the expression found in ref. [19] for the two-loop (NNLLA) impact factor $\Phi_{\text{Reg}}^{(2)}(\nu, n)$ defined in ref. [15]. Inserting eq. (4.6.37) into that expression, we obtain,

$$\begin{aligned} \Phi_{\text{Reg}}^{(2)}(\nu, n) = & \frac{1}{2} \left[\Phi_{\text{Reg}}^{(1)}(\nu, n) \right]^2 - E_{\nu,n}^{(1)} E_{\nu,n} + \frac{1}{8} [D_\nu E_{\nu,n}]^2 + \frac{5}{64} N^2 (N^2 + 4 V^2) \\ & - \frac{\zeta_2}{4} (2 E_{\nu,n}^2 + N^2 + 6 V^2) + \frac{17}{4} \zeta_4. \end{aligned} \quad (4.6.38)$$

Here $\Phi_{\text{Reg}}^{(1)}$ is the one-loop (NLLA) impact factor, and $E_{\nu,n}$ and $E_{\nu,n}^{(1)}$ are the LLA and NLLA BFKL eigenvalues [15, 19]. These functions all are combinations of polygamma (ψ) functions and their derivatives, plus accompanying rational terms in ν and n . For example,

$$E_{\nu,n} = \psi \left(1 + i\nu + \frac{|n|}{2} \right) + \psi \left(1 - i\nu + \frac{|n|}{2} \right) - 2\psi(1) - \frac{1}{2} \frac{|n|}{\nu^2 + \frac{n^2}{4}}. \quad (4.6.39)$$

Additional rational dependence on ν and n enters eq. (4.6.38) via the combinations

$$V \equiv \frac{i\nu}{\nu^2 + \frac{|n|^2}{4}}, \quad N \equiv \frac{n}{\nu^2 + \frac{|n|^2}{4}}. \quad (4.6.40)$$

We recall that the NNLLA BFKL eigenvalue $E_{\nu,n}^{(2)}$ also has been determined [19], up to nine rational parameters, a_i , $i = 0, 1, 2, \dots, 8$. These parameters enter the NNLLA coefficient function $g_1^{(4)}(w, w^*)$. If the above exercise can be repeated at four loops, then it will be possible to fix all of these parameters in the same way, and obtain an unambiguous result for the NNLLA approximation to the MRK limit.

Finally, we ask whether we could have determined all coefficients from the collinear vanishing of $R_6^{(3)}$ and the MRK limit alone, *i.e.* without using the near-collinear information from BSV. The answer is yes, if we assume extra purity and if we also take the value of α_2 from ref. [45]. After imposing collinear vanishing, we have two parameters left: α_2 and the coefficient of $\zeta_2 R_6^{(2)}$. We can fix the latter coefficient in terms of α_2 using the known NLLA coefficient $g_3^{(1)}$ in the MRK limit. (The LLA coefficient $g_3^{(2)}$ automatically comes out correct.) Then we compare to the NNLLA coefficient $g_3^{(0)}$. We find that we can fix d_2 and γ'' to the values in eq. (4.6.37), but that α_2 is linked to d_1 by the equation,

$$\alpha_2 = \frac{d_1}{8} + \frac{5}{32}. \quad (4.6.41)$$

If we do take α_2 from ref. [45], then the near-collinear limit of our result for $R_6^{(3)}$ provides an unambiguous test of BSV's approach at three loops, through $\mathcal{O}(T^2)$.

4.7 Final formula for $R_6^{(3)}$ and its quantitative behavior

Now that we have used the (near) collinear limits to fix all undetermined constants in eq. (4.4.48) for $R_6^{(3)}$, we can write an expression for the full function, either in terms of multiple polylogarithms or integral representations. We absorb the $c_i r_i(u, v)$ terms in eq. (4.4.48) into R_{ep} . In total we have,

$$R_6^{(3)}(u, v, w) = R_{\text{ep}}(u, v, w) + R_{\text{ep}}(v, w, u) + R_{\text{ep}}(w, u, v) + P_6(u, v, w) + \frac{413}{24} \zeta_6 + (\zeta_3)^2. \quad (4.7.1)$$

Expressions for $R_6^{(3)}$ in terms of multiple polylogarithms, valid in Regions I and II, are too lengthy to present here, but they are attached to this document in computer-readable format. To represent R_{ep} as an integral, we make use of its extra purity and similarity to $\Omega^{(2)}(u, v, w)$, writing a formula similar to eq. (4.4.43):

$$R_{\text{ep}}(u, v, w) = - \int_1^u du_t \frac{[R_{\text{ep}}^u + (u \leftrightarrow v)](u_t, v_t, w_t)}{u_t(u_t - 1)}, \quad (4.7.2)$$

with v_t and w_t as defined in eq. (4.4.44). Note that the function Q_ϕ in eq. (4.4.43) is given, via eq. (4.4.41), as $-\Omega^{(2),u} + (u \leftrightarrow v)$, the analogous combination of coproduct components entering eq. (4.7.2). The function R_{ep}^u is defined in appendix C.3.

We may also define $R_6^{(3)}$ via the $\{5, 1\}$ component of its coproduct, which is easily constructed from the corresponding coproducts of R_{ep} in appendix C.3, and of the product function P_6 . The general form of the $\{5, 1\}$ component of the coproduct is,

$$\begin{aligned} \Delta_{5,1} \left(R_6^{(3)} \right) &= R_6^{(3),u} \otimes \ln u + R_6^{(3),v} \otimes \ln v + R_6^{(3),w} \otimes \ln w \\ &\quad + R_6^{(3),1-u} \otimes \ln(1-u) + R_6^{(3),1-v} \otimes \ln(1-v) + R_6^{(3),1-w} \otimes \ln(1-w) \\ &\quad + R_6^{(3),y_u} \otimes \ln y_u + R_6^{(3),y_v} \otimes \ln y_v + R_6^{(3),y_w} \otimes \ln y_w. \end{aligned} \quad (4.7.3)$$

Many of the elements are related to each other, *e.g.* by the total symmetry of $R_6^{(3)}$:

$$\begin{aligned} R_6^{(3),1-u} &= -R_6^{(3),u}, & R_6^{(3),1-v} &= -R_6^{(3),v}, & R_6^{(3),1-w} &= -R_6^{(3),w}, \\ R_6^{(3),v}(u, v, w) &= R_6^{(3),u}(v, w, u), & R_6^{(3),w}(u, v, w) &= R_6^{(3),u}(w, u, v), \\ R_6^{(3),yv}(u, v, w) &= R_6^{(3),yu}(v, w, u), & R_6^{(3),yw}(u, v, w) &= R_6^{(3),yu}(w, u, v). \end{aligned} \quad (4.7.4)$$

The two independent functions may be written as,

$$\begin{aligned} R_6^{(3),yu} &= \frac{1}{32} \left\{ -4 \left(H_1(u, v, w) + H_1(u, w, v) \right) - 2 H_1(v, u, w) \right. \\ &\quad + \frac{3}{2} \left(J_1(u, v, w) + J_1(v, w, u) + J_1(w, u, v) \right) \\ &\quad \left. - 4 \left[H_2^u + H_2^v + H_2^w + \frac{1}{2} \left(\ln^2 u + \ln^2 v + \ln^2 w \right) - 9 \zeta_2 \right] \tilde{\Phi}_6(u, v, w) \right\}, \end{aligned} \quad (4.7.5)$$

and

$$R_6^{(3),u} = \frac{1}{32} \left[A(u, v, w) + A(u, w, v) \right], \quad (4.7.6)$$

where

$$\begin{aligned}
A = & M_1(u, v, w) - M_1(w, u, v) + \frac{32}{3} \left(Q_{\text{ep}}(v, w, u) - Q_{\text{ep}}(v, u, w) \right) \\
& + (4 \ln u - \ln v + \ln w) \Omega^{(2)}(u, v, w) + (\ln u + \ln v) \Omega^{(2)}(v, w, u) \\
& + 24H_5^u - 14H_{4,1}^u + \frac{5}{2}H_{3,2}^u + 42H_{3,1,1}^u + \frac{13}{2}H_{2,2,1}^u - 36H_{2,1,1,1}^u \\
& + H_2^u \left[-5H_3^u + \frac{1}{2}H_{2,1}^u + 7\zeta_3 \right] + \frac{1}{2} \ln^2 u (H_3^u - 12H_{2,1}^u + 3\zeta_3) + \frac{1}{4} \ln^3 u (H_2^u - \zeta_2) \\
& + \ln u \left[-14(H_4^u - \zeta_4) + 19H_{3,1}^u - \frac{57}{2}H_{2,1,1}^u + \frac{1}{4}(H_2^u)^2 + \frac{7}{4}\zeta_2 H_2^u \right] \\
& + \zeta_2 \left(\frac{33}{4}H_3^u + H_{2,1}^u \right) - 2H_{4,1}^u - \frac{5}{2}H_{3,2}^u + 30H_{3,1,1}^u + \frac{19}{2}H_{2,2,1}^u - 12H_{2,1,1,1}^u \\
& + H_2^v \left(H_3^v - \frac{9}{2}H_{2,1}^v + \frac{9}{4}\zeta_2 \ln v - 7\zeta_3 \right) - \frac{1}{2} \ln^2 v (H_3^v + 4H_{2,1}^v + 3\zeta_3) \\
& + \ln v \left[2H_4^v + 5H_{3,1}^v - \frac{15}{2}H_{2,1,1}^v - \frac{5}{4}(H_2^v)^2 + 6\zeta_4 \right] - \frac{1}{4} \ln^3 v (H_2^v - \zeta_2) \\
& - \frac{1}{4}\zeta_2 (H_3^v - 28H_{2,1}^v) + \frac{1}{6} \left(H_2^u + \frac{1}{2} \ln^2 u \right) \left(-5H_3^v - 17H_{2,1}^v - 7 \ln v H_2^v + \frac{3}{2} \ln^3 v \right) \\
& + \frac{1}{6} \left(H_2^v + \frac{1}{2} \ln^2 v \right) \left(-43H_3^u + 41H_{2,1}^u - 5 \ln u H_2^u - \frac{21}{2} \ln^3 u \right) - 4 \ln u H_2^v H_2^w \\
& + \ln u \left[16H_4^v - 4H_{3,1}^v - 5(H_2^v)^2 - 6 \ln v (2H_3^v - H_{2,1}^v) + 3 \ln^2 v (H_2^v - 2\zeta_2) + 12\zeta_2 H_2^v \right] \\
& + \frac{1}{2} \ln^2 u \left[4(H_3^v + H_{2,1}^v) + \ln v H_2^v \right] + \ln v \left[2H_{3,1}^u - \frac{1}{2}(H_2^u)^2 + 2\zeta_2 H_2^u \right] \\
& + \ln w \left[-6H_{3,1}^v - \frac{1}{2}(H_2^v)^2 - 2 \ln v (2H_3^v - H_{2,1}^v) + \ln^2 v H_2^v - 2\zeta_2 (3H_2^v + \ln^2 v) \right] \\
& + \frac{1}{2} \ln^2 w (4H_3^v - \ln v H_2^v) + \frac{1}{2} \left(H_2^v + \frac{1}{2} \ln^2 v \right) (8H_{2,1}^w + 4 \ln w H_2^w - \ln^3 w) \\
& + 2 \ln^2 v (H_{2,1}^u + \ln u H_2^u) - \ln u \ln w \left[4H_3^v + 2H_{2,1}^v + \frac{3}{2} \ln u \left(H_2^v + \frac{1}{2} \ln^2 v \right) \right] \\
& + \ln v \ln w \left[-2H_{2,1}^u - \frac{1}{2} \ln v H_2^u - 2 \ln u \left(H_2^u + 2H_2^v + \frac{3}{8} \ln v \ln w - 6\zeta_2 \right) \right].
\end{aligned} \tag{4.7.7}$$

Since the $\{5, 1\}$ component of the coproduct specifies all the first derivatives of $R_6^{(3)}$, eqs. (4.7.5) and (4.7.6) should be supplemented by the value of $R_6^{(3)}$ at one point. For example, the value at $(u, v, w) = (1, 1, 1)$ will suffice (see below), or the constraint that it vanishes in all collinear limits.

In the remainder of this section, we use the multiple polylogarithmic and integral representations to obtain numerical values for $R_6^{(3)}$ for a variety of interesting contours and surfaces within the positive octant of the (u, v, w) space. We also obtain compact formulae for $R_6^{(3)}$ along specific lines through the space.

4.7.1 The line $(u, u, 1)$

On the line $(u, u, 1)$, the two- and three-loop remainder functions can be expressed solely in terms of HPLs of a single argument, $1 - u$. The two-loop function is,

$$R_6^{(2)}(u, u, 1) = H_4^u - H_{3,1}^u + 3 H_{2,1,1}^u + H_1^u (H_3^u - H_{2,1}^u) - \frac{1}{2} (H_2^u)^2 - (\zeta_2)^2, \quad (4.7.8)$$

while the three-loop function is,

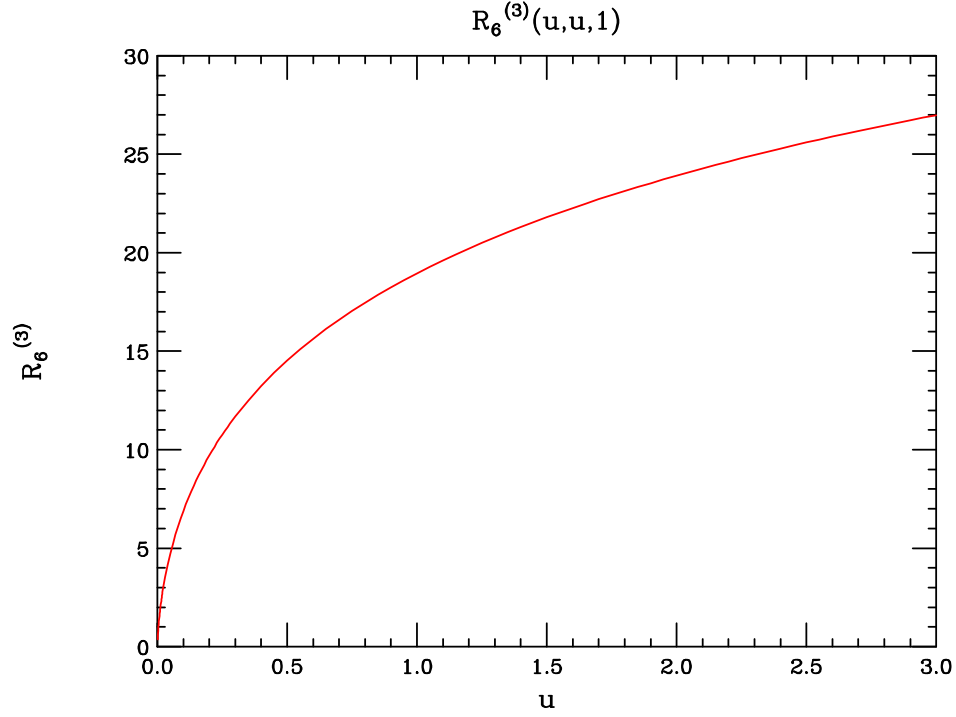
$$\begin{aligned} R_6^{(3)}(u, u, 1) = & -3 H_6^u + 2 H_{5,1}^u - 9 H_{4,1,1}^u - 2 H_{3,2,1}^u + 6 H_{3,1,1,1}^u - 15 H_{2,1,1,1,1}^u \\ & - \frac{1}{4} (H_3^u)^2 - \frac{1}{2} H_3^u H_{2,1}^u + \frac{3}{4} (H_{2,1}^u)^2 - \frac{5}{12} (H_2^u)^3 \\ & + \frac{1}{2} H_2^u \left[3 (H_4^u + H_{2,1,1}^u) + H_{3,1}^u \right] \\ & - H_1^u (3 H_5^u - 2 H_{4,1}^u + 9 H_{3,1,1}^u + 2 H_{2,2,1}^u - 6 H_{2,1,1,1}^u - H_2^u H_3^u) \\ & - \frac{1}{4} (H_1^u)^2 \left[3 (H_4^u + H_{2,1,1}^u) - 5 H_{3,1}^u + \frac{1}{2} (H_2^u)^2 \right] \\ & - \zeta_2 \left[H_4^u + H_{3,1}^u + 3 H_{2,1,1}^u + H_1^u (H_3^u + H_{2,1}^u) - (H_1^u)^2 H_2^u - \frac{3}{2} (H_2^u)^2 \right] \\ & - \zeta_4 \left[(H_1^u)^2 + 2 H_2^u \right] + \frac{413}{24} \zeta_6 + (\zeta_3)^2. \end{aligned} \quad (4.7.9)$$

Setting $u = 1$ in the above formula leads to

$$R_6^{(3)}(1, 1, 1) = \frac{413}{24} \zeta_6 + (\zeta_3)^2. \quad (4.7.10)$$

We remark that the four-loop cusp anomalous dimension in planar $\mathcal{N} = 4$ SYM,

$$\gamma_K^{(4)} = -\frac{219}{2} \zeta_6 - 4(\zeta_3)^2, \quad (4.7.11)$$

Figure 4.3: $R_6^{(3)}(u, u, 1)$ as a function of u .

has a different value for the ratio of the ζ_6 coefficient to the $(\zeta_3)^2$ coefficient.

The value of the two-loop remainder function at this same point is

$$R_6^{(2)}(1, 1, 1) = -(\zeta_2)^2 = -\frac{5}{2}\zeta_4. \quad (4.7.12)$$

The numerical value of the three-loop to two-loop ratio at the point $(1, 1, 1)$ is:

$$\frac{R_6^{(3)}(1, 1, 1)}{R_6^{(2)}(1, 1, 1)} = -7.004088513718\dots \quad (4.7.13)$$

We will see that over large swaths of the positive octant, the ratio $R_6^{(3)}/R_6^{(2)}$ does not stray too far from -7 .

We plot the function $R_6^{(3)}(u, u, 1)$ in fig. 4.3. We also give the leading term in the

expansions of $R_6^{(2)}(u, u, 1)$ and $R_6^{(3)}(u, u, 1)$ around $u = 0$,

$$\begin{aligned} R_6^{(2)}(u, u, 1) &= u \left[-\frac{1}{2} \ln^2 u + 2 \ln u + \zeta_2 - 3 \right] + \mathcal{O}(u^2), \\ R_6^{(3)}(u, u, 1) &= u \left[-\frac{1}{4} \ln^3 u + \left(\zeta_2 + \frac{9}{4} \right) \ln^2 u - \left(\frac{5}{2} \zeta_2 + 9 \right) \ln u - \frac{11}{2} \zeta_4 - \zeta_3 + \frac{3}{2} \zeta_2 + 15 \right] \\ &\quad + \mathcal{O}(u^2). \end{aligned} \tag{4.7.14}$$

Hence the ratio $R_6^{(3)}/R_6^{(2)}$ diverges logarithmically as $u \rightarrow 0$ along this line:

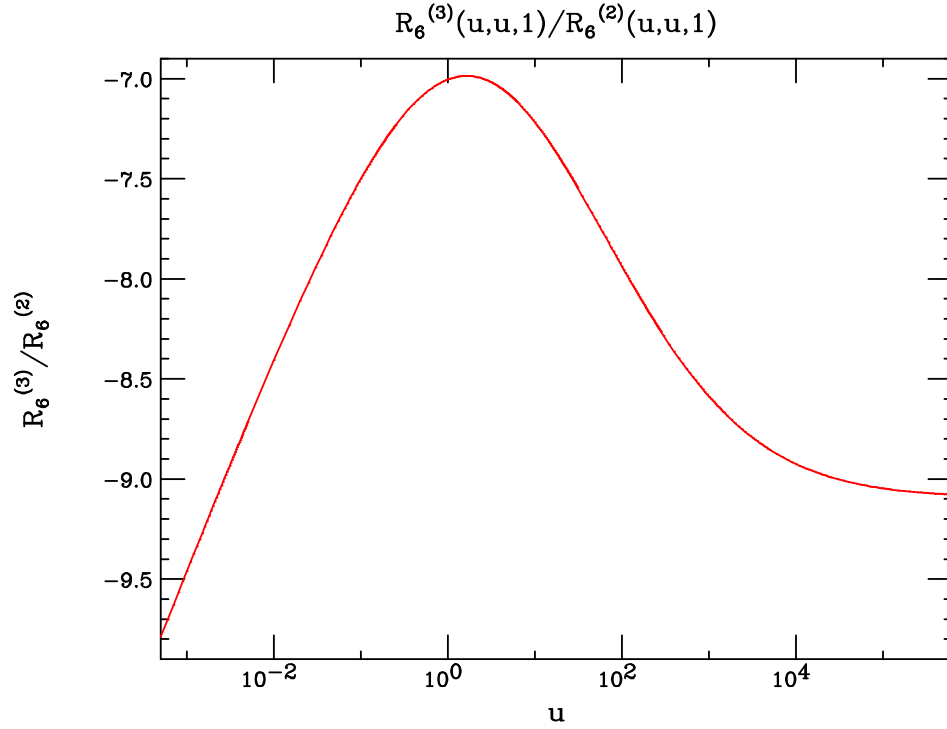
$$\frac{R_6^{(3)}(u, u, 1)}{R_6^{(2)}(u, u, 1)} \sim \frac{1}{2} \ln u, \quad \text{as } u \rightarrow 0. \tag{4.7.15}$$

This limit captures a piece of the near-collinear limit $T \rightarrow 0$, the case in which $S \rightarrow 0$ at the same rate, as discussed in section 4.5 near eq. (4.5.10). The fact that $R_6^{(3)}$ has one more power of $\ln u$ than does $R_6^{(2)}$ is partly from its extra leading power of $\ln T$ (the leading singularity behaves like $(\ln T)^{L-1}$), but also from an extra $\ln S^2$ factor in a subleading $\ln T$ term.

As $u \rightarrow \infty$, the leading behavior at two and three loops is,

$$\begin{aligned} R_6^{(2)}(u, u, 1) &= -\frac{27}{4} \zeta_4 + \frac{1}{u} \left[\frac{1}{3} \ln^3 u + \ln^2 u + (\zeta_2 + 2) \ln u + \zeta_2 + 2 \right] + \mathcal{O}\left(\frac{1}{u^2}\right), \\ R_6^{(3)}(u, u, 1) &= \frac{6097}{96} \zeta_6 + \frac{5}{4} (\zeta_3)^2 + \frac{1}{u} \left[-\frac{1}{10} \ln^5 u - \frac{1}{2} \ln^4 u - \frac{1}{3} (5\zeta_2 + 6) \ln^3 u \right. \\ &\quad \left. + \left(\frac{1}{2} \zeta_3 - 5\zeta_2 - 6 \right) \ln^2 u - \left(\frac{141}{8} \zeta_4 - \zeta_3 + 10\zeta_2 + 12 \right) \ln u \right. \\ &\quad \left. - 2\zeta_5 + 2\zeta_2 \zeta_3 - \frac{141}{8} \zeta_4 + \zeta_3 - 10\zeta_2 - 12 \right] + \mathcal{O}\left(\frac{1}{u^2}\right). \end{aligned} \tag{4.7.16}$$

As $u \rightarrow \infty$ along the line $(u, u, 1)$, the two- and three-loop remainder functions, and

Figure 4.4: $R_6^{(3)}/R_6^{(2)}$ on the line $(u, u, 1)$.

thus their ratio $R_6^{(3)}/R_6^{(2)}$, approach a constant. For the ratio it is:

$$\frac{R_6^{(3)}(u, u, 1)}{R_6^{(2)}(u, u, 1)} \sim -\left[\frac{50}{3} \frac{(\zeta_3)^2}{\pi^4} + \frac{871}{972} \pi^2\right] = -9.09128803107\dots, \quad \text{as } u \rightarrow \infty. \quad (4.7.17)$$

We plot the ratio $R_6^{(3)}/R_6^{(2)}$ on the line $(u, u, 1)$ in fig. 4.4. The logarithmic scale for u highlights how little the ratio varies over a broad range in u .

The line $(u, u, 1)$ is special in that the remainder function is extra pure on it. That

is, applying the operator $u(1-u) d/du$ returns a pure function for $L = 2, 3$:

$$\begin{aligned}
u(1-u) \frac{dR_6^{(2)}(u, u, 1)}{du} &= H_{2,1}^u - H_3^u, \\
u(1-u) \frac{dR_6^{(3)}(u, u, 1)}{du} &= 3H_5^u - 2H_{4,1}^u + 9H_{3,1,1}^u + 2H_{2,2,1}^u - 6H_{2,1,1,1}^u - H_2^u H_3^u \\
&\quad + H_1^u \left[\frac{3}{2}(H_4^u + H_{2,1,1}^u) - \frac{5}{2}H_{3,1}^u + \frac{1}{4}(H_2^u)^2 \right] \\
&\quad + \zeta_2 \left[H_3^u + H_{2,1}^u - 2H_1^u H_2^u \right] \\
&\quad + 2\zeta_4 H_1^u.
\end{aligned} \tag{4.7.18}$$

The extra-pure property is related to the fact that the asymptotic behavior as $u \rightarrow \infty$ is merely a constant, with no $\ln u$ terms. Indeed, if one applies $u(1-u) d/du$ to any positive power of $\ln u$, the result diverges at large u like u times a power of $\ln u$, which is not the limiting behavior of any combination of HPLs in \mathcal{H}_u .

4.7.2 The line $(1, 1, w)$

We next consider the line $(1, 1, w)$. As was the case for the line $(u, u, 1)$, we can express the two- and three-loop remainder functions on the line $(1, 1, w)$ solely in terms of HPLs of a single argument. However, in contrast to $(u, u, 1)$, the expressions on the line $(1, 1, w)$ are not extra-pure functions of w .

The two-loop result is,

$$\begin{aligned}
R_6^{(2)}(1, 1, w) &= \frac{1}{2} \left[H_4^w - H_{3,1}^w + 3H_{2,1,1}^w - \frac{1}{4}(H_2^w)^2 + H_1^w(H_3^w - 2H_{2,1}^w) \right. \\
&\quad \left. + \frac{1}{2}(H_2^w - \zeta_2)(H_1^w)^2 - 5\zeta_4 \right].
\end{aligned} \tag{4.7.19}$$

It is not extra pure on this line, because the quantity

$$w(1-w) \frac{dR_6^{(2)}(1, 1, w)}{dw} = \frac{1}{4}(2-w)(2H_{2,1}^w - H_1^w H_2^w) - \frac{1}{2}H_3^w + \frac{\zeta_2}{2}(1-w)H_1^w \tag{4.7.20}$$

contains explicit factors of w .

The three-loop result is,

$$\begin{aligned}
R_6^{(3)}(1, 1, w) = & -\frac{3}{2} H_6^w + H_{5,1}^w - \frac{9}{2} H_{4,1,1}^w - H_{3,2,1}^w + 3 H_{3,1,1,1}^w - \frac{15}{2} H_{2,1,1,1,1}^w \\
& - \frac{1}{8} H_3^w (H_3^w + 2 H_{2,1}^w) + \frac{3}{8} (H_{2,1}^w)^2 + \frac{1}{2} H_2^w \left(H_4^w + H_{3,1}^w - \frac{1}{6} (H_2^w)^2 \right) \\
& - \frac{1}{2} H_1^w \left[3 H_5^w + H_{3,2}^w + 6 H_{3,1,1}^w + H_{2,2,1}^w - 9 H_{2,1,1,1}^w - H_2^w H_3^w + \frac{1}{2} H_2^w H_{2,1}^w \right. \\
& \quad \left. + \frac{1}{8} H_1^w \left(-5 H_4^w + 5 H_{3,1}^w - 9 H_{2,1,1}^w + (H_2^w)^2 - H_1^w (H_3^w - H_{2,1}^w) \right) \right] \\
& - \frac{1}{2} \zeta_2 \left[H_4^w + H_{3,1}^w + 3 H_{2,1,1}^w - (H_2^w)^2 + H_1^w \left(H_3^w - 2 H_{2,1}^w + \frac{1}{2} H_1^w H_2^w \right) \right] \\
& + \zeta_4 \left[-H_2^w + \frac{17}{8} (H_1^w)^2 \right] + \frac{413}{24} \zeta_6 + (\zeta_3)^2.
\end{aligned} \tag{4.7.21}$$

It is easy to check that it is also not extra pure. We plot the function $R_6^{(3)}(1, 1, w)$ in fig. 4.5.

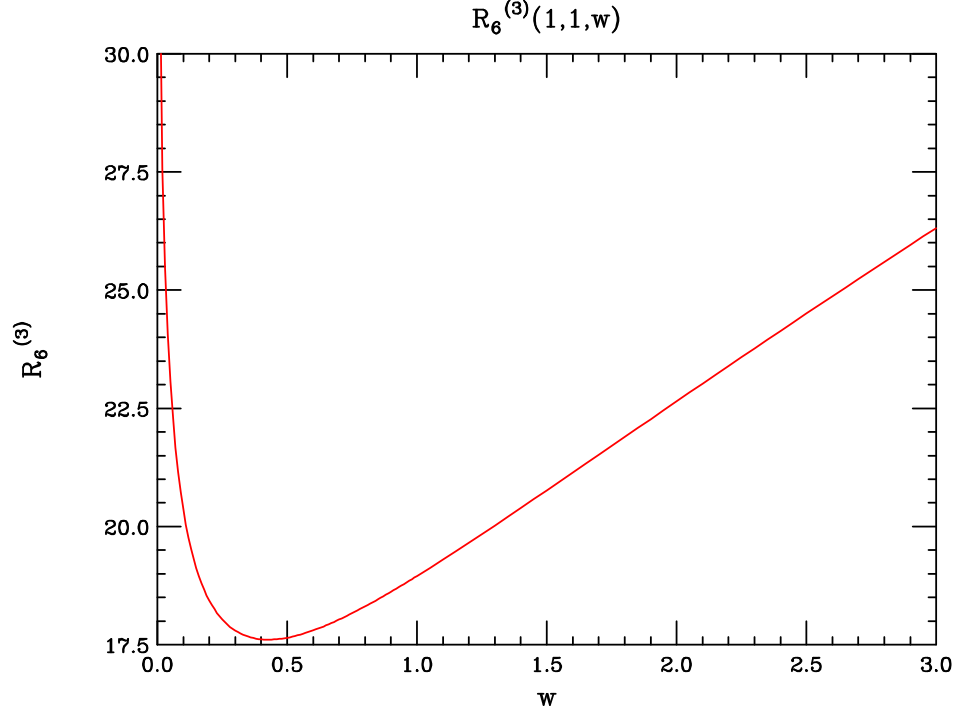
At small w , the two- and three-loop remainder functions diverge logarithmically,

$$\begin{aligned}
R_6^{(2)}(1, 1, w) &= \frac{1}{2} \zeta_3 \ln w - \frac{15}{16} \zeta_4 + \mathcal{O}(w), \\
R_6^{(3)}(1, 1, w) &= \frac{7}{32} \zeta_4 \ln^2 w - \left(\frac{5}{2} \zeta_5 + \frac{3}{4} \zeta_2 \zeta_3 \right) \ln w + \frac{77}{12} \zeta_6 + \frac{1}{2} (\zeta_3)^2 + \mathcal{O}(w).
\end{aligned} \tag{4.7.22}$$

At large w , they also diverge logarithmically,

$$\begin{aligned}
R_6^{(2)}(1, 1, w) &= -\frac{1}{96} \ln^4 w - \frac{3}{8} \zeta_2 \ln^2 w + \frac{\zeta_3}{2} \ln w - \frac{69}{16} \zeta_4 + \mathcal{O}\left(\frac{1}{w}\right), \\
R_6^{(3)}(1, 1, w) &= \frac{1}{960} \ln^6 w + \frac{\zeta_2}{12} \ln^4 w - \frac{\zeta_3}{8} \ln^3 w + 5 \zeta_4 \ln^2 w - \left(\frac{13}{4} \zeta_5 + 2 \zeta_2 \zeta_3 \right) \ln w \\
& \quad + \frac{1197}{32} \zeta_6 + \frac{9}{8} (\zeta_3)^2 + \mathcal{O}\left(\frac{1}{w}\right).
\end{aligned} \tag{4.7.23}$$

As discussed in the previous subsection, the lack of extra purity on the line $(1, 1, w)$

Figure 4.5: $R_6^{(3)}(1, 1, w)$ as a function of w .

is related to the logarithmic divergence in this asymptotic direction.

4.7.3 The line (u, u, u)

The symmetrical diagonal line (u, u, u) has the nice feature that the remainder function at strong coupling can be written analytically. Using AdS/CFT to map the problem to a minimal area one, and applying integrability, Alday, Gaiotto and Maldacena obtained the strong-coupling result [157],

$$R_6^{(\infty)}(u, u, u) = -\frac{\pi}{6} + \frac{\phi^2}{3\pi} + \frac{3}{8} \left[\ln^2 u + 2 \operatorname{Li}_2(1-u) \right] - \frac{\pi^2}{12}, \quad (4.7.24)$$

where $\phi = 3 \cos^{-1}(1/\sqrt{4u})$. The extra constant term $-\pi^2/12$ is needed in order for $R_6^{(\infty)}(u, v, w)$ to vanish properly in the collinear limits [169].²

²We thank Pedro Vieira for providing us with this constant.

In perturbation theory, the function $R_6^{(L)}(u, v, w)$ is less simple to represent on the line (u, u, u) than on the lines $(u, u, 1)$ and $(1, 1, w)$. It cannot be written solely in terms of HPLs with argument $(1 - u)$. At two loops, using eq. (4.2.14), the only obstruction is the function $\Omega^{(2)}(u, u, u)$,

$$R_6^{(2)}(u, u, u) = \frac{3}{4} \left[\Omega^{(2)}(u, u, u) + 4 H_4^u - 2 H_{3,1}^u - 2 (H_2^u)^2 + 2 H_1^u (2 H_3^u - H_{2,1}^u) - \frac{1}{4} (H_1^u)^4 - \zeta_2 (2 H_2^u + (H_1^u)^2) + \frac{8}{3} \zeta_4 \right]. \quad (4.7.25)$$

One way to proceed is to convert the first-order partial differential equations for all the hexagon functions of (u, v, w) into ordinary differential equations in u for the same functions evaluated on the line (u, u, u) . The differential equation for the three-loop remainder function itself is,

$$\begin{aligned} \frac{dR_6^{(3)}(u, u, u)}{du} = & \frac{3}{32} \left\{ \frac{1-u}{u\sqrt{\Delta}} \left[-10H_1(u, u, u) + \frac{9}{2}J_1(u, u, u) - 4\tilde{\Phi}_6(u, u, u) \left(3H_2^u + \frac{3}{2}(H_1^u)^2 - 9\zeta_2 \right) \right] \right. \\ & + \frac{8}{u(1-u)} \left[-\frac{3}{2}H_1^u \Omega^{(2)}(u, u, u) + 6H_5^u - 4H_{4,1}^u + 18H_{3,1,1}^u + 4H_{2,2,1}^u - 12H_{2,1,1,1}^u \right. \\ & + H_2^u (H_{2,1}^u - 3H_3^u) - H_1^u \left(H_4^u + 4H_{3,1}^u - 9H_{2,1,1}^u - \frac{11}{4}(H_2^u)^2 \right) \\ & + (H_1^u)^2 (H_{2,1}^u - 5H_3^u) + (H_1^u)^3 H_2^u + \frac{5}{8} (H_1^u)^5 \\ & \left. \left. + \zeta_2 (2H_3^u + 2H_{2,1}^u - 3H_1^u H_2^u - (H_1^u)^3) - 5\zeta_4 H_1^u \right] \right\}, \quad (4.7.26) \end{aligned}$$

with similar differential equations for $\Omega^{(2)}(u, u, u)$, $H_1(u, u, u)$ and $J_1(u, u, u)$. Interestingly, the parity-even weight-five functions M_1 and Q_{ep} do not enter eq. (4.7.26).

We can solve the differential equations by using series expansions around three points: $u = 0$, $u = 1$, and $u = \infty$. If we take enough terms in each expansion (of order 30–40 terms suffices), then the ranges of validity of the expansions will overlap.

At $u = 1$, Δ vanishes, and so do all the parity-odd functions, so we divide them by $\sqrt{\Delta}$ before series expanding in $(u - 1)$. These expansions, and those of the parity-even functions, are regular, with no logarithmic coefficients, as expected for a point in the interior of the positive octant. (Indeed, we can perform an analogous three-dimensional series expansion of all hexagon functions of (u, v, w) about $(1, 1, 1)$; this is actually a convenient way to fix the beyond-the-symbol terms in the coproducts, by using consistency of the mixed partial derivatives.)

At $u = 0$, the series expansions also contain powers of $\ln u$ in their coefficients. At $u = \infty$, there are two types of terms in the generic series expansion: a series expansion in $1/u$ with coefficients that are powers of $\ln u$, and a series expansion in odd powers of $1/\sqrt{u}$ with an overall factor of π^3 , and coefficients that can contain powers of $\ln u$. The square-root behavior can be traced back to the appearance of factors of $\sqrt{\Delta(u, u, u)} = (1 - u)\sqrt{1 - 4u}$ in the differential equations, such as eq. (4.7.26).

The constants of integration are easy to determine at $u = 1$ (where most of the hexagon function are defined to be zero). They can be determined numerically (and sometimes analytically) at $u = 0$ and $u = \infty$, either by evaluating the multiple polylogarithmic expressions, or by matching the series expansions with the one around $u = 1$.

At small u , the series expansions at two and three loops have the following form:

$$\begin{aligned}
 R_6^{(2)}(u, u, u) &= \frac{3}{4} \zeta_2 \ln^2 u + \frac{17}{16} \zeta_4 + \frac{3}{4} u \left[\ln^3 u + \ln^2 u + (5 \zeta_2 - 2) \ln u + 3 \zeta_2 - 6 \right] \\
 &\quad + \mathcal{O}(u^2), \\
 R_6^{(3)}(u, u, u) &= -\frac{63}{8} \zeta_4 \ln^2 u - \frac{1691}{192} \zeta_6 + \frac{1}{4} (\zeta_3)^2 \\
 &\quad + \frac{3}{16} u \left[\ln^5 u + \ln^4 u - 4(3 \zeta_2 + 1) \ln^3 u + 4(\zeta_3 - 2 \zeta_2 - 3) \ln^2 u \right. \\
 &\quad \left. - 2(97 \zeta_4 - 4 \zeta_3 - 4 \zeta_2 - 12) \ln u - 60 \zeta_4 - 8 \zeta_3 + 120 \right] \\
 &\quad + \mathcal{O}(u^2),
 \end{aligned}
 \tag{4.7.27}$$

while the strong-coupling result is,

$$R_6^{(\infty)}(u, u, u) = \left(\frac{3}{8} - \frac{3}{4\pi}\right) \ln^2 u + \frac{\pi^2}{24} - \frac{\pi}{6} + u \left[\left(\frac{3}{4} - \frac{3}{\pi}\right) \ln u - \frac{3}{4}\right] + \mathcal{O}(u^2). \quad (4.7.28)$$

Note that the leading term at three loops diverges logarithmically, but only as $\ln^2 u$. Alday, Gaiotto and Maldacena [157] observed that this property holds at two loops and at strong coupling, and predicted that it should hold to all orders.

At large u , the two- and three-loop remainder functions behave as,

$$\begin{aligned} R_6^{(2)}(u, u, u) &= -\frac{5}{8}\zeta_4 - \frac{3\pi^3}{4u^{1/2}} \\ &\quad + \frac{1}{16u} \left[2 \ln^3 u + 15 \ln^2 u + 6(6\zeta_2 + 11) \ln u + 24\zeta_3 + 126\zeta_2 + 138 \right] \\ &\quad - \frac{\pi^3}{32u^{3/2}} + \mathcal{O}\left(\frac{1}{u^2}\right), \\ R_6^{(3)}(u, u, u) &= -\frac{29}{48}\zeta_6 + \zeta_3^2 + \frac{3\pi^5}{4u^{1/2}} \\ &\quad + \frac{1}{32u} \left[-\frac{3}{10} \ln^5 u - \frac{15}{4} \ln^4 u - (22\zeta_2 + 33) \ln^3 u \right. \\ &\quad \quad + (12\zeta_3 - 159\zeta_2 - 207) \ln^2 u \\ &\quad \quad - (747\zeta_4 - 48\zeta_3 + 690\zeta_2 + 846) \ln u \\ &\quad \quad \left. - 96\zeta_5 + 72\zeta_2\zeta_3 - \frac{4263}{2}\zeta_4 + 96\zeta_3 - 1434\zeta_2 - 1710 \right] \\ &\quad + \frac{\pi^3}{32u^{3/2}} (-36 \ln u + 6\zeta_2 - 70) + \mathcal{O}\left(\frac{1}{u^2}\right), \end{aligned} \quad (4.7.29)$$

while the strong-coupling behavior is,

$$R_6^{(\infty)}(u, u, u) = -\frac{5\pi^2}{24} + \frac{7\pi}{12} - \frac{3}{2u^{1/2}} + \frac{3}{4u} \left[\ln u + 1 + \frac{1}{\pi} \right] - \frac{1}{16u^{3/2}} + \mathcal{O}\left(\frac{1}{u^2}\right). \quad (4.7.30)$$

In fig. 4.6 we plot the two- and three-loop and strong-coupling remainder functions on the line (u, u, u) . In order to highlight the remarkably similar shapes of the three functions for small and moderate values of u , we rescale $R_6^{(2)}$ by the constant factor (4.7.13), so that it matches $R_6^{(3)}$ at $u = 1$. We perform a similar rescaling of

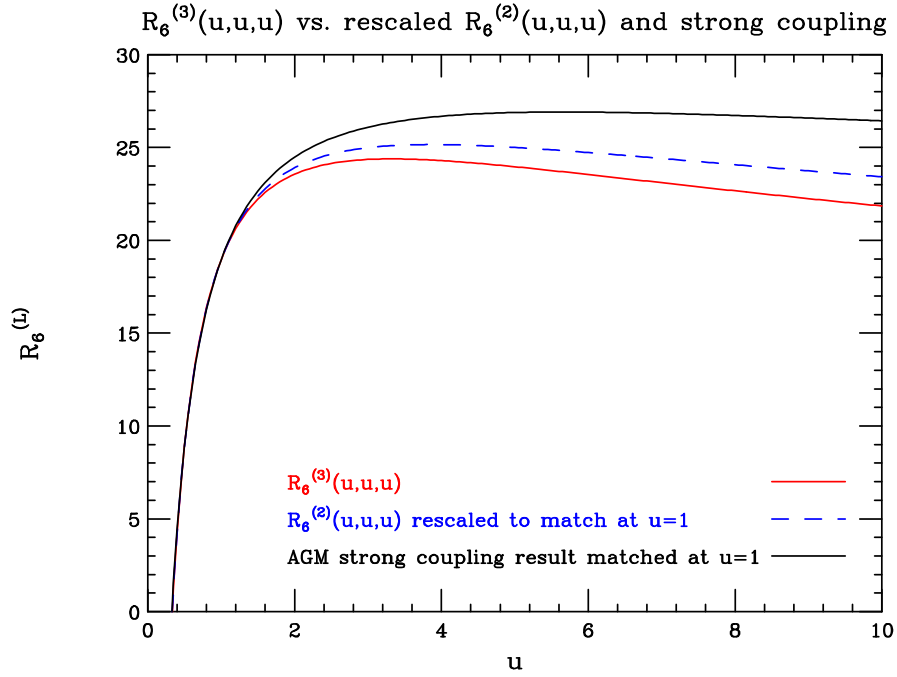


Figure 4.6: $R_6^{(2)}$, $R_6^{(3)}$, and the strong-coupling result on the line (u, u, u) .

the strong-coupling result, multiplying it by

$$\frac{R_6^{(3)}(1, 1, 1)}{R_6^{(\infty)}(1, 1, 1)} = -63.4116164\dots, \quad (4.7.31)$$

where $R_6^{(\infty)}(1, 1, 1) = \pi/6 - \pi^2/12$. A necessary condition for the shapes to be so similar is that the limiting behavior of the ratios as $u \rightarrow 0$ is almost the same as the ratios' values at $u = 1$. From eq. (4.7.27), the three-loop to two-loop ratio as $u \rightarrow 0$ is,

$$\frac{R_6^{(3)}(u, u, u)}{R_6^{(2)}(u, u, u)} \sim -\frac{21}{5} \zeta_2 = -6.908723\dots, \quad \text{as } u \rightarrow 0, \quad (4.7.32)$$

which is within 1.5% of the ratio at $(1, 1, 1)$, eq. (4.7.13). The three-loop to strong-coupling ratio is,

$$\frac{R_6^{(3)}(u, u, u)}{R_6^{(\infty)}(u, u, u)} \sim -\frac{21}{1 - 2/\pi} \zeta_4 = -62.548224\dots, \quad \text{as } u \rightarrow 0, \quad (4.7.33)$$

which is again within 1.5% of the corresponding ratio (4.7.33) at $u = 1$.

The similarity of the perturbative and strong-coupling curves for small and moderate u suggests that if a smooth extrapolation of the remainder function from weak to strong coupling can be achieved, on the line (u, u, u) it will have a form that is almost independent of u , for $u < 1$.

On the other hand, the curves in fig. 4.6 diverge from each other at large u , although they each approach a constant value as $u \rightarrow \infty$. The three-to-two-loop ratio at very large u , from eq. (4.7.29), eventually approaches $-1.227\dots$, which is quite different from -7 . The three-to-strong-coupling ratio approaches $-3.713\dots$, which is very different from -63.4 .

On the line (u, u, u) , all three curves in fig. 4.6 cross zero very close to $u = 1/3$. The respective zero crossing points for $L = 2, 3, \infty$ are:

$$u_0^{(2)} = 0.33245163\dots, \quad u_0^{(3)} = 0.3342763\dots, \quad u_0^{(\infty)} = 0.32737425\dots \quad (4.7.34)$$

Might the zero crossings in perturbation theory somehow converge to the strong-coupling value at large L ? We will return to the issue of the sign of $R_6^{(L)}$ below.

Another way to examine the progression of perturbation theory, and its possible extrapolation to strong coupling, is to use the Wilson loop ratio adopted by BSV, which is related to the remainder function by eq. (4.5.23). This relation holds for strong coupling as well as weak coupling, since the cusp anomalous dimension is known exactly [168]. In the near-collinear limit, considering the Wilson loop ratio has the advantage that the strong-coupling OPE behaves sensibly. The remainder function differs from this ratio by the one-loop function $X(u, v, w)$, whose near-collinear limit does not resemble a strong-coupling OPE at all. On the other hand, the Wilson loop ratio breaks all of the S_3 permutation symmetries of the remainder function. This is not an issue for the line (u, u, u) , since none of the S_3 symmetries survive on this line. However, there is also the issue that $X(u, u, u)$ as determined from eq. (4.5.24) diverges logarithmically as $u \rightarrow 1$.

In fig. 4.7 we plot the perturbative coefficients of $\ln[1 + \mathcal{W}_{\text{hex}}(a/2)]$, as well as the strong-coupling value, restricting ourselves to the range $0 < u < 1$ where $X(u, u, u)$

remains real. Now there is also a one-loop term, from multiplying $X(u, u, u)$ by the cusp anomalous dimension in eq. (4.5.23). We normalize the results in this case by dividing the coefficient at a given loop order by the corresponding coefficient of the cusp anomalous dimension, and similarly at strong coupling. Equivalently, from eq. (4.5.23), we plot

$$\frac{R_6^{(L)}(u, u, u)}{\gamma_K^{(L)}} + \frac{1}{8}X(u, u, u), \quad (4.7.35)$$

for $L = 1, 2, 3, \infty$.

The Wilson loop ratio diverges at both $u = 0$ and $u = 1$. The divergence at $u = 1$ comes only from X and is controlled by the cusp anomalous dimension. This forces the curves to converge in this region. The $\ln^2 u$ divergence as $u \rightarrow 0$ gets contributions from both X and R_6 . The latter contributions are not proportional to the cusp anomalous dimensions, causing all the curves to split apart at small u . Because $X(u, u, u)$ crosses zero at $u = 0.394\dots$, which is a bit different from the almost identical zero crossings in eq. (4.7.34) and in fig. 4.6, the addition of X in fig. 4.7 splits the zero crossings apart a little. However, in the bulk of the range, the perturbative coefficients do alternate in sign from one to three loops, following the sign alternation of the cusp anomaly coefficients, and suggesting that a smooth extrapolation from weak to strong coupling may be possible for this observable as well.

4.7.4 Planes of constant w

Having examined the remainder function on a few one-dimensional lines, we now turn to its behavior on various two-dimensional surfaces. We will now restrict our analysis to the unit cube, $0 \leq u, v, w \leq 1$. To provide a general picture of how the remainder function behaves throughout this region, we show in fig. 4.8 the function evaluated on planes with constant w , as a function of u and v . The plane $w = 1$ is in pink, $w = \frac{3}{4}$ in purple, $w = \frac{1}{2}$ in dark blue, and $w = \frac{1}{4}$ in light blue. The function goes to zero for the collinear-EMRK corner point $(u, v, w) = (0, 0, 1)$ (the right corner of the pink sheaf). Except for this point, $R_6^{(3)}(u, v, w)$ diverges as either $u \rightarrow 0$ or $v \rightarrow 0$.

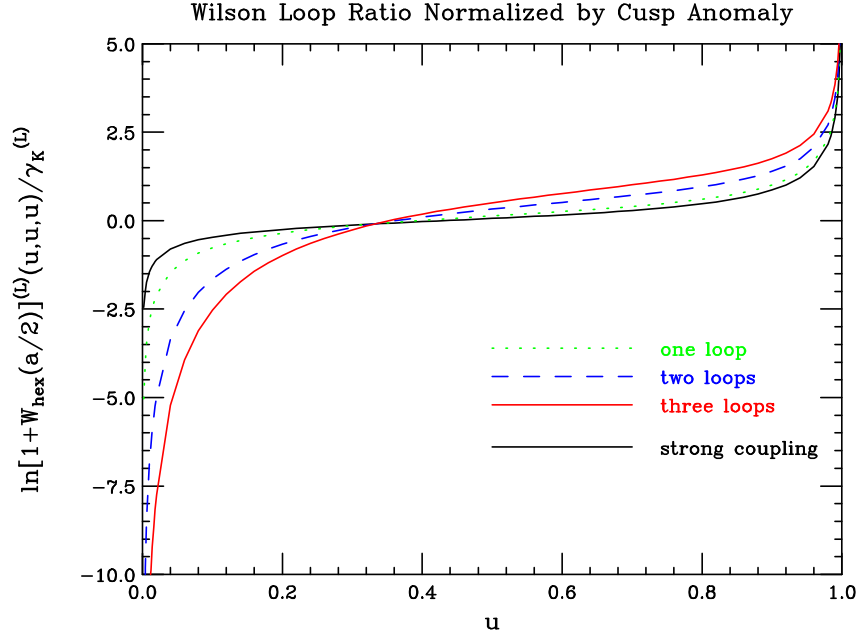


Figure 4.7: Comparison between the Wilson loop ratio at one to three loops, and the strong coupling value, evaluated on the line (u, u, u) .

While the plot might suggest that the function is monotonic in w within the unit cube, our analytic expression for the $(1, 1, w)$ line in section 4.7.2, and fig. 4.5, shows that at the left corner, where $u = v = 1$, the function does turn over closer to $w = 0$. (In fact, while it cannot be seen clearly from the plot, the $w = \frac{1}{4}$ surface actually intersects the $w = \frac{1}{2}$ surface near this corner.)

4.7.5 The plane $u + v - w = 1$

Next we consider the plane $u + v - w = 1$. Its intersection with the unit cube is the triangle bounded by the lines $(1, v, v)$ and $(w, 1, w)$, which are equivalent to the line $(u, u, 1)$ discussed in section 4.7.1, and by the collinear limit line $(u, 1 - u, 0)$, on which the remainder function vanishes.

In fig. 4.9 we plot the ratio $R_6^{(3)}/R_6^{(2)}$ on this triangle. The back edges can be identified with the $u < 1$ portion of fig. 4.4, although here they are plotted on a linear scale rather than a logarithmic scale. The plot is symmetrical under $u \leftrightarrow v$. In the

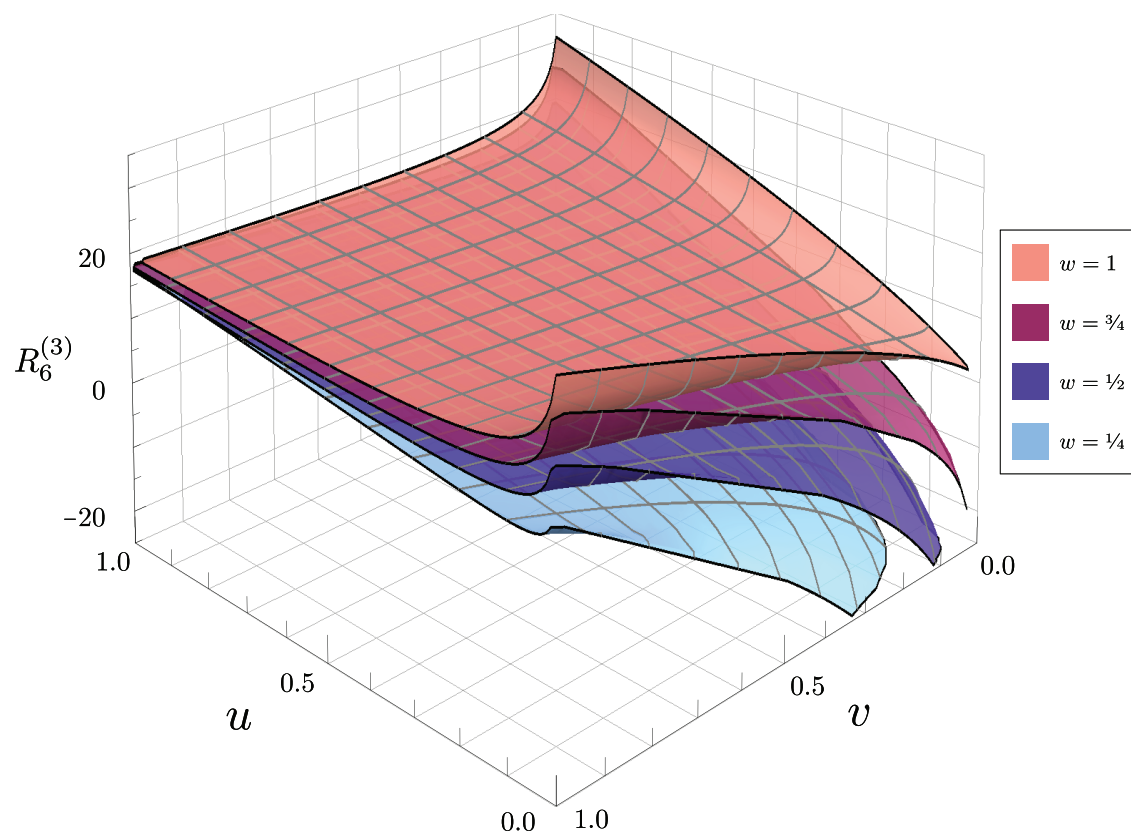


Figure 4.8: The remainder function $R_6^{(3)}(u, v, w)$ on planes of constant w , plotted in u and v . The top surface corresponds to $w = 1$, while lower surfaces correspond to $w = \frac{3}{4}$, $w = \frac{1}{2}$ and $w = \frac{1}{4}$, respectively.

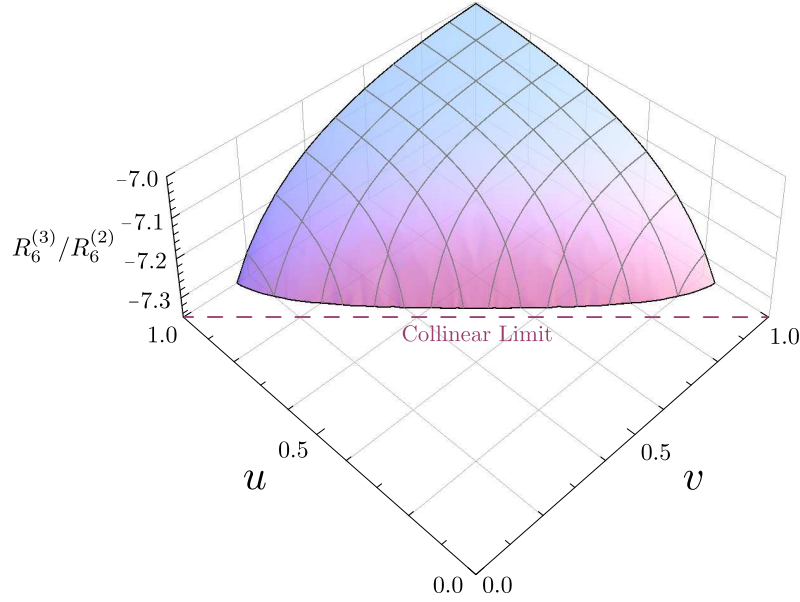


Figure 4.9: The ratio $R_6^{(3)}(u, v, w)/R_6^{(2)}(u, v, w)$ on the plane $u+v+w=1$, as a function of u and v .

bulk of the triangle, the ratio does not stray far from -7 . The only place it deviates is in the approach to the collinear limit, the front edge of the triangle corresponding to $T \rightarrow 0$ in the notation of section 4.5. Both $R_6^{(2)}$ and $R_6^{(3)}$ vanish like T times powers of $\ln T$ as $T \rightarrow 0$. However, because the leading singularity behaves like $(\ln T)^{L-1}$ at L loops, $R_6^{(3)}$ contains an extra power of $\ln T$ in its vanishing, and so the ratio diverges like $\ln T$. Otherwise, the shapes of the two functions agree remarkably well on this triangle.

4.7.6 The plane $u + v + w = 1$

The plane $u + v + w = 1$ intersects the unit cube along the three collinear lines. In fig. 4.10 we give a contour plot of $R_6^{(3)}(u, v, w)$ on the equilateral triangle lying between these lines. The plot has the full S_3 symmetry of the triangle under permutations of (u, v, w) . Because $R_6^{(3)}$ has to vanish on the boundary, one might expect that it should not get too large in the interior. Indeed, its furthest deviation from zero is

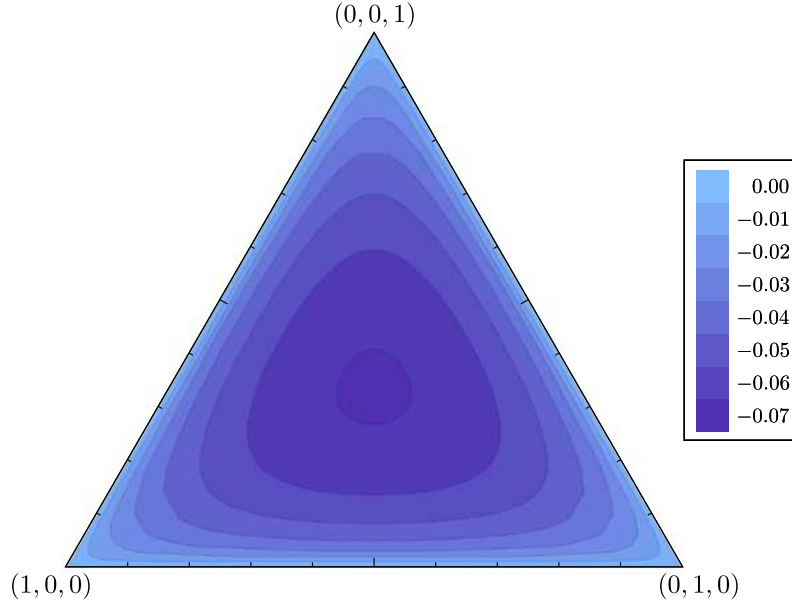


Figure 4.10: Contour plot of $R_6^{(3)}(u, v, w)$ on the plane $u + v + w = 1$ and inside the unit cube. The corners are labeled with their (u, v, w) values. Color indicates depth; each color corresponds to roughly a range of 0.01. The function must vanish at the edges, each of which corresponds to a collinear limit. Its minimum is slightly under -0.07 .

slightly under -0.07 , at the center of the triangle.

From the discussion in section 4.7.3 and fig. 4.6, we know that along the line (u, u, u) the two- and three-loop remainder functions almost always have the opposite sign. The only place they have the same sign on this line is for a very short interval $u \in [0.3325, 0.3343]$ (see eq. (4.7.34)). This interval happens to contain the point $(1/3, 1/3, 1/3)$, which is the intersection of the line (u, u, u) with the plane in fig. 4.10, right at the center of the triangle. In fact, throughout the entire unit cube, the only region where $R_6^{(2)}$ and $R_6^{(3)}$ have the same sign is a very thin pouch-like region surrounding this triangle. In other words, the zero surfaces of $R_6^{(2)}$ and $R_6^{(3)}$ are close to the plane $u + v + w = 1$, just slightly on opposite sides of it in the two cases. (We do not plot $R_6^{(2)}$ on the triangle here, but it is easy to verify that it is also uniformly negative in the region of fig. 4.10. Its furthest deviation from zero is about -0.0093 , again occurring at the center of the triangle.)

4.7.7 The plane $u = v$

In fig. 4.11 we plot $R_6^{(3)}(u, v, w)$ on the plane $u = v$, as a function of u and w inside the unit cube. This plane crosses the surface $\Delta = 0$ on the curve $w = (1 - 2u)^2$, plotted as the dashed parabola. Hence it allows us to observe that $R_6^{(3)}$ is perfectly continuous across the $\Delta = 0$ surface. We can also see that the function diverge as w goes to zero, and as u and v go to zero, everywhere except for the two places that this plane intersects the collinear limits, namely the points $(u, v, w) = (1/2, 1/2, 0)$ and $(u, v, w) = (0, 0, 1)$. The line of intersection of the $u = v$ plane and the $u + v + w = 1$ plane passes through both of these points, and fig. 4.11 shows that $R_6^{(3)}$ is very close to zero on this line.

Based on considerations related to the positive Grassmannian [133], it was recently conjectured [170] that the three-loop remainder function should have a uniform sign in the “positive region”, or what we call Region I: the portion of the unit cube where $\Delta > 0$ and $u + v + w < 1$, which corresponds to positive external kinematics in terms of momentum twistors. On the surface $u = v$, this region lies in front of the parabola shown in fig. 4.11. It was already checked [170] that the two-loop remainder function has a uniform (positive) sign in Region I. Fig. 4.11 illustrates that the uniform sign behavior (with a negative sign) is indeed true at three loops on the plane $u = v$. We have checked many other points with $u \neq v$ in Region I, and $R_6^{(3)}$ was negative for every point we checked, so the conjecture looks solid.

Furthermore, a uniform sign behavior for $R_6^{(2)}$ and $R_6^{(3)}$ also holds in the other regions of the unit cube with $\Delta > 0$, namely Regions II, III, and IV, which are all equivalent under S_3 transformations of the cross ratios. In these regions, the overall signs are reversed: $R_6^{(2)}$ is uniformly negative and $R_6^{(3)}$ is uniformly positive. For the plane $u = v$, fig. 4.11 shows the uniform positive sign of $R_6^{(3)}$ in Region II, which lies behind the parabola in the upper-left portion of the figure.

Based on the two- and three-loop data, sign flips in $R_6^{(L)}$ only seem to occur where $\Delta < 0$, and in fact very close to $u + v + w = 1$.

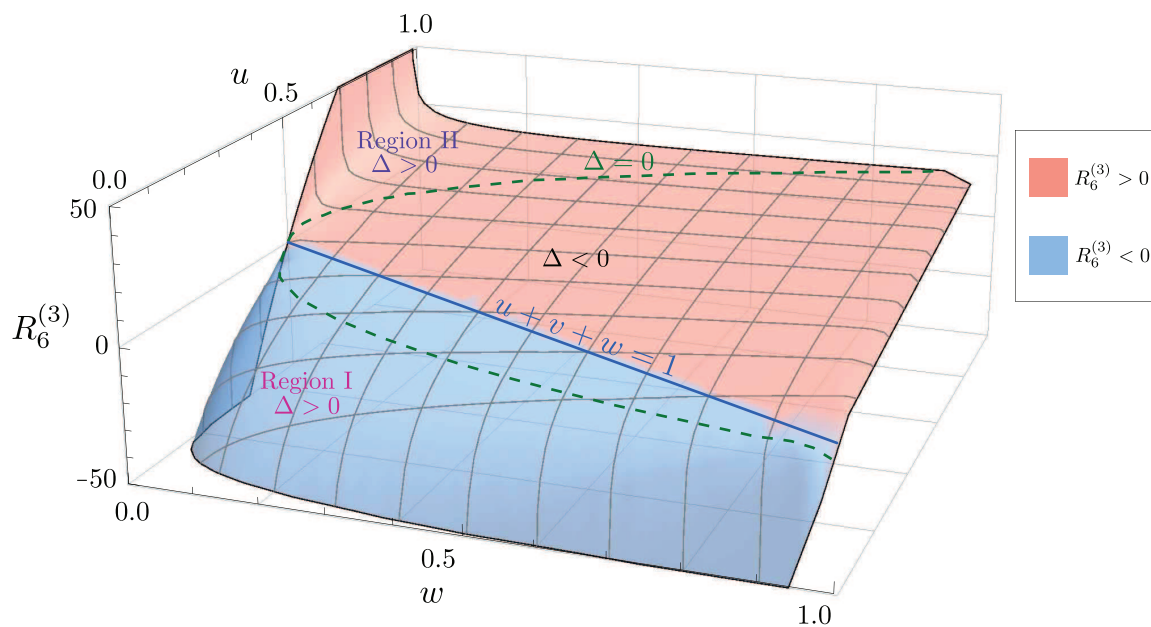


Figure 4.11: Plot of $R_6^{(3)}(u, v, w)$ on the plane $u = v$, as a function of u and w . The region where $R_6^{(3)}$ is positive is shown in pink, while the negative region is blue. The border between these two regions almost coincides with the intersection with the $u + v + w = 1$ plane, indicated with a solid line. The dashed parabola shows the intersection with the $\Delta = 0$ surface; inside the parabola $\Delta < 0$, while in the top-left and bottom-left corners $\Delta > 0$.

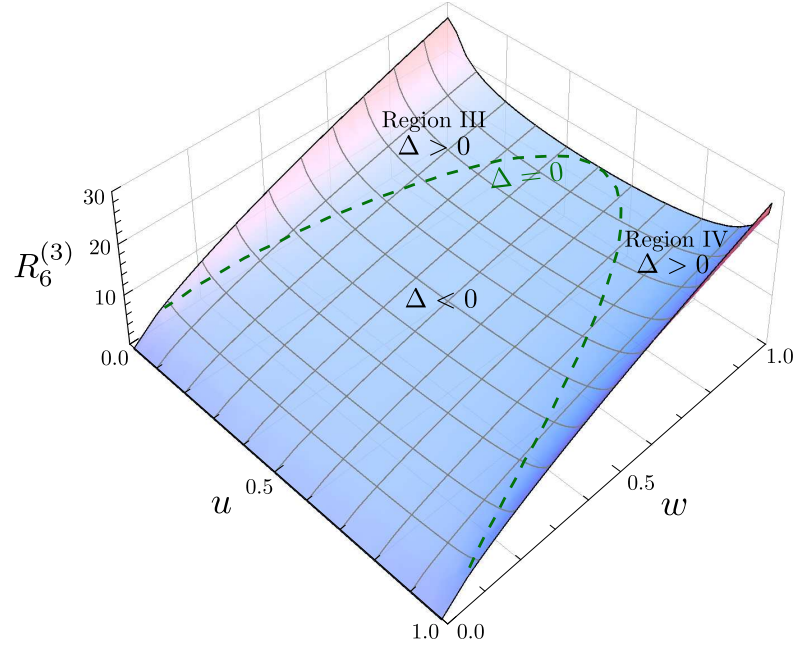


Figure 4.12: $R_6^{(3)}(u, v, w)$ on the plane $u + v = 1$, as a function of u and w .

4.7.8 The plane $u + v = 1$

In fig. 4.12 we plot $R_6^{(3)}$ on the plane $u + v = 1$. This plane provides information complementary to that on the plane $u = v$, since the two planes intersect at right angles. Like the $u = v$ plane, this plane shows smooth behavior over the $\Delta = 0$ surface, which intersects the plane $u + v = 1$ in the parabola $w = 4u(1 - u)$. It also shows that the function vanishes smoothly in the $w \rightarrow 0$ collinear limit.

4.8 Conclusions

In this paper, we successfully applied a bootstrap, or set of consistency conditions, in order to determine the three-loop remainder function $R_6^{(3)}(u, v, w)$ directly from a few assumed analytic properties. We bypassed altogether the problem of constructing and integrating multi-loop integrands. This work represents the completion of a program begun in ref. [14], in which the symbol $\mathcal{S}(R_6^{(3)})$ was determined via a Wilson loop OPE and certain conditions on the final entries, up to two undetermined rational numbers that were fixed soon thereafter [45].

In order to promote the symbol to a function, we first had to characterize the space of globally well-defined functions of three variables with the correct analytic properties, which we call hexagon functions. Hexagon functions are in one-to-one correspondence with the integrable symbols whose entries are drawn from the nine letters $\{u_i, 1 - u_i, y_i\}$, with the first entry restricted to $\{u_i\}$. We specified the hexagon functions at function level, iteratively in the transcendental weight, by using their coproduct structure. In this approach, integrability of the symbol is promoted to the function-level constraint of consistency of mixed partial derivatives. Additional constraints prevent branch-cuts from appearing except at physical locations ($u_i = 0, \infty$). These requirements fix the beyond-the-symbol terms in the $\{n - 1, 1\}$ coproduct components of the hexagon functions, and hence they fix the hexagon functions themselves (up to the arbitrary addition of lower-weight functions multiplied by zeta values). We found explicit representations of all the hexagon functions through weight five, and of $R_6^{(3)}$ itself at weight six, in terms of multiple polylogarithms whose arguments involve simple combinations of the y variables. We also used the coproduct structure to obtain systems of coupled first-order partial differential equations, which could be integrated numerically at generic values of the cross ratios, or solved analytically in various limiting kinematic regions.

Using our understanding of the space of hexagon functions, we constructed an ansatz for the function $R_6^{(3)}$ containing 11 rational numbers, free parameters multiplying lower-transcendentality hexagon functions. The vanishing of $R_6^{(3)}$ in the collinear limits fixed all but one of these parameters. The last parameter was fixed using the

near-collinear limits, in particular the $T^1 \ln T$ terms which we obtained from the OPE and integrability-based predictions of Basso, Sever and Vieira [150]. (The $T^1 \ln^0 T$ terms are also needed to fix the last symbol-level parameter [150], independently of ref. [45].)

With all parameters fixed, we could unambiguously extract further terms in the near-collinear limit. We find perfect agreement with Basso, Sever and Vieira’s results through order T^2 [152]. We have also evaluated the remainder function in the multi-Regge limit. This limit provides additional consistency checks, and allows us to fix three undetermined parameters in an expression [19] for the NNLLA impact parameter $\Phi_{\text{Reg}}^{(2)}(\nu, n)$ in the BFKL-factorized form of the remainder function [15].

Finally, we found simpler analytic representations for $R_6^{(3)}$ along particular lines in the three-dimensional (u, v, w) space; we plotted the function along these and other lines, and on some two-dimensional surfaces within the unit cube $0 \leq u_i \leq 1$. Throughout much of the unit cube, and sometimes much further out from the origin, we found the approximate numerical relation $R_6^{(3)} \approx -7 R_6^{(2)}$. The relation has only been observed to break down badly in regions where the functions vanish: the collinear limits, and very near the plane $u + v + w = 1$. On the diagonal line (u, u, u) , we observed that the two-loop, three-loop, and strong-coupling [157] remainder functions are almost indistinguishable in shape for $0 < u < 1$.

We have verified numerically a conjecture [170] that the remainder function should have a uniform sign in the “positive” region $\{u, v, w > 0; \Delta > 0; u + v + w < 1\}$. It also appears to have an (opposite) uniform sign in the complementary region $\{u, v, w > 0; \Delta > 0; u + v + w > 1\}$. The only zero-crossings we have found for either $R_6^{(2)}$ or $R_6^{(3)}$ in the positive octant are very close to the plane $u + v + w = 1$, in a region where Δ is negative.

Our work opens up a number of avenues for further research. A straightforward application is to the NMHV ratio function. Knowledge of the complete space of hexagon functions through weight five allowed us to construct the six-point MHV remainder function at three loops. The components of the three-loop six-point NMHV ratio function are also expected [71] to be weight-six hexagon functions. Therefore they should be constructable just as $R_6^{(3)}$ was, provided that enough physical information

can be supplied to fix all the free parameters.

It is also straightforward in principle to push the remainder function to higher loops. The symbol of the four-loop remainder function was heavily constrained [19] by the same information used at three loops [14], but of order 100 free parameters were left undetermined. With the knowledge of the near-collinear limits provided by Basso, Sever and Vieira [150, 152], those parameters can now all be fixed. Indeed, all the function-level ambiguities can be fixed as well [153]. This progress will allow many of the numerical observations made in this paper at three loops, to be explored at four loops in the near future. Going beyond four loops may also be feasible, depending primarily on computational issues — and provided that no inconsistencies arise related to failure of an underlying assumption.

It is remarkable that scattering amplitudes in planar $\mathcal{N} = 4$ super-Yang-Mills — polygonal (super) Wilson loops — are so heavily constrained by symmetries and other analytic properties, that a full bootstrap at the integrated level is practical, at least in perturbation theory. We have demonstrated this practicality explicitly for the six-point MHV remainder function. The number of cross ratios increases linearly with the number of points. More importantly, the number of letters in the symbol grows quite rapidly, even at two loops [46], increasing the complexity of the problem. However, with enough understanding of the relevant transcendental functions for more external legs [171, 172], it may still be possible to implement a similar procedure in these cases as well. In the longer term, the existence of near-collinear boundary conditions, for which there is now a fully nonperturbative bootstrap based on the OPE and integrability [150], should inspire the search for a fully nonperturbative formulation that also penetrates the interior of the kinematical phase space for particle scattering.

Chapter 5

The four-loop remainder function

5.1 Introduction

In the previous chapter, we introduced a set of polylogarithmic functions, which we call *hexagon functions*, whose symbols are built out of the nine letters eq. (1.1.3) and whose branch cut locations are restricted to the points where the cross ratios u_i either vanish or approach infinity. We developed a method, based on the coproduct on multiple polylogarithms (or, equivalently, a corresponding set of first-order partial differential equations), that allows for the construction of hexagon functions at arbitrary weight. Using this method, we determined the three-loop remainder function as a particular weight-six hexagon function.

In this chapter, we extend the analysis and construct the four-loop remainder function, which is a hexagon function of weight eight. As in the three-loop case, we begin by constructing the symbol. Referring to the discussion in section 1.7.2, the symbol may be written as

$$\mathcal{S}(R_6^{(4)}) = \sum_{i=1}^{113} \alpha_i S_i, \quad (5.1.1)$$

where α_i are undetermined rational numbers. The S_i are drawn from the complete set of eight-fold tensor products (*i.e.* symbols of weight eight) which satisfy the first entry condition and which obey the following properties:

0. All entries in the symbol are drawn from the set $\{u_i, 1 - u_i, y_i\}_{i=1,2,3}$, where the y_i 's are defined in eq. (1.1.4).
1. The symbol is integrable.
2. The symbol is totally symmetric under S_3 permutations of the cross ratios u_i .
3. The symbol is invariant under the transformation $y_i \rightarrow 1/y_i$.
4. The symbol vanishes in all simple collinear limits.
5. The symbol is in agreement with the predictions coming from the collinear OPE of ref. [38]. We implement this condition on the leading singularity exactly as was done at three loops [14].
6. The final entry of the symbol is drawn from the set $\{u_i/(1 - u_i), y_i\}_{i=1,2,3}$.

Imposing the above constraints on the most general ansatz of all 9^8 possible words will yield eq. (5.1.1); however, performing the linear algebra on such a large system is challenging. Therefore, it is useful to employ the shortcuts described in section 4.3.1: the first- and second-entry conditions reduce somewhat the size of the initial ansatz, and applying the integrability condition iteratively softens the exponential growth of the ansatz with the weight. Even still, the computation requires a dedicated method, since out-of-the-box linear algebra packages cannot handle such large systems. We implemented a batched Gaussian elimination algorithm, performing the back substitution with `FORM` [173], similar to the method described in ref. [174].

As discussed in section 1.7.2, the factorization formula of Fadin and Lipatov in the multi-Regge limit provides additional constraints on the 113 parameters entering eq. (5.1.1),

7. The symbol is in agreement with the prediction coming from BFKL factorization [15].

We may also apply constraints in the near-collinear limit by matching onto the recent predictions by Basso, Sever, and Vieira (BSV) based on the OPE for flux tube excitations [150],

8. The symbol is in agreement to order T^1 with the OPE prediction of the near-collinear expansion [150].
9. The symbol is in agreement to order T^2 with the OPE prediction of the near-collinear expansion [152].

The dimension of the ansatz after applying each of these constraints successively is summarized in table 5.1.

Constraint	Dimension
1. Integrability	5897
2. Total S_3 symmetry	1224
3. Parity invariance	874
4. Collinear vanishing (T^0)	622
5. Consistency with the leading discontinuity of the collinear OPE	482
6. Final entry	113
7. Multi-Regge limit	80
8. Near-collinear OPE (T^1)	4
9. Near-collinear OPE (T^2)	0

Table 5.1: Dimensions of the space of weight-eight symbols after applying the successive constraints. The final result is unique, including normalization, so the vector space of possible solutions has dimension zero.

In section 4.5, we applied the last two constraints at function-level to fully determine the three-loop remainder function. In fact, we will soon apply them at function-level in the four-loop case as well, but first we will apply them at symbol-level in order to determine the constants not fixed by the first seven constraints. For this purpose, it is necessary to expand $\mathcal{S}(R_6^{(4)})$ in the near-collinear limit, which, in the variables of eq. (4.5.1), is governed by $T \rightarrow 0$. To this end, we formulate the expansion of an arbitrary pure function in a manner that can easily be extended to the symbol. This is not entirely trivial because the expansion will in general contain powers of $\ln T$,

and some care must be given to keep track of them. Consider a pure function $F(T)$ for which $F(0) = 0$. We can immediately write,

$$\left[F(T)\right]_1 = \int_0^T dT_1 \left[F'(T_1)\right]_0 \quad (5.1.2)$$

where $[\cdot]_i$ indicates the T^i term of the expansion around 0. Owing to the presence of logarithms, it is possible that in evaluating $[F'(T)]_0$ we might generate a pole in T . Letting,

$$F'(T) = \frac{f_{-1}(T)}{T} + f_0(T) + \mathcal{O}(T^1) \quad (5.1.3)$$

we have,

$$\left[F'(T)\right]_0 = \frac{1}{T} \left[f_{-1}(T)\right]_1 + \left[f_0(T)\right]_0. \quad (5.1.4)$$

Notice that $f_{-1}(0) = 0$ (since otherwise $F(0) \neq 0$), so we can calculate $[f_{-1}(T)]_1$ by again applying eqn. (5.1.2), this time with $F \rightarrow f_{-1}$. Therefore eq. (5.1.2) defines a recursive procedure for extracting the first term in the expansion around $T = 0$. The recursion will terminate after a finite number of steps for a pure function.

The only data necessary to execute this procedure is the ability to evaluate the function when $T = 0$, and the ability to take derivatives. Since both of these operations carry over to the symbol, we can apply this method directly to $S(R_6^{(4)})$. To be specific, we write

$$S(R_6^{(4)}) = A_0 \otimes R_0 + A_1 \otimes R_1 \otimes T + A_2 \otimes R_2 \otimes T \otimes T + A_3 \otimes R_3 \otimes T \otimes T \otimes T, \quad (5.1.5)$$

where $R_i \neq T$ is defined to have length one and the A_i have length $7 - i$. This decomposition has made use of Constraint 5, consistency with the leading discontinuity predicted by the OPE: at ℓ loops, the OPE predicts the leading logarithm of T to be $\ln^{(\ell-1)} T$, which implies that no term in the symbol of $R_6^{(4)}$ can contain more than three T entries. We also note that although we have made explicit the T entries at the back end of the symbol, there may be up to $3 - i$ other T entries hidden inside

A_i . Applying eqn. (5.1.2), we obtain,

$$\begin{aligned} \left[\mathcal{S}(R_6^{(4)}) \right]_1 &= \int_0^T dT_0 \left[\frac{R'_0(T_0)}{R_0(T_0)} A_0 \right]_0 + \int_0^T dT_0 \int_0^{T_0} \frac{dT_1}{T_1} \left[\frac{R'_1(T_1)}{R_1(T_1)} A_1 \right]_0 \\ &\quad + \int_0^T dT_0 \int_0^{T_0} \frac{dT_1}{T_1} \int_0^{T_1} \frac{dT_2}{T_2} \left[\frac{R'_2(T_2)}{R_2(T_2)} A_2 \right]_0 \\ &\quad + \int_0^T dT_0 \int_0^{T_0} \frac{dT_1}{T_1} \int_0^{T_1} \frac{dT_2}{T_2} \int_0^{T_2} \frac{dT_3}{T_3} \left[\frac{R'_3(T_3)}{R_3(T_3)} A_3 \right]_0. \end{aligned} \quad (5.1.6)$$

As indicated by the brackets $[\cdot]_0$, the integrands should be expanded around $T = 0$ to order T^0 . To expand the A_i , one should first unshuffle all factors of T from the symbol, and then identify them as logarithms. Only after performing this identification should the integrations be performed. Notice that the integrals over T_0 have no $1/T_0$ in the measure, and as such they will generate terms of mixed transcendentality.

Equation (5.1.6) gives the expansion of $\mathcal{S}(R_6^{(4)})$ to order T^1 , but it is easy to extend this method to extract more terms in the expansion. To obtain the T^n term, we first subtract off the expansion through order T^{n-1} and divide by T^{n-1} , yielding a function that vanishes when $T = 0$. Then we can proceed as above and calculate the T^1 term, which will correspond to the T^n term of the original function.

Proceeding in this manner, we obtain the expansion of the symbol of $R_6^{(4)}$ through order T^2 . To compare this expansion with the data from the OPE, we must first disregard all terms containing factors of π or ζ_n , since these constants are not captured by the symbol. Performing the comparison, we find that the information at order T^1 is sufficient to fix all but four of the remaining parameters. At order T^2 , all four of these constants are determined and many additional cross-checks are satisfied. The final expression for the symbol of $R_6^{(4)}$ has 1,544,205 terms and is provided in a computer-readable file attached to this document.

We now turn to the problem of promoting the symbol to a function. In principle, the procedure is identical to that described in chapter 4; indeed, with enough computational power we could construct the full basis of hexagon functions at weight seven (or even eight), and replicate the analysis of chapter 4. In practice, it is difficult to build the full basis of hexagon functions beyond weight five or six, and so we briefly

describe a more efficient procedure that requires only a subset of the full basis.

To begin, we construct a function-level ansatz for $\Delta_{5,1,1,1}(R_6^{(4)})$. The ansatz is a four-fold tensor product whose first slot is a weight-five function and whose last three slots are logarithms. The symbol of the weight-five functions can be read off of the symbol of $R_6^{(4)}$ and identified with functions in the weight-five hexagon basis. Therefore we can immediately write down,

$$\Delta_{5,1,1,1}(R_6^{(4)}) = \sum_{s_i, s_j, s_k \in \mathcal{S}_u} [R_6^{(4)}]^{s_i, s_j, s_k} \otimes \ln s_i \otimes \ln s_j \otimes \ln s_k \quad (5.1.7)$$

where $[R_6^{(4)}]^{s_i, s_j, s_k}$ are the most general linear combinations of weight-five hexagon functions with the correct symbol and correct parity. There will be many arbitrary parameters associated with ζ values multiplying lower-weight functions.

Many of these parameters can be fixed by demanding that $\sum_{s_i \in \mathcal{S}_u} [R_6^{(4)}]^{s_i, s_j, s_k}$ be the $\{5, 1\}$ component of the coproduct for some weight-six function for every choice of j and k . This is simply the integrability constraint, discussed extensively in chapter 4, applied to the first two slots of the four-fold tensor product in eq. (5.1.7). We also require that each weight-six functions have the proper branch cut structure; again, this constraint may be applied using the techniques discussed in chapter 4. Finally, we must guarantee that the weight-six function have all of the symmetries exhibited by their symbols. For example, if a particular coproduct entry vanishes at symbol-level, we require that it vanish at function-level as well. We also demand that the function have definite parity since the symbol-level expressions have this property.

After imposing these mathematical consistency conditions, we will have constructed the $\{5, 1\}$ component of the coproduct for each of the weight-six functions entering $\Delta_{6,1,1}(R_6^{(4)})$, as well as all the integration constants necessary to define the corresponding integral representations (see section 4.4). There are many undetermined parameters, but they all correspond to ζ values multiplying lower-weight hexagon functions, so they cannot be fixed at this stage.

It is also also straightforward to represent $\Delta_{6,1,1}(R_6^{(4)})$ directly in terms of multiple polylogarithms in Region I. To this end, we describe how to integrate directly the $\{n-1, 1\}$ component of the coproduct of a weight- n function in terms of multiple

polylogarithms. The method is very similar to the integral given in eq. (4.3.8), which maps symbols directly into multiple polylogarithms. Instead of starting from the symbol, we start from the $\{n-1, 1\}$ coproduct component, and therefore we only have to perform one integration, corresponding to the final iteration of the n -fold iterated integration in eq. (4.3.8). As discussed in section 4.3, we are free to integrate along a contour that goes from the origin $t_i = 0$ to the point $t_i = y_i$ sequentially along the directions t_u , t_v and t_w . The integration is over $\omega = d \log \phi$ with $\phi \in \mathcal{S}_y$, and the integrand is a combination of weight- $(n-1)$ multiple polylogarithms in Region I; together, these two facts imply that the integral may always be evaluated trivially by invoking the definition of multiple polylogarithms, eq. (C.1.1).

Applying this method to the case at hand, we obtain an expression for $\Delta_{6,1,1}(R_6^{(4)})$ in terms of multiple polylogarithms in Region I. Again, we enforce mathematical consistency by requiring integrability in the first two slots, proper branch cut locations, and well-defined parity. We then integrate the expression using the same method, yielding an expression for $\Delta_{7,1}(R_6^{(4)})$. Finally, we iterate the procedure once more and obtain a representation for $R_6^{(4)}$ itself. At each stage we keep track of all the undetermined parameters. Any parameter that survives all the way to the weight-eight ansatz for $R_6^{(4)}$ must be associated with a ζ value multiplying a lower-weight hexagon functions with the proper symmetries and branch cut locations. There are 68 such functions. The counting of parameters is presented in table 5.2.

It is straightforward to expand our 68-parameter ansatz for $R_6^{(4)}$ in the near-collinear limit. Indeed, the methods discussed in section 4.5 can be applied directly to this case. We carried out this expansion through order T^3 , though even at order T^1 the result is too lengthy to present here. The expansion is available in a computer-readable format attached to this document.

Demanding that our ansatz vanish in the strict collinear limit fixes all but ten of the constants, while consistency with the OPE at order T^1 fixes nine more, leaving one constant that is fixed at order T^2 . The rest of the data at order T^2 provides many nontrivial consistency checks of the result. The final expression for $R_6^{(4)}$ in terms of multiple polylogarithms in Region I is attached to this document in a computer-readable format.

k	MZVs of weight k	Functions of weight $8 - k$	Total parameters
2	ζ_2	38	38
3	ζ_3	14	14
4	ζ_4	6	6
5	$\zeta_2\zeta_3, \zeta_5$	2	4
6	ζ_3^2, ζ_6	1	2
7	$\zeta_2\zeta_5, \zeta_3\zeta_4, \zeta_7$	0	0
8	$\zeta_2\zeta_3^2, \zeta_3\zeta_5, \zeta_8, \zeta_{5,3}$	1	4
			68

Table 5.2: Characterization of the beyond-the-symbol ambiguities in $R_6^{(4)}$ after imposing all mathematical consistency conditions.

5.2 Multi-Regge limit

The multi-Regge limit of the four-loop remainder function can be extracted by using the techniques described in section 4.6. We find expressions for the two previously undetermined functions in this limit,

$$\begin{aligned}
g_1^{(4)}(w, w^*) = & \frac{3}{128} [L_2^-]^2 [L_0^-]^2 - \frac{3}{32} [L_2^-]^2 [L_1^+]^2 + \frac{19}{384} [L_0^-]^2 [L_1^+]^4 \\
& + \frac{73}{1536} [L_0^-]^4 [L_1^+]^2 - \frac{17}{48} L_3^+ [L_1^+]^3 + \frac{1}{4} L_0^- L_{4,1}^- - \frac{3}{4} L_0^- L_{2,1,1,1}^- \\
& + \frac{1}{96} L_{2,1}^- [L_0^-]^3 - \frac{29}{64} L_1^+ L_3^+ [L_0^-]^2 - \frac{11}{30720} [L_0^-]^6 - \frac{1}{8} [L_{2,1}^-]^2 \\
& + \frac{11}{480} [L_1^+]^6 + \frac{5}{32} [L_3^+]^2 - \frac{1}{4} L_4^- L_2^- + \frac{1}{4} L_2^- L_{2,1,1}^- + \frac{19}{8} L_5^+ L_1^+ \\
& + \frac{5}{4} L_1^+ L_{3,1,1}^+ + \frac{1}{2} L_1^+ L_{2,2,1}^+ + \frac{1}{8} \zeta_3^2 - \frac{3}{2} \zeta_5 L_1^+ + \zeta_2 \zeta_3 L_1^+ \\
& + \frac{27}{8} \zeta_4 \left([L_1^+]^2 - \frac{1}{4} [L_0^-]^2 \right) + \frac{1}{8} \zeta_3 \left([L_1^+]^3 - L_3^+ + \frac{15}{4} L_1^+ [L_0^-]^2 \right) \\
& - \frac{1}{2} \zeta_2 \left(\frac{11}{384} [L_0^-]^4 + \frac{7}{8} [L_1^+]^4 + \frac{1}{2} [L_1^+]^2 [L_0^-]^2 - 3 L_1^+ L_3^+ \right. \\
& \quad \left. - L_0^- L_{2,1}^- + \frac{3}{4} [L_2^-]^2 \right), \tag{5.2.1}
\end{aligned}$$

and,

$$\begin{aligned}
g_0^{(4)}(w, w^*) = & \frac{5}{64} L_1^+ [L_2^-]^2 [L_0^-]^2 - \frac{1}{16} [L_2^-]^2 [L_1^+]^3 - \frac{21}{64} L_3^+ [L_0^-]^2 [L_1^+]^2 \\
& + \frac{7}{144} [L_0^-]^4 [L_1^+]^3 + \frac{1007}{46080} L_1^+ [L_0^-]^6 + \frac{1}{4} L_2^- L_{2,1,1}^- L_1^+ - \frac{125}{8} L_7^+ \\
& + \frac{9}{320} [L_0^-]^2 [L_1^+]^5 - \frac{7}{192} L_{2,1}^- L_1^+ [L_0^-]^3 + \frac{129}{64} L_5^+ [L_0^-]^2 \\
& - \frac{5}{24} L_3^+ [L_0^-]^4 + \frac{3}{32} L_{3,1,1}^+ [L_0^-]^2 - \frac{1}{16} L_{2,2,1}^+ [L_0^-]^2 - \frac{1}{16} L_0^- L_{2,1}^- [L_1^+]^3 \\
& + \frac{25}{16} L_5^+ [L_1^+]^2 - \frac{7}{48} L_3^+ [L_1^+]^4 + \frac{1}{210} [L_1^+]^7 - \frac{1}{4} L_4^- L_2^- L_1^+ \\
& - \frac{5}{16} L_2^- L_0^- L_{3,1}^+ + \frac{1}{4} L_0^- L_{4,1}^- L_1^+ - \frac{1}{8} L_0^- L_{2,1}^- L_3^+ - \frac{1}{4} L_0^- L_{2,1,1,1}^- L_1^+ \\
& + \frac{1}{2} L_{4,1,2}^+ + \frac{11}{4} L_{4,2,1}^+ + \frac{3}{4} L_{3,3,1}^+ - \frac{1}{2} L_{2,1,2,1,1}^+ - \frac{3}{2} L_{2,2,1,1,1}^+ \\
& + \frac{7}{8} L_{3,1,1}^+ [L_1^+]^2 + 5 L_{5,1,1}^+ - 4 L_{3,1,1,1,1}^+ + \frac{1}{4} L_{2,2,1}^+ [L_1^+]^2 \\
& + \frac{25}{4} \zeta_7 + \frac{3}{4} \zeta_2 \zeta_5 + \frac{3}{2} \zeta_3^2 L_1^+ + \zeta_5 \left(\frac{17}{16} [L_0^-]^2 - \frac{5}{2} [L_1^+]^2 \right) \\
& + \zeta_2 \zeta_3 \left(\frac{5}{4} [L_1^+]^2 - \frac{9}{16} [L_0^-]^2 \right) + \zeta_4 \left(\frac{9}{4} [L_1^+]^3 + \frac{11}{16} L_1^+ [L_0^-]^2 - \frac{15}{2} L_3^+ \right) \\
& + \zeta_3 \left(\frac{7}{48} [L_1^+]^4 + \frac{7}{256} [L_0^-]^4 - \frac{3}{4} L_1^+ L_3^+ + \frac{1}{2} [L_1^+]^2 [L_0^-]^2 + \frac{1}{4} [L_2^-]^2 \right) \\
& - \zeta_2 \left(\frac{1}{5} [L_1^+]^5 + \frac{19}{192} L_1^+ [L_0^-]^4 + \frac{19}{48} [L_1^+]^3 [L_0^-]^2 - \frac{15}{8} [L_1^+]^2 L_3^+ \right. \\
& \quad \left. - \frac{25}{32} [L_0^-]^2 L_3^+ - L_1^+ L_0^- L_{2,1}^- + \frac{21}{4} L_5^+ + \frac{3}{2} L_{2,2,1}^+ + 3 L_{3,1,1}^+ \right).
\end{aligned} \tag{5.2.2}$$

These expressions match with those of eqs. (1.7.14) and (1.7.15), provided that the constants in chapter 1 take the values,

$$\begin{aligned}
a_0 &= 0, & a_1 &= -\frac{1}{6}, & a_2 &= -5, & a_3 &= 1, & a_4 &= \frac{4}{3}, \\
a_5 &= -\frac{4}{3}, & a_6 &= \frac{17}{180}, & a_7 &= \frac{15}{4}, & a_8 &= -29,
\end{aligned} \tag{5.2.3}$$

and

$$\begin{aligned}
b_1 &= \frac{97}{1220}, & b_2 &= \frac{127}{3660}, & b_3 &= \frac{1720}{183}, & b_4 &= \frac{622}{183}, & b_5 &= \frac{644}{305}, & b_6 &= \frac{2328}{305} \\
b_7 &= -1, & b_8 &= -\frac{554}{305}, & b_9 &= -\frac{10416}{305}, & b_{10} &= \frac{248}{3}, & b_{11} &= -\frac{11}{6}, & b_{12} &= 49, \\
b_{13} &= -112, & b_{14} &= \frac{83}{12}, & b_{15} &= -\frac{1126}{61}, & b_{16} &= \frac{849}{122}, & b_{17} &= \frac{83}{6}, & b_{18} &= -10.
\end{aligned} \tag{5.2.4}$$

These constants, in turn, determine the NNLLA BFKL eigenvalue and N³LLA impact factor,

$$\begin{aligned}
E_{\nu,n}^{(2)} &= \frac{1}{8} \left\{ \frac{1}{6} D_\nu^4 E_{\nu,n} - V D_\nu^3 E_{\nu,n} + (V^2 + 2\zeta_2) D_\nu^2 E_{\nu,n} - V (N^2 + 8\zeta_2) D_\nu E_{\nu,n} \right. \\
&\quad \left. + \zeta_3 (4V^2 + N^2) + 44\zeta_4 E_{\nu,n} + 16\zeta_2 \zeta_3 + 80\zeta_5 \right\},
\end{aligned} \tag{5.2.5}$$

and,

$$\begin{aligned}
\Phi_{\text{Reg}}^{(3)} &= -\frac{1}{48} \left\{ E_{\nu,n}^6 + \frac{9}{4} E_{\nu,n}^4 N^2 + \frac{57}{16} E_{\nu,n}^2 N^4 + \frac{189}{64} N^6 + \frac{15}{2} E_{\nu,n}^2 N^2 V^2 + \frac{123}{8} N^4 V^2 \right. \\
&\quad + 9N^2 V^4 - 3 \left(4E_{\nu,n}^3 V + 5E_{\nu,n} N^2 V \right) D_\nu E_{\nu,n} \\
&\quad + 3 \left(E_{\nu,n}^2 + \frac{3}{4} N^2 + 2V^2 \right) [D_\nu E_{\nu,n}]^2 + 6E_{\nu,n} \left(E_{\nu,n}^2 + \frac{3}{4} N^2 + V^2 \right) D_\nu^2 E_{\nu,n} \\
&\quad - 12V [D_\nu E_{\nu,n}] [D_\nu^2 E_{\nu,n}] - 6E_{\nu,n} V D_\nu^3 E_{\nu,n} + 2 [D_\nu E_{\nu,n}] [D_\nu^3 E_{\nu,n}] \\
&\quad \left. + 2 [D_\nu^2 E_{\nu,n}]^2 + E_{\nu,n} D_\nu^4 E_{\nu,n} \right\} \\
&\quad - \frac{1}{8} \zeta_2 \left[3E_{\nu,n}^4 + 2E_{\nu,n}^2 N^2 - \frac{1}{16} N^4 - 6E_{\nu,n}^2 V^2 - 16N^2 V^2 - 12E_{\nu,n} V D_\nu E_{\nu,n} \right. \\
&\quad \left. + [D_\nu E_{\nu,n}]^2 + 4E_{\nu,n} D_\nu^2 E_{\nu,n} \right] \\
&\quad - \frac{1}{2} \zeta_3 \left[3E_{\nu,n}^3 + \frac{5}{2} E_{\nu,n} N^2 + E_{\nu,n} V^2 - 3V D_\nu E_{\nu,n} + \frac{13}{6} D_\nu^2 E_{\nu,n} \right] \\
&\quad - \frac{1}{4} \zeta_4 \left[27E_{\nu,n}^2 + N^2 - 45V^2 \right] - 5(2\zeta_5 + \zeta_2 \zeta_3) E_{\nu,n} - \frac{219}{8} \zeta_6 - \frac{14}{3} \zeta_3^2,
\end{aligned} \tag{5.2.6}$$

where V and N are as given in chapter 1,

$$\begin{aligned} V &\equiv -\frac{1}{2} \left[\frac{1}{i\nu + \frac{|n|}{2}} - \frac{1}{-i\nu + \frac{|n|}{2}} \right] = \frac{i\nu}{\nu^2 + \frac{|n|^2}{4}}, \\ N &\equiv \text{sgn}(n) \left[\frac{1}{i\nu + \frac{|n|}{2}} + \frac{1}{-i\nu + \frac{|n|}{2}} \right] = \frac{n}{\nu^2 + \frac{|n|^2}{4}}. \end{aligned} \quad (5.2.7)$$

These data suggest an intriguing connection between the BFKL eigenvalues $E_{\nu,n}$, $E_{\nu,n}^{(1)}$, and $E_{\nu,n}^{(2)}$ and the weak-coupling expansion of the energy $E(u)$ of a gluonic excitation of the GKP string as a function of its rapidity, given in ref. [175]. First we rewrite the expressions for $E_{\nu,n}$, $E_{\nu,n}^{(1)}$, and $E_{\nu,n}^{(2)}$ explicitly in terms of ψ functions and their derivatives,

$$\begin{aligned} E_{\nu,n} &= \psi(\xi^+) + \psi(\xi^-) - 2\psi(1) - \frac{1}{2} \text{sgn}(n)N \\ E_{\nu,n}^{(1)} &= -\frac{1}{4} \left[\psi^{(2)}(\xi^+) + \psi^{(2)}(\xi^-) - \text{sgn}(n)N \left(\frac{1}{4}N^2 + V^2 \right) \right] \\ &\quad + \frac{1}{2}V \left[\psi^{(1)}(\xi^+) - \psi^{(1)}(\xi^-) \right] - \zeta_2 E_{\nu,n} - 3\zeta_3 \\ E_{\nu,n}^{(2)} &= \frac{1}{8} \left\{ \frac{1}{6} \left[\psi^{(4)}(\xi^+) + \psi^{(4)}(\xi^-) - 60 \text{sgn}(n)N \left(V^4 + \frac{1}{2}V^2N^2 + \frac{1}{80}N^4 \right) \right] \right. \\ &\quad - V \left[\psi^{(3)}(\xi^+) - \psi^{(3)}(\xi^-) - 3 \text{sgn}(n)VN(4V^2 + N^2) \right] \\ &\quad + (V^2 + 2\zeta_2) \left[\psi^{(2)}(\xi^+) + \psi^{(2)}(\xi^-) - \text{sgn}(n)N \left(3V^2 + \frac{1}{4}N^2 \right) \right] \\ &\quad - V(N^2 + 8\zeta_2) \left[\psi'(\xi^+) - \psi'(\xi^-) - \text{sgn}(n)VN \right] + \zeta_3(4V^2 + N^2) \\ &\quad \left. + 44\zeta_4 E_{\nu,n} + 16\zeta_2\zeta_3 + 80\zeta_5 \right\}, \end{aligned} \quad (5.2.8)$$

where $\xi^\pm \equiv 1 \pm i\nu + \frac{|n|}{2}$. Next, we keep only the pure ψ terms, dropping anything with a V or an N ,

$$\begin{aligned}
E_{\nu,n} \Big|_{\psi \text{ only}} &= \psi(\xi^+) + \psi(\xi^-) - 2\psi(1) \\
E_{\nu,n}^{(1)} \Big|_{\psi \text{ only}} &= -\frac{1}{4} \left[\psi^{(2)}(\xi^+) + \psi^{(2)}(\xi^-) \right] - \zeta_2 \left[\psi(\xi^+) + \psi(\xi^-) - 2\psi(1) \right] - 3\zeta_3 \\
E_{\nu,n}^{(2)} \Big|_{\psi \text{ only}} &= \frac{1}{8} \left\{ \frac{1}{6} \left[\psi^{(4)}(\xi^+) + \psi^{(4)}(\xi^-) \right] + 2\zeta_2 \left[\psi^{(2)}(\xi^+) + \psi^{(2)}(\xi^-) \right] \right. \\
&\quad \left. + 44\zeta_4 \left[\psi(\xi^+) + \psi(\xi^-) - 2\psi(1) \right] + 16\zeta_2\zeta_3 + 80\zeta_5 \right\}.
\end{aligned} \tag{5.2.9}$$

Finally we write,

$$-\omega(\nu, n) \Big|_{\psi \text{ only}} = a \left(E_{\nu,n} \Big|_{\psi \text{ only}} + a E_{\nu,n}^{(1)} \Big|_{\psi \text{ only}} + a^2 E_{\nu,n}^{(2)} \Big|_{\psi \text{ only}} + \cdots \right). \tag{5.2.10}$$

Now we compare this formula to equation (4.21) of ref. [175] for the energy $E(u)$ of a gauge field ($\ell = 1$) and its bound state ($\ell > 1$),

$$\begin{aligned}
E(u) &= \ell + \Gamma_{\text{cusp}}(g) \left[\psi_0^{(+)}(s, u) - \psi_0(1) \right] - 2g^4 \left[\psi_2^{(+)}(s, u) + 6\zeta_3 \right] \\
&\quad + \frac{g^6}{3} \left[\psi_4^{(+)}(s, u) + 2\pi^2 \psi_2^{(+)}(s, u) + 24\zeta_3 \psi_1^{(+)}(s-1, u) + 8(\pi^2 \zeta_3 + 30\zeta_5) \right] \\
&\quad + \mathcal{O}(g^8),
\end{aligned}$$

where $g^2 = a/2$ is the loop expansion parameter, $s = 1 + \ell/2$,

$$\Gamma_{\text{cusp}}(g) = 4g^2 \left(1 - 2\zeta_2 g^2 + 22\zeta_4 g^4 + \cdots \right), \tag{5.2.11}$$

and,

$$\psi_n^{(\pm)}(s, u) \equiv \frac{1}{2} \left[\psi^{(n)}(s + iu) \pm \psi^{(n)}(s - iu) \right]. \tag{5.2.12}$$

Neglecting the constant offset at a^0 , eq. (5.2.11) matches perfectly with eq. (5.2.10) at order a^1 and a^2 , provided we identify,

$$\ell = |n|, \quad u = \nu. \tag{5.2.13}$$

The correspondence continues to order a^3 if we also drop the term $24\zeta_3\psi_1^{(+)}(s-1, u)$. It would be very interesting to understand the origin of this correspondence, and if there is a physical meaning to the operation of dropping all terms with a N or a V . We leave this question for future work and return our attention to the quantitative behavior of the four-loop remainder function.

5.3 Quantitative behavior

5.3.1 The line $(u, u, 1)$

As noted in section 4.7.1, the two- and three-loop remainder functions can be expressed solely in terms of HPLs of a single argument, $1-u$, on the line $(u, u, 1)$. The same is true at four loops, though the resulting expression is rather lengthy. To save space, we first expand all products of HPL's using the shuffle algebra. The result will have weight vectors consisting entirely of 0's and 1's, which we can interpret as binary numbers. Finally, we can write these binary numbers in decimal, making sure to keep track of the length of the original weight vector, which we write as a superscript. For example,

$$H_1^u H_{2,1}^u = H_1^u H_{0,1,1}^u = 3H_{0,1,1,1}^u + H_{1,0,1,1}^u \rightarrow 3h_7^{[4]} + h_{11}^{[4]}. \quad (5.3.1)$$

In this notation, $R_6^{(2)}(u, u, 1)$ and $R_6^{(3)}(u, u, 1)$ read,

$$R_6^{(2)}(u, u, 1) = h_1^{[4]} - h_3^{[4]} + h_9^{[4]} - h_{11}^{[4]} - \frac{5}{2}\zeta_4, \quad (5.3.2)$$

$$\begin{aligned} R_6^{(3)}(u, u, 1) = & -3h_1^{[6]} + 5h_3^{[6]} + \frac{3}{2}h_5^{[6]} - \frac{9}{2}h_7^{[6]} - \frac{1}{2}h_9^{[6]} - \frac{3}{2}h_{11}^{[6]} - h_{13}^{[6]} - \frac{3}{2}h_{17}^{[6]} \\ & + \frac{3}{2}h_{19}^{[6]} - \frac{1}{2}h_{21}^{[6]} - \frac{3}{2}h_{23}^{[6]} - 3h_{33}^{[6]} + 5h_{35}^{[6]} + \frac{3}{2}h_{37}^{[6]} - \frac{9}{2}h_{39}^{[6]} \\ & - \frac{1}{2}h_{41}^{[6]} - \frac{3}{2}h_{43}^{[6]} - h_{45}^{[6]} - \frac{3}{2}h_{49}^{[6]} + \frac{3}{2}h_{51}^{[6]} - \frac{1}{2}h_{53}^{[6]} - \frac{3}{2}h_{55}^{[6]} \\ & + \zeta_2 \left[-h_1^{[4]} + 3h_3^{[4]} + 2h_5^{[4]} - h_9^{[4]} + 3h_{11}^{[4]} + 2h_{13}^{[4]} \right] \\ & + \zeta_4 \left[-2h_1^{[2]} - 2h_3^{[2]} \right] + \zeta_3^2 + \frac{413}{24}\zeta_6, \end{aligned} \quad (5.3.3)$$

and the 4-loop remainder function on the line $(u, u, 1)$ is,

$$\begin{aligned}
R_6^{(4)}(u, u, 1) = & 15h_1^{[8]} - 41h_3^{[8]} - \frac{31}{2}h_5^{[8]} + \frac{105}{2}h_7^{[8]} - \frac{7}{2}h_9^{[8]} + \frac{53}{2}h_{11}^{[8]} + 12h_{13}^{[8]} - 42h_{15}^{[8]} \\
& + \frac{5}{2}h_{17}^{[8]} + \frac{11}{2}h_{19}^{[8]} + \frac{9}{2}h_{21}^{[8]} - \frac{41}{2}h_{23}^{[8]} + h_{25}^{[8]} - 13h_{27}^{[8]} - 7h_{29}^{[8]} - 5h_{31}^{[8]} \\
& + 6h_{33}^{[8]} - 11h_{35}^{[8]} - 3h_{37}^{[8]} + 3h_{39}^{[8]} - 4h_{43}^{[8]} - 4h_{45}^{[8]} - 11h_{47}^{[8]} + \frac{3}{2}h_{49}^{[8]} - \frac{3}{2}h_{51}^{[8]} \\
& - 3h_{53}^{[8]} - 5h_{55}^{[8]} + \frac{3}{2}h_{57}^{[8]} - \frac{3}{2}h_{59}^{[8]} + 9h_{65}^{[8]} - 25h_{67}^{[8]} - 9h_{69}^{[8]} + 27h_{71}^{[8]} - 2h_{73}^{[8]} \\
& + 9h_{75}^{[8]} + 2h_{77}^{[8]} - 23h_{79}^{[8]} + 2h_{81}^{[8]} - h_{85}^{[8]} - 8h_{87}^{[8]} + 2h_{89}^{[8]} - 3h_{91}^{[8]} + \frac{5}{2}h_{97}^{[8]} \\
& - \frac{7}{2}h_{99}^{[8]} - \frac{1}{2}h_{101}^{[8]} + \frac{5}{2}h_{103}^{[8]} + \frac{1}{2}h_{105}^{[8]} + \frac{1}{2}h_{107}^{[8]} + \frac{1}{2}h_{109}^{[8]} - \frac{5}{2}h_{111}^{[8]} + 15h_{129}^{[8]} \\
& - 41h_{131}^{[8]} - \frac{31}{2}h_{133}^{[8]} + \frac{105}{2}h_{135}^{[8]} - \frac{7}{2}h_{137}^{[8]} + \frac{53}{2}h_{139}^{[8]} + 12h_{141}^{[8]} - 42h_{143}^{[8]} \\
& + \frac{5}{2}h_{145}^{[8]} + \frac{11}{2}h_{147}^{[8]} + \frac{9}{2}h_{149}^{[8]} - \frac{41}{2}h_{151}^{[8]} + h_{153}^{[8]} - 13h_{155}^{[8]} - 7h_{157}^{[8]} \\
& - 5h_{159}^{[8]} + 6h_{161}^{[8]} - 11h_{163}^{[8]} - 3h_{165}^{[8]} + 3h_{167}^{[8]} - 4h_{171}^{[8]} - 4h_{173}^{[8]} \\
& - 11h_{175}^{[8]} + \frac{3}{2}h_{177}^{[8]} - \frac{3}{2}h_{179}^{[8]} - 3h_{181}^{[8]} - 5h_{183}^{[8]} + \frac{3}{2}h_{185}^{[8]} - \frac{3}{2}h_{187}^{[8]} \\
& + 9h_{193}^{[8]} - 25h_{195}^{[8]} - 9h_{197}^{[8]} + 27h_{199}^{[8]} - 2h_{201}^{[8]} + 9h_{203}^{[8]} + 2h_{205}^{[8]} - 23h_{207}^{[8]} \\
& + 2h_{209}^{[8]} - h_{213}^{[8]} - 8h_{215}^{[8]} + 2h_{217}^{[8]} - 3h_{219}^{[8]} + \frac{5}{2}h_{225}^{[8]} - \frac{7}{2}h_{227}^{[8]} - \frac{1}{2}h_{229}^{[8]} \\
& + \frac{5}{2}h_{231}^{[8]} + \frac{1}{2}h_{233}^{[8]} + \frac{1}{2}h_{235}^{[8]} + \frac{1}{2}h_{237}^{[8]} - \frac{5}{2}h_{239}^{[8]} \\
& + \zeta_2 \left[2h_1^{[6]} - 14h_3^{[6]} - \frac{15}{2}h_5^{[6]} + \frac{37}{2}h_7^{[6]} - \frac{5}{2}h_9^{[6]} + \frac{25}{2}h_{11}^{[6]} + 7h_{13}^{[6]} - \frac{1}{2}h_{17}^{[6]} \right. \\
& \quad + \frac{5}{2}h_{19}^{[6]} + \frac{7}{2}h_{21}^{[6]} + \frac{9}{2}h_{23}^{[6]} - 3h_{25}^{[6]} + 3h_{27}^{[6]} + 2h_{33}^{[6]} - 14h_{35}^{[6]} - \frac{15}{2}h_{37}^{[6]} \\
& \quad + \frac{37}{2}h_{39}^{[6]} - \frac{5}{2}h_{41}^{[6]} + \frac{25}{2}h_{43}^{[6]} + 7h_{45}^{[6]} - \frac{1}{2}h_{49}^{[6]} + \frac{5}{2}h_{51}^{[6]} + \frac{7}{2}h_{53}^{[6]} \\
& \quad \left. + \frac{9}{2}h_{55}^{[6]} - 3h_{57}^{[6]} + 3h_{59}^{[6]} \right] \\
& + \zeta_4 \left[\frac{15}{2}h_1^{[4]} - \frac{55}{2}h_3^{[4]} - \frac{41}{2}h_5^{[4]} + \frac{15}{2}h_9^{[4]} - \frac{55}{2}h_{11}^{[4]} - \frac{41}{2}h_{13}^{[4]} \right] \\
& + \left(\zeta_2 \zeta_3 - \frac{5}{2} \zeta_5 \right) \left[h_3^{[3]} + h_7^{[3]} \right] - \left(\zeta_3^2 - \frac{73}{4} \zeta_6 \right) \left[h_1^{[2]} + h_3^{[2]} \right] \\
& - \frac{3}{2} \zeta_2 \zeta_3^2 - \frac{5}{2} \zeta_3 \zeta_5 - \frac{471}{4} \zeta_8 + \frac{3}{2} \zeta_{5,3} .
\end{aligned} \tag{5.3.4}$$

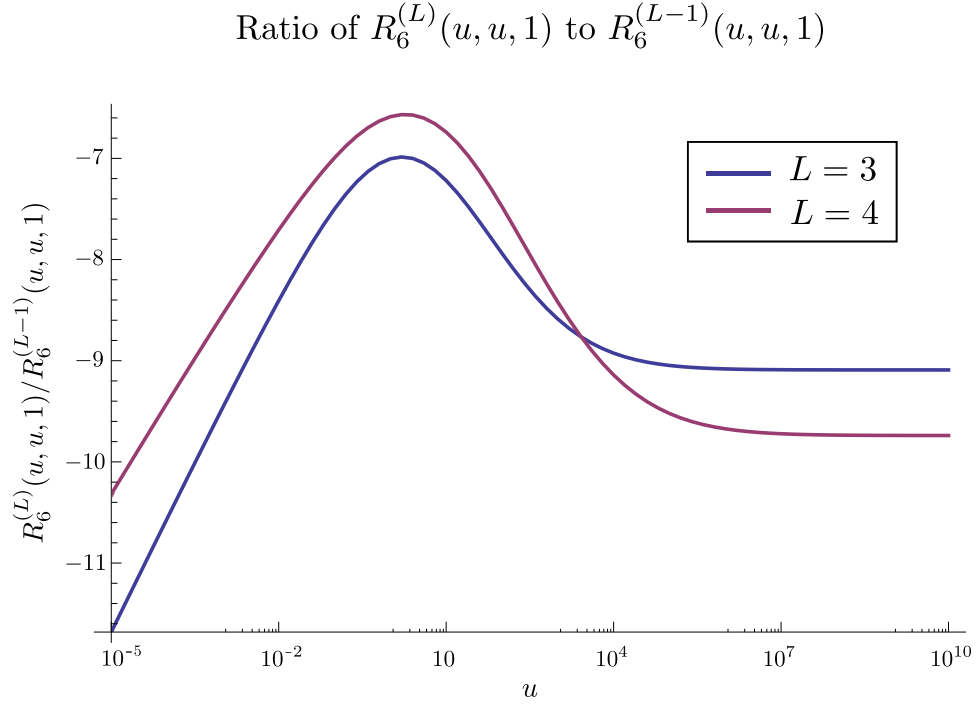


Figure 5.1: The successive ratios $R_6^{(L)}/R_6^{(L-1)}$ on the line $(u, u, 1)$.

These expressions are all extra-pure. It is easy to check this property by verifying their symmetry under the operation,

$$h_m^{[n]} \rightarrow h_{m+2^{n-1}}^{[n]}, \quad (5.3.5)$$

where the lower index is taken mod 2^n . This operation exchanges $0 \leftrightarrow 1$ in the initial term of the weight vectors, which corresponds to the final entry of the symbol.

Setting $u = 1$ in the above formulas leads to

$$\begin{aligned} R_6^{(2)}(1, 1, 1) &= -(\zeta_2)^2 = -\frac{5}{2}\zeta_4 = -2.705808084278\dots, \\ R_6^{(3)}(1, 1, 1) &= \frac{413}{24}\zeta_6 + (\zeta_3)^2 = 18.95171932342\dots \\ R_6^{(4)}(1, 1, 1) &= -\frac{3}{2}\zeta_2\zeta_3^2 - \frac{5}{2}\zeta_3\zeta_5 - \frac{471}{4}\zeta_8 + \frac{3}{2}\zeta_{5,3} = -124.8549111141\dots \end{aligned} \quad (5.3.6)$$

The numerical values of the L -loop to the $(L-1)$ -loop ratios at the point $(1, 1, 1)$ are remarkably close,

$$\begin{aligned}\frac{R_6^{(3)}(1, 1, 1)}{R_6^{(2)}(1, 1, 1)} &= -7.004088513718\dots, \\ \frac{R_6^{(4)}(1, 1, 1)}{R_6^{(3)}(1, 1, 1)} &= -6.588051932566\dots\end{aligned}\tag{5.3.7}$$

In fact, the ratios are also similar away from this point, as can be seen in fig. 5.1. The logarithmic scale for u highlights how little the ratios vary over a broad range in u , as well as how the u -dependence differs minimally between the successive ratios.

We also give the leading term in the expansion of $R_6^{(4)}(u, u, 1)$ around $u = 0$,

$$\begin{aligned}R_6^{(4)}(u, u, 1) &= u \left[-\frac{5}{48} \ln^4 u + \left(\frac{3}{4} \zeta_2 + \frac{5}{3} \right) \ln^3 u - \left(\frac{27}{4} \zeta_4 - \frac{1}{2} \zeta_3 + 5 \zeta_2 + \frac{25}{2} \right) \ln^2 u \right. \\ &\quad + \left(15 \zeta_4 - 3 \zeta_3 + 13 \zeta_2 + 50 \right) \ln u \\ &\quad + \left. \frac{219}{8} \zeta_6 + \zeta_3^2 + 5 \zeta_5 + \zeta_2 \zeta_3 - \frac{71}{8} \zeta_4 + 6 \zeta_3 - 10 \zeta_2 - \frac{175}{2} \right] \\ &\quad + \mathcal{O}(u^2).\end{aligned}\tag{5.3.8}$$

We note the intriguing observation that the maximum-transcendentality piece of the $u^1 \ln^0 u$ term is proportional to the four-loop cusp anomalous dimension, $\frac{219}{8} \zeta_6 + \zeta_3^2 = -\frac{1}{4} \gamma_K^{(4)}$. In fact, the corresponding pieces of the two- and three-loop results (eq. (5.3.8)) correspond to $-\frac{1}{4} \gamma_K^{(2)}$ and $-\frac{1}{4} \gamma_K^{(3)}$.

Comparing with eq. (5.3.8), we see that the ratios $R_6^{(L)}/R_6^{(L-1)}$ both diverge logarithmically as $u \rightarrow 0$ along this line:

$$\begin{aligned}\frac{R_6^{(3)}(u, u, 1)}{R_6^{(2)}(u, u, 1)} &\sim \frac{1}{2} \ln u, & \text{as } u \rightarrow 0, \\ \frac{R_6^{(4)}(u, u, 1)}{R_6^{(3)}(u, u, 1)} &\sim \frac{5}{12} \ln u, & \text{as } u \rightarrow 0.\end{aligned}\tag{5.3.9}$$

The slight difference in these coefficients is reflected in the slight difference in slopes in the region of small u in fig. 5.1.

As $u \rightarrow \infty$, the leading behavior at four loops is,

$$\begin{aligned}
R_6^{(4)}(u, u, 1) = & -\frac{88345}{144}\zeta_8 - \frac{19}{4}\zeta_2(\zeta_3)^2 - \frac{63}{4}\zeta_3\zeta_5 + \frac{5}{4}\zeta_{5,3} \\
& + \frac{1}{u} \left[\frac{1}{42}\ln^7 u + \frac{1}{6}\ln^6 u + \left(1 + \frac{4}{5}\zeta_2\right)\ln^5 u - \left(\frac{11}{12}\zeta_3 - 4\zeta_2 - 5\right)\ln^4 u \right. \\
& + \left(\frac{605}{24}\zeta_4 - \frac{11}{3}\zeta_3 + 16\zeta_2 + 20\right)\ln^3 u \\
& - \left(7\zeta_5 + 9\zeta_2\zeta_3 - \frac{605}{8}\zeta_4 + 11\zeta_3 - 48\zeta_2 - 60\right)\ln^2 u \\
& + \left(\frac{6257}{32}\zeta_6 + \frac{13}{4}(\zeta_3)^2 - 14\zeta_5 - 18\zeta_2\zeta_3 + \frac{605}{4}\zeta_4 - 22\zeta_3 \right. \\
& \quad \left. + 96\zeta_2 + 120\right)\ln u \\
& - \frac{13}{2}\zeta_7 - 25\zeta_2\zeta_5 - \frac{173}{4}\zeta_3\zeta_4 + \frac{6257}{32}\zeta_6 + \frac{13}{4}(\zeta_3)^2 - 14\zeta_5 \\
& \quad \left. - 18\zeta_2\zeta_3 + \frac{605}{4}\zeta_4 - 22\zeta_3 + 96\zeta_2 + 120 \right] \\
& + \mathcal{O}\left(\frac{1}{u^2}\right).
\end{aligned} \tag{5.3.10}$$

Just like at two- and three-loops, $R_6^{(4)}(u, u, 1)$ approaches a constant as $u \rightarrow \infty$. Comparing with eq. (4.7.17), we find

$$\begin{aligned}
\frac{R_6^{(3)}(u, u, 1)}{R_6^{(2)}(u, u, 1)} & \sim -9.09128803107\dots, \quad \text{as } u \rightarrow \infty. \\
\frac{R_6^{(4)}(u, u, 1)}{R_6^{(3)}(u, u, 1)} & \sim -9.73956178163\dots, \quad \text{as } u \rightarrow \infty.
\end{aligned} \tag{5.3.11}$$

5.3.2 The line $(u, 1, 1)$

Next we consider the line $(u, 1, 1)$, which, due to the total S_3 symmetry of $R_6(u, v, w)$, is equivalent to the line $(1, 1, w)$ discussed in section 4.7.2. As was the case at two- and three-loops, we can express $R_6^{(4)}(u, 1, 1)$ solely in terms of HPLs of a single argument.

Using the notation of section 5.3.1, the two-loop result is,

$$R_6^{(2)}(u, 1, 1) = \frac{1}{2}h_1^{[4]} + \frac{1}{4}h_5^{[4]} + \frac{1}{2}h_9^{[4]} + \frac{1}{2}h_{13}^{[4]} - \frac{1}{2}\zeta_2 h_3^{[2]} - \frac{5}{2}\zeta_4, \quad (5.3.12)$$

the three-loop result is,

$$\begin{aligned} R_6^{(3)}(u, 1, 1) = & -\frac{3}{2}h_1^{[6]} + \frac{1}{2}h_3^{[6]} - \frac{1}{4}h_5^{[6]} - \frac{3}{4}h_9^{[6]} + \frac{1}{4}h_{11}^{[6]} - \frac{1}{4}h_{13}^{[6]} - h_{17}^{[6]} \\ & + \frac{1}{2}h_{19}^{[6]} - \frac{1}{2}h_{21}^{[6]} - \frac{1}{2}h_{25}^{[6]} + \frac{1}{2}h_{27}^{[6]} - \frac{3}{2}h_{33}^{[6]} + \frac{1}{2}h_{35}^{[6]} - \frac{1}{4}h_{37}^{[6]} \\ & - \frac{3}{4}h_{41}^{[6]} + \frac{1}{2}h_{43}^{[6]} - \frac{5}{4}h_{49}^{[6]} + \frac{3}{4}h_{51}^{[6]} - \frac{1}{4}h_{53}^{[6]} - \frac{3}{4}h_{57}^{[6]} + \frac{3}{4}h_{59}^{[6]} \\ & + \zeta_2 \left[-\frac{1}{2}h_1^{[4]} + \frac{1}{2}h_3^{[4]} + \frac{1}{2}h_5^{[4]} - \frac{1}{2}h_9^{[4]} - \frac{1}{2}h_{13}^{[4]} \right] \\ & - \zeta_4 \left[h_1^{[2]} - \frac{17}{4}h_3^{[2]} \right] + \zeta_3^2 + \frac{413}{24}\zeta_6, \end{aligned} \quad (5.3.13)$$

and the four-loop result is,

$$\begin{aligned}
R_6^{(4)}(u, 1, 1) = & \frac{15}{2}h_1^{[8]} - \frac{13}{2}h_3^{[8]} - \frac{3}{4}h_5^{[8]} + \frac{3}{4}h_7^{[8]} + \frac{9}{4}h_9^{[8]} - \frac{3}{4}h_{11}^{[8]} + \frac{1}{2}h_{13}^{[8]} + \frac{15}{4}h_{17}^{[8]} \\
& - \frac{5}{2}h_{19}^{[8]} + \frac{1}{2}h_{21}^{[8]} + \frac{5}{8}h_{23}^{[8]} + \frac{5}{4}h_{25}^{[8]} - \frac{1}{2}h_{27}^{[8]} - \frac{1}{8}h_{29}^{[8]} + \frac{9}{2}h_{33}^{[8]} - \frac{17}{4}h_{35}^{[8]} \\
& - \frac{3}{8}h_{37}^{[8]} + \frac{3}{4}h_{39}^{[8]} + \frac{11}{8}h_{41}^{[8]} - \frac{11}{8}h_{43}^{[8]} - \frac{5}{8}h_{45}^{[8]} + \frac{9}{4}h_{49}^{[8]} - \frac{9}{4}h_{51}^{[8]} - \frac{3}{4}h_{53}^{[8]} \\
& + \frac{3}{4}h_{55}^{[8]} + \frac{3}{4}h_{57}^{[8]} + \frac{21}{4}h_{65}^{[8]} - \frac{23}{4}h_{67}^{[8]} - \frac{7}{8}h_{69}^{[8]} + \frac{3}{4}h_{71}^{[8]} + \frac{11}{8}h_{73}^{[8]} - \frac{13}{8}h_{75}^{[8]} \\
& - \frac{5}{8}h_{77}^{[8]} + \frac{23}{8}h_{81}^{[8]} - \frac{25}{8}h_{83}^{[8]} - \frac{5}{8}h_{85}^{[8]} + \frac{7}{8}h_{87}^{[8]} + \frac{9}{8}h_{89}^{[8]} - \frac{3}{8}h_{91}^{[8]} + \frac{1}{8}h_{93}^{[8]} \\
& + \frac{11}{4}h_{97}^{[8]} - 5h_{99}^{[8]} - \frac{11}{8}h_{101}^{[8]} + \frac{7}{8}h_{103}^{[8]} + \frac{3}{4}h_{105}^{[8]} - \frac{5}{4}h_{107}^{[8]} - \frac{5}{8}h_{109}^{[8]} + \frac{7}{8}h_{113}^{[8]} \\
& - \frac{23}{8}h_{115}^{[8]} - \frac{9}{8}h_{117}^{[8]} + \frac{7}{8}h_{119}^{[8]} + \frac{15}{2}h_{129}^{[8]} - \frac{13}{2}h_{131}^{[8]} - \frac{3}{4}h_{133}^{[8]} + \frac{3}{4}h_{135}^{[8]} \\
& + \frac{9}{4}h_{137}^{[8]} - h_{139}^{[8]} + \frac{1}{4}h_{141}^{[8]} + \frac{15}{4}h_{145}^{[8]} - 3h_{147}^{[8]} + \frac{1}{4}h_{149}^{[8]} + h_{151}^{[8]} + \frac{5}{4}h_{153}^{[8]} \\
& + \frac{1}{4}h_{157}^{[8]} + \frac{9}{2}h_{161}^{[8]} - \frac{21}{4}h_{163}^{[8]} - \frac{7}{8}h_{165}^{[8]} + \frac{9}{8}h_{167}^{[8]} + \frac{9}{8}h_{169}^{[8]} - \frac{9}{8}h_{171}^{[8]} - \frac{1}{2}h_{173}^{[8]} \\
& + 2h_{177}^{[8]} - \frac{11}{4}h_{179}^{[8]} - \frac{7}{8}h_{181}^{[8]} + \frac{9}{8}h_{183}^{[8]} + \frac{3}{8}h_{185}^{[8]} + \frac{3}{8}h_{187}^{[8]} + 6h_{193}^{[8]} - 7h_{195}^{[8]} \\
& - \frac{5}{4}h_{197}^{[8]} + \frac{9}{8}h_{199}^{[8]} + \frac{3}{2}h_{201}^{[8]} - \frac{3}{2}h_{203}^{[8]} - \frac{3}{8}h_{205}^{[8]} + \frac{25}{8}h_{209}^{[8]} - \frac{31}{8}h_{211}^{[8]} - \frac{1}{4}h_{213}^{[8]} \\
& + \frac{11}{8}h_{215}^{[8]} + h_{217}^{[8]} + \frac{1}{4}h_{221}^{[8]} + \frac{7}{2}h_{225}^{[8]} - 7h_{227}^{[8]} - \frac{17}{8}h_{229}^{[8]} + \frac{5}{4}h_{231}^{[8]} + \frac{5}{8}h_{233}^{[8]} \\
& - \frac{13}{8}h_{235}^{[8]} - \frac{7}{8}h_{237}^{[8]} + \frac{5}{4}h_{241}^{[8]} - \frac{19}{4}h_{243}^{[8]} - \frac{7}{4}h_{245}^{[8]} + \frac{5}{4}h_{247}^{[8]} \\
& + \zeta_2 \left[h_1^{[6]} - 3h_3^{[6]} - \frac{7}{4}h_5^{[6]} + \frac{1}{4}h_7^{[6]} - \frac{1}{4}h_9^{[6]} + \frac{1}{4}h_{11}^{[6]} + \frac{1}{2}h_{13}^{[6]} + \frac{1}{4}h_{17}^{[6]} - \frac{3}{4}h_{19}^{[6]} \right. \\
& \quad + \frac{1}{2}h_{21}^{[6]} - \frac{1}{4}h_{23}^{[6]} - \frac{3}{4}h_{27}^{[6]} - \frac{1}{2}h_{29}^{[6]} + h_{33}^{[6]} - \frac{5}{2}h_{35}^{[6]} - \frac{3}{2}h_{37}^{[6]} - \frac{1}{2}h_{39}^{[6]} \\
& \quad \left. - h_{43}^{[6]} - \frac{1}{2}h_{45}^{[6]} + \frac{3}{4}h_{49}^{[6]} - \frac{9}{4}h_{51}^{[6]} - \frac{5}{4}h_{53}^{[6]} - \frac{1}{2}h_{55}^{[6]} + \frac{3}{4}h_{57}^{[6]} - \frac{5}{4}h_{59}^{[6]} \right] \\
& + \zeta_4 \left[\frac{15}{4}h_1^{[4]} - 5h_3^{[4]} - \frac{47}{8}h_5^{[4]} + \frac{3}{2}h_7^{[4]} + \frac{15}{4}h_9^{[4]} + \frac{3}{2}h_{11}^{[4]} + \frac{9}{2}h_{13}^{[4]} \right] \\
& + \left(\zeta_2\zeta_3 - \frac{5}{2}\zeta_5 \right) \left[\frac{3}{2}h_3^{[3]} + h_7^{[3]} \right] + \zeta_6 \left[\frac{73}{8}h_1^{[2]} - \frac{461}{16}h_3^{[2]} \right] - \frac{1}{2}\zeta_3^2 \left[h_1^{[2]} + h_3^{[2]} \right] \\
& - \frac{3}{2}\zeta_2\zeta_3^2 - \frac{5}{2}\zeta_3\zeta_5 - \frac{471}{4}\zeta_8 + \frac{3}{2}\zeta_{5,3} .
\end{aligned}
\tag{5.3.14}$$

Using eq. (5.3.5), it is easy to check that none of these functions are extra-pure.

At both large and small u , these functions all diverge logarithmically. At two- and three-loops, this can be seen from eqs. (4.7.22) and (4.7.23). At four loops, we find at small u ,

$$R_6^{(4)}(u, 1, 1) = \frac{1}{24} \left(\frac{7}{2} \zeta_5 - \zeta_2 \zeta_3 \right) \ln^3 u - \frac{639}{256} \zeta_6 \ln^2 u + \left(\frac{829}{64} \zeta_7 + \frac{69}{16} \zeta_3 \zeta_4 + \frac{39}{8} \zeta_2 \zeta_5 \right) \ln u - \frac{3}{16} \zeta_2 \zeta_3^2 - \frac{57}{16} \zeta_3 \zeta_5 - \frac{123523}{2880} \zeta_8 + \frac{19}{80} \zeta_{5,3} + \mathcal{O}(u), \quad (5.3.15)$$

and at large u ,

$$R_6^{(4)}(u, 1, 1) = -\frac{37}{322560} \ln^8 u - \frac{1}{80} \zeta_2 \ln^6 u + \frac{7}{320} \zeta_3 \ln^5 u - \frac{533}{384} \zeta_4 \ln^4 u + \left(\frac{47}{48} \zeta_5 + \frac{53}{48} \zeta_2 \zeta_3 \right) \ln^3 u - \left(\frac{6019}{128} \zeta_6 + \frac{11}{16} \zeta_3^2 \right) \ln^2 u + \left(\frac{195}{8} \zeta_7 + \frac{923}{32} \zeta_3 \zeta_4 + \frac{33}{2} \zeta_2 \zeta_5 \right) \ln u - 3 \zeta_2 \zeta_3^2 - \frac{25}{2} \zeta_3 \zeta_5 - \frac{1488641}{4608} \zeta_8 + \frac{1}{4} \zeta_{5,3} + \mathcal{O} \left(\frac{1}{u} \right). \quad (5.3.16)$$

The ratios $R_6^{(L)}(u, 1, 1)/R_6^{(L-1)}(u, 1, 1)$ also diverge in both limits,

$$\begin{aligned} \frac{R_6^{(3)}(u, 1, 1)}{R_6^{(2)}(u, 1, 1)} &\sim \left(\frac{7\pi^4}{1440\zeta_3} \right) \ln u = \left(0.393921796467 \dots \right) \ln u, & \text{as } u \rightarrow 0, \\ \frac{R_6^{(4)}(u, 1, 1)}{R_6^{(3)}(u, 1, 1)} &\sim \left(\frac{60\zeta_5}{\pi^4} - \frac{20\zeta_3}{7\pi^2} \right) \ln u = \left(0.290722549640 \dots \right) \ln u, & \text{as } u \rightarrow 0, \end{aligned} \quad (5.3.17)$$

and,

$$\begin{aligned} \frac{R_6^{(3)}(u, 1, 1)}{R_6^{(2)}(u, 1, 1)} &\sim -\frac{1}{10} \ln^2 u, & \text{as } u \rightarrow \infty, \\ \frac{R_6^{(4)}(u, 1, 1)}{R_6^{(3)}(u, 1, 1)} &\sim -\frac{37}{336} \ln^2 u, & \text{as } u \rightarrow \infty. \end{aligned} \quad (5.3.18)$$

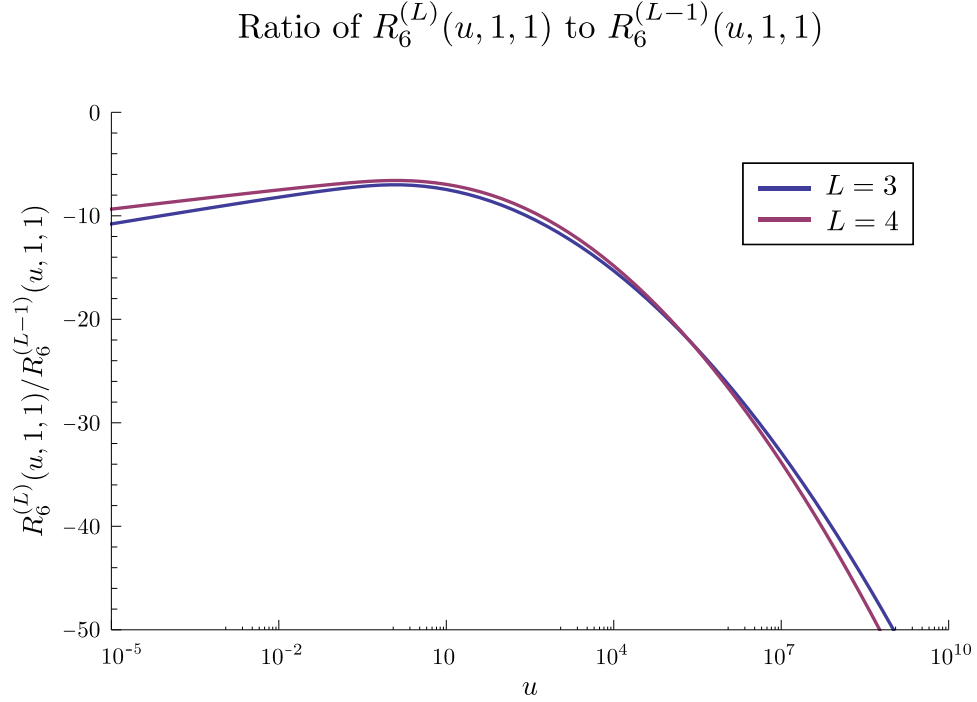


Figure 5.2: The successive ratios $R_6^{(L)}/R_6^{(L-1)}$ on the line $(u, 1, 1)$.

In fig. 5.2, we plot the ratios $R_6^{(L)}(u, 1, 1)/R_6^{(L-1)}(u, 1, 1)$ for a large range of u . The ratios are strikingly similar throughout the entire region.

5.3.3 The line (u, u, u)

As discussed in section 4.7.3, the remainder function at strong coupling can be written analytically on the symmetrical diagonal line (u, u, u) ,

$$R_6^{(\infty)}(u, u, u) = -\frac{\pi}{6} + \frac{\phi^2}{3\pi} + \frac{3}{8} \left[\ln^2 u + 2 \operatorname{Li}_2(1-u) \right] - \frac{\pi^2}{12}, \quad (5.3.19)$$

where $\phi = 3 \cos^{-1}(1/\sqrt{4u})$. In perturbation theory, the function $R_6^{(L)}(u, u, u)$ cannot be written solely in terms of HPLs with argument $(1-u)$. However, it is possible to use the coproduct structure to derive differential equations which may be solved by using series expansions around the three points $u = 0$, $u = 1$, and $u = \infty$. This

method was applied in section 4.7.3 at two and three loops, and here we extend it to the four loop case.

The expansion around $u = 0$ takes the form,

$$\begin{aligned}
R_6^{(4)}(u, u, u) = & \left(\frac{1791}{32} \zeta_6 - \frac{3}{4} \zeta_3^2 \right) \ln^2 u + \frac{32605}{512} \zeta_8 - \frac{5}{2} \zeta_3 \zeta_5 - \frac{9}{8} \zeta_2 (\zeta_3)^2 \\
& + u \left[\frac{5}{192} \ln^7 u + \frac{5}{192} \ln^6 u - \left(\frac{19}{16} \zeta_2 + \frac{5}{32} \right) \ln^5 u \right. \\
& + \frac{5}{16} \left(\zeta_3 - 3\zeta_2 - \frac{1}{2} \right) \ln^4 u + \left(\frac{1129}{64} \zeta_4 + \frac{5}{8} \zeta_3 + 3\zeta_2 + \frac{15}{8} \right) \ln^3 u \\
& - \left(\frac{21}{8} \zeta_5 + \frac{3}{2} \zeta_2 \zeta_3 - \frac{669}{64} \zeta_4 + \frac{3}{2} \zeta_3 - 6\zeta_2 - \frac{75}{8} \right) \ln^2 u \\
& + \left(\frac{32073}{128} \zeta_6 - 3(\zeta_3)^2 - \frac{27}{4} \zeta_5 - \frac{3}{2} \zeta_2 \zeta_3 - \frac{165}{32} \zeta_4 - \frac{15}{4} \zeta_3 \right. \\
& \quad \left. - \frac{15}{2} \zeta_2 - \frac{75}{4} \right) \ln u + \frac{3}{4} \zeta_2 \zeta_5 - \frac{21}{16} \zeta_3 \zeta_4 + \frac{7119}{128} \zeta_6 \\
& \left. + \frac{3}{4} (\zeta_3)^2 + \frac{27}{4} \zeta_5 + \frac{3}{2} \zeta_2 \zeta_3 + \frac{45}{32} \zeta_4 + \frac{21}{2} \zeta_3 - \frac{15}{2} \zeta_2 - \frac{525}{4} \right] \\
& + \mathcal{O}(u^2).
\end{aligned} \tag{5.3.20}$$

The leading term at four loops diverges logarithmically, but, just like at two and three loops, the divergence appears only as $\ln^2 u$. This is another piece of evidence in support of the claim by Alday, Gaiotto and Maldacena [157] that this property should hold to all orders in perturbation theory. Because of this fact, the ratios $R_6^{(3)}(u, u, u)/R_6^{(2)}(u, u, u)$ and $R_6^{(4)}(u, u, u)/R_6^{(3)}(u, u, u)$ approach constants in the limit $u \rightarrow 0$,

$$\begin{aligned}
\frac{R_6^{(3)}(u, u, u)}{R_6^{(2)}(u, u, u)} & \sim -\frac{7\pi^2}{10} = -6.90872308076 \dots, \quad \text{as } u \rightarrow 0, \\
\frac{R_6^{(4)}(u, u, u)}{R_6^{(3)}(u, u, u)} & \sim -\frac{199\pi^2}{294} + \frac{60(\zeta_3)^2}{7\pi^4} = -6.55330020271, \quad \text{as } u \rightarrow 0.
\end{aligned} \tag{5.3.21}$$

At large u , the expansion behaves as,

$$\begin{aligned}
R_6^{(4)}(u, u, u) = & \frac{3}{2}\zeta_2(\zeta_3)^2 - 10\zeta_3\zeta_5 + \frac{1713}{64}\zeta_8 - \frac{3}{4}\zeta_{5,3} - \frac{4\pi^7}{5u^{1/2}} \\
& + \frac{1}{32u} \left[\frac{1}{56}\ln^7 u + \frac{5}{16}\ln^6 u + \left(\frac{51}{20}\zeta_2 + \frac{33}{8}\right)\ln^5 u \right. \\
& \quad - \left(\frac{11}{2}\zeta_3 - \frac{249}{8}\zeta_2 - \frac{345}{8}\right)\ln^4 u \\
& \quad + \left(\frac{1237}{4}\zeta_4 - 50\zeta_3 + \frac{547}{2}\zeta_2 + \frac{705}{2}\right)\ln^3 u \\
& \quad - \left(168\zeta_5 + 222\zeta_2\zeta_3 - \frac{17607}{8}\zeta_4 + 330\zeta_3 - \frac{3441}{2}\zeta_2 - \frac{4275}{2}\right)\ln^2 u \\
& \quad + \left(\frac{52347}{8}\zeta_6 + 144(\zeta_3)^2 - 744\zeta_5 - 1032\zeta_2\zeta_3 + \frac{38397}{4}\zeta_4 \right. \\
& \quad \quad \left. - 1416\zeta_3 + 7041\zeta_2 + 8595\right)\ln u - 360\zeta_7 - 2499\zeta_3\zeta_4 \\
& \quad - 1200\zeta_2\zeta_5 + \frac{134553}{16}\zeta_6 + 426(\zeta_3)^2 - 1596\zeta_5 - 2292\zeta_2\zeta_3 \\
& \quad \left. + \frac{80289}{4}\zeta_4 - 2976\zeta_3 + 14193\zeta_2 + 17235 \right] \\
& + \frac{\pi^3}{32u^{3/2}} \left[3\ln^3 u + \frac{45}{2}\ln^2 u + \left(306\zeta_2 + 99\right)\ln u - 96\zeta_4 + 36\zeta_3 \right. \\
& \quad \left. + 671\zeta_2 + \frac{469}{2} \right] + \mathcal{O}\left(\frac{1}{u^2}\right).
\end{aligned} \tag{5.3.22}$$

The ratios $R_6^{(3)}(u, u, u)/R_6^{(2)}(u, u, u)$ and $R_6^{(4)}(u, u, u)/R_6^{(3)}(u, u, u)$ approach constants in the limit $u \rightarrow \infty$,

$$\begin{aligned}
\frac{R_6^{(3)}(u, u, u)}{R_6^{(2)}(u, u, u)} & \sim -1.22742782334\dots, \quad \text{as } u \rightarrow \infty, \\
\frac{R_6^{(4)}(u, u, u)}{R_6^{(3)}(u, u, u)} & \sim 21.6155002540\dots, \quad \text{as } u \rightarrow \infty.
\end{aligned} \tag{5.3.23}$$

In contrast to the expansions around $u = 0$ and $u = \infty$, the expansion around $u = 1$

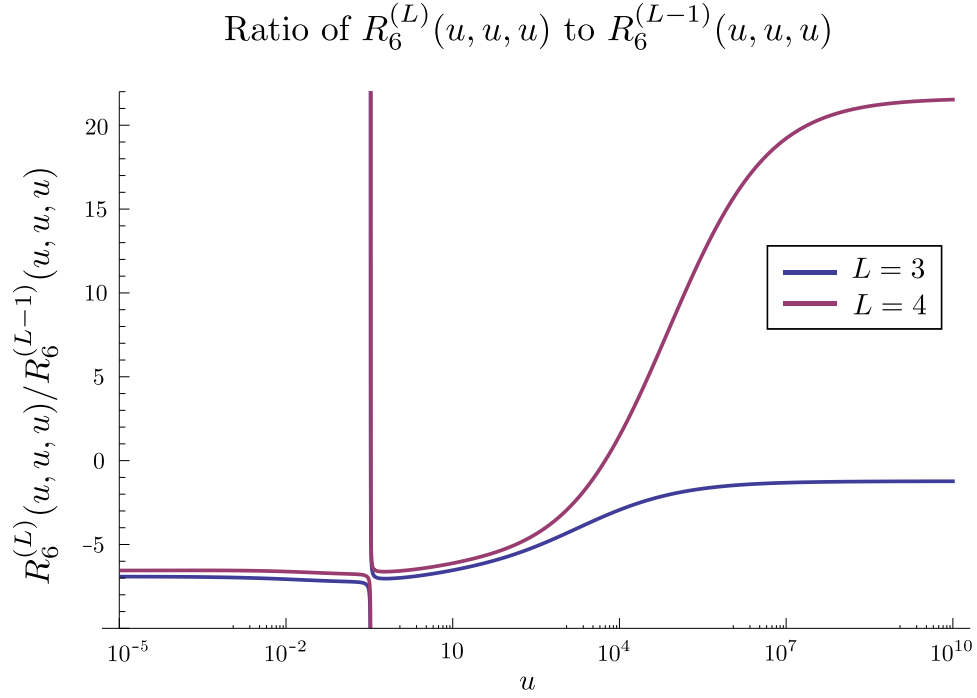


Figure 5.3: The successive ratios $R_6^{(L)}/R_6^{(L-1)}$ on the line (u, u, u) .

is regular,

$$\begin{aligned}
 R_6^{(4)}(u, u, u) = & -\frac{3}{2}\zeta_2\zeta_3^2 - \frac{5}{2}\zeta_3\zeta_5 - \frac{471}{4}\zeta_8 + \frac{3}{2}\zeta_{5,3} \\
 & + \left(\frac{219}{8}\zeta_6 - \frac{3}{2}(\zeta_3)^2 + \frac{45}{4}\zeta_4 + 3\zeta_2 + \frac{45}{2} \right) (1-u) + \mathcal{O}\left((1-u)^2\right).
 \end{aligned}
 \tag{5.3.24}$$

We take 100 terms in each expansion and piece them together to obtain a numerical representation for the function $R_6^{(4)}(u, u, u)$ that is valid along the entire line. In the regions of overlap, we find agreement to at least 15 digits. In fig. 5.3, we plot the ratios $R_6^{(L)}(u, u, u)/R_6^{(L-1)}(u, u, u)$ for a large range of u .

As noted in eq. (4.7.34), the two and three loop remainder functions vanish along the line (u, u, u) near the point $u = \frac{1}{3}$. The same is true at four loops, and we find

the zero-crossing point to be,

$$u_0^{(4)} = 0.33575561 \dots \quad (5.3.25)$$

As can be seen from fig. 5.3, $R_6^{(4)}(u, u, u)$ actually crosses zero in a second place,

$$u_{0,2}^{(4)} = 5529.65453 \dots \quad (5.3.26)$$

Aside from the small region near where $R_6^{(2)}(u, u, u)$ and $R_6^{(3)}(u, u, u)$ vanish, the general agreement between the two successive ratios is excellent for relatively small u , say $u < 1000$. For large u , the ratios approach constant values that differ by a factor of about -17.6 (see eq. (5.3.23)).

In fig. 5.4, we plot the two-, three-, and four-loop and strong-coupling remainder functions on the line (u, u, u) . In order to compare their relative shapes, we rescale each function by its value at $(1, 1, 1)$. The remarkable similarity in shape that was noticed at two and three loops persists at four loops, particularly for the region $0 < u < 1$.

As discussed in section 4.7.3, a necessary condition for the shapes to be so similar is that the limiting behavior of the ratios as $u \rightarrow 0$ is almost the same as the ratios' values at $u = 1$. Comparing eq. (5.3.21) to eq. (5.3.7), we find,

$$\begin{aligned} \frac{R_6^{(3)}(u, u, u)}{R_6^{(2)}(u, u, u)} \bigg/ \frac{R_6^{(3)}(1, 1, 1)}{R_6^{(2)}(1, 1, 1)} &\sim 0.986 \dots, & \text{as } u \rightarrow 0, \\ \frac{R_6^{(4)}(u, u, u)}{R_6^{(3)}(u, u, u)} \bigg/ \frac{R_6^{(4)}(1, 1, 1)}{R_6^{(3)}(1, 1, 1)} &\sim 0.995 \dots, & \text{as } u \rightarrow 0, \end{aligned} \quad (5.3.27)$$

which are indeed quite close to 1. The agreement is slightly better between the three- and four-loop points than it is between the two- and three-loop points. We can also

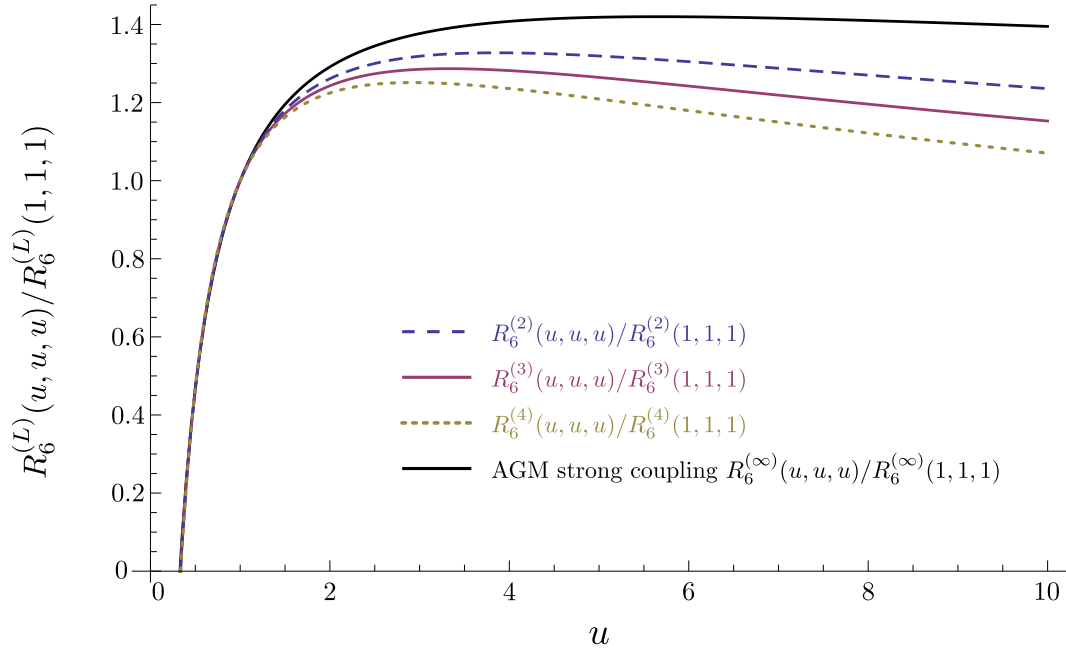
Rescaled $R_6^{(L)}(u, u, u)$ and strong coupling

Figure 5.4: The remainder function on the line (u, u, u) plotted at two, three, and four loops and at strong coupling. The functions have been rescaled by their values at the point $(1, 1, 1)$.

see how well these points agree with strong coupling values,

$$\begin{aligned}
 \frac{R_6^{(\infty)}(u, u, u)}{R_6^{(2)}(u, u, u)} \bigg/ \frac{R_6^{(\infty)}(1, 1, 1)}{R_6^{(2)}(1, 1, 1)} &\sim 1, & \text{as } u \rightarrow 0, \\
 \frac{R_6^{(\infty)}(u, u, u)}{R_6^{(3)}(u, u, u)} \bigg/ \frac{R_6^{(\infty)}(1, 1, 1)}{R_6^{(3)}(1, 1, 1)} &\sim 1.014, & \text{as } u \rightarrow 0, \\
 \frac{R_6^{(\infty)}(u, u, u)}{R_6^{(4)}(u, u, u)} \bigg/ \frac{R_6^{(\infty)}(1, 1, 1)}{R_6^{(4)}(1, 1, 1)} &\sim 1.019, & \text{as } u \rightarrow 0,
 \end{aligned} \tag{5.3.28}$$

The ratio between the two-loop and strong-coupling points is exactly 1, while the corresponding ratios for three and four loops deviate slightly from one. The deviations increase as L increases, suggesting that the shapes of the weak-coupling curves on the

line (u, u, u) are getting slightly further from the shape of the strong coupling curve, at least for small L . This observation is also evident in fig. 5.4 at large u .

5.4 Conclusions

In this chapter, we presented the four-loop remainder function, which is a dual-conformally invariant function that describes six-point MHV scattering amplitudes in planar $\mathcal{N} = 4$ super Yang-Mills theory. The result was bootstrapped from a limited set of assumptions about the analytic properties of the relevant function space. Following the strategy of ref. [14], we constructed an ansatz for the symbol and constrained this ansatz using various physical and mathematical consistency conditions. A unique expression for the symbol was obtained by applying information from the near-collinear expansion, as generated by the OPE for flux tube excitations [150]. The symbol, in turn, was lifted to a full function, using the methods described in chapter 4. In particular, a mathematically-consistent ansatz for the function was obtained by applying the coproduct bootstrap of section 4.3.3. All of the function-level parameters of this ansatz were fixed by again applying information from the near-collinear expansion.

The final expression for the four-loop remainder function is quite lengthy, but its functional form simplifies dramatically on various one-dimensional lines in the three-dimensional space of cross ratios. While the analytic form for the function on these lines is rather different at two, three, and four loops, a numerical evaluation shows that they are in fact quite similar for large fractions of the parameter space, at least up to an overall rescaling. On the line where all three cross ratios are equal, an analytical result at strong coupling is available. The perturbative results show good agreement with the strong-coupling result, particularly in the region where the common cross ratio is less than one. This agreement suggests that an interpolation from weak to strong coupling may depend rather weakly on the kinematic variables, at least on this one-dimensional line.

Given the full functional form of the four-loop remainder function, it is straightforward to extract its limit in multi-Regge kinematics. This information allowed us to

fix all of the previously undetermined constants in the NNLLA BFKL eigenvalue and the N³LLA impact factor. We also observed an intriguing correspondence between the BFKL eigenvalue and the energy of a gluonic excitation of the GKP string. It would be very interesting to better understand this correspondence.

There are many avenues for future research. In principle, the methods of this work could be extended to five loops and beyond. The primary limitation is computational power and the availability of boundary data, such as the near-collinear limit, to fix the proliferation of constants. It is remarkable that a fully nonperturbative formulation of the near-collinear limit now exists. Ultimately, the hope is that the full analytic structure of perturbative scattering amplitudes, as exposed here through four loops for the six-point case, might in some way pave the way for a nonperturbative formulation for generic kinematics.

Appendix A

Single-valued harmonic polylogarithms and the multi-Regge limit

A.1 Single-valued harmonic polylogarithms

A.1.1 Expression of the L^\pm functions in terms of ordinary HPLs

In this appendix we present the expressions for the $\mathbb{Z}_2 \times \mathbb{Z}_2$ eigenfunctions $L_w^\pm(z)$ defined in eq. (1.3.19) as linear combinations of ordinary HPLs of the form $H_{w_1}(z) H_{w_2}(\bar{z})$ up to weight 5. All expressions up to weight 6 are attached as ancillary files in computer-readable format. We give results only for the Lyndon words, as all other cases can be reduced to the latter. In the following, we use the condensed notation (1.3.27) for the HPL arguments z and \bar{z} to improve the readability of the formulas.

A.1.2 Lyndon words of weight 1

$$L_0^- = H_0 + \overline{H}_0 = \log |z|^2, \quad (\text{A.1.1})$$

$$L_1^+ = H_1 + \overline{H}_1 + \frac{1}{2}H_0 + \frac{1}{2}\overline{H}_0 = -\log |1-z|^2 + \frac{1}{2}\log |z|^2, \quad (\text{A.1.2})$$

A.1.3 Lyndon words of weight 2

$$\begin{aligned} L_2^- &= \frac{1}{4}[-2H_{1,0} + 2\overline{H}_{1,0} + 2H_0\overline{H}_1 - 2\overline{H}_0H_1 + 2H_2 - 2\overline{H}_2] \\ &= \text{Li}_2(z) - \text{Li}_2(\bar{z}) + \frac{1}{2}\log |z|^2(\log(1-z) - \log(1-\bar{z})), \end{aligned} \quad (\text{A.1.3})$$

A.1.4 Lyndon words of weight 3

$$\begin{aligned} L_3^+ &= \frac{1}{4}[2H_0\overline{H}_{0,0} + 2H_0\overline{H}_{1,0} + 2\overline{H}_0H_{0,0} + 2\overline{H}_0H_{1,0} + 2H_1\overline{H}_{0,0} + 2\overline{H}_1H_{0,0} \\ &\quad + 2H_{0,0,0} + 2H_{1,0,0} + 2\overline{H}_{0,0,0} + 2\overline{H}_{1,0,0} + 2H_3 + 2\overline{H}_3] \\ &= \text{Li}_3(z) + \text{Li}_3(\bar{z}) - \frac{1}{2}\log |z|^2[\text{Li}_2(\bar{z}) + \text{Li}_2(z)] - \frac{1}{4}\log^2 |z|^2\log |1-z|^2 \\ &\quad + \frac{1}{12}\log^3 |z|^2, \\ L_{2,1}^- &= \frac{1}{4}[H_0\overline{H}_{1,0} + \overline{H}_0H_{1,0} + H_1\overline{H}_{0,0} + \overline{H}_1H_{0,0} + 2H_0\overline{H}_{0,0} + 2H_0\overline{H}_{1,1} \\ &\quad + 2\overline{H}_0H_{0,0} + 2\overline{H}_0H_{1,1} + H_{1,0,0} + 2H_{0,0,0} + 2H_{2,0} + 2H_{2,1} + 2H_{1,1,0} \\ &\quad + \overline{H}_{1,0,0} + 2\overline{H}_{0,0,0} + 2\overline{H}_{2,0} + 2\overline{H}_{2,1} + 2\overline{H}_{1,1,0} + 2H_0\overline{H}_2 + 2\overline{H}_0H_2 \\ &\quad + 2H_1\overline{H}_2 + 2\overline{H}_1H_2 + H_3 + \overline{H}_3 - 4\zeta_3] \\ &= -\text{Li}_3(1-z) - \text{Li}_3(1-\bar{z}) - \frac{1}{2}[\text{Li}_3(z) + \text{Li}_3(\bar{z})] + \frac{1}{4}\log |z|^2[\text{Li}_2(z) + \text{Li}_2(\bar{z})] \\ &\quad - \frac{1}{2}\log |1-z|^2[\text{Li}_2(z) + \text{Li}_2(\bar{z})] - \frac{1}{8}\log^2 |z|^2\log |1-z|^2 + \frac{1}{12}\log^3 |z|^2 \\ &\quad - \frac{1}{4}\log \frac{z}{\bar{z}}[\log^2(1-z) - \log^2(1-\bar{z})] + \zeta_2\log |1-z|^2 + \zeta_3, \end{aligned} \quad (\text{A.1.4})$$

A.1.5 Lyndon words of weight 4

$$\begin{aligned}
L_{3,1}^+ = & \frac{1}{4} [H_0 \bar{H}_{2,0} + H_0 \bar{H}_{1,0,0} - \bar{H}_0 H_{2,0} - \bar{H}_0 H_{1,0,0} - H_1 \bar{H}_{0,0,0} + \bar{H}_1 H_{0,0,0} \\
& + H_{0,0} \bar{H}_2 + H_{0,0} \bar{H}_{1,0} - \bar{H}_{0,0} H_2 - \bar{H}_{0,0} H_{1,0} + 2 H_0 \bar{H}_{1,1,0} - 2 \bar{H}_0 H_{1,1,0} \\
& + 2 H_{0,0} \bar{H}_{1,1} - 2 \bar{H}_{0,0} H_{1,1} + H_{3,0} - H_{2,0,0} - H_{1,0,0,0} + 2 H_{3,1} - 2 H_{1,1,0,0} \\
& + \bar{H}_{2,0,0} + \bar{H}_{1,0,0,0} - \bar{H}_{3,0} - 2 \bar{H}_{3,1} + 2 \bar{H}_{1,1,0,0} - H_0 \bar{H}_3 + \bar{H}_0 H_3 - 2 H_1 \bar{H}_3 \\
& + 2 \bar{H}_1 H_3 + 4 H_1 \zeta_3 + H_4 - 4 \bar{H}_1 \zeta_3 - \bar{H}_4] ,
\end{aligned} \tag{A.1.6}$$

$$\begin{aligned}
L_4^- = & \frac{1}{4} [2 H_0 \bar{H}_{1,0,0} - 2 \bar{H}_0 H_{1,0,0} - 2 H_1 \bar{H}_{0,0,0} + 2 \bar{H}_1 H_{0,0,0} + 2 H_{0,0} \bar{H}_{1,0} \\
& - 2 \bar{H}_{0,0} H_{1,0} - 2 H_{1,0,0,0} + 2 \bar{H}_{1,0,0,0} + 2 H_4 - 2 \bar{H}_4] ,
\end{aligned} \tag{A.1.7}$$

$$\begin{aligned}
L_{2,1,1}^- = & \frac{1}{4} [H_0 \bar{H}_{1,0,0} + H_0 \bar{H}_{1,2} + H_0 \bar{H}_{1,1,0} - \bar{H}_0 H_{1,0,0} - \bar{H}_0 H_{1,2} - \bar{H}_0 H_{1,1,0} \\
& - H_1 \bar{H}_{0,0,0} - H_1 \bar{H}_{2,0} + \bar{H}_1 H_{0,0,0} + \bar{H}_1 H_{2,0} + H_{0,0} \bar{H}_{1,0} + H_{0,0} \bar{H}_{1,1} \\
& - \bar{H}_{0,0} H_{1,0} - \bar{H}_{0,0} H_{1,1} + H_2 \bar{H}_{1,0} - \bar{H}_2 H_{1,0} + 2 H_0 \bar{H}_{1,1,1} - 2 \bar{H}_0 H_{1,1,1} \\
& - 2 H_1 \bar{H}_{2,1} + 2 \bar{H}_1 H_{2,1} + 2 H_2 \bar{H}_{1,1} - 2 \bar{H}_2 H_{1,1} + H_{3,1} + H_{2,2} \\
& - H_{1,0,0,0} - H_{1,2,0} - H_{1,1,0,0} + 2 H_{2,1,1} - 2 H_{1,1,1,0} + \bar{H}_{1,0,0,0} + \bar{H}_{1,2,0} + \bar{H}_{1,1,0,0} \\
& - \bar{H}_{3,1} - \bar{H}_{2,2} - 2 \bar{H}_{2,1,1} + 2 \bar{H}_{1,1,1,0} - H_1 \bar{H}_3 + \bar{H}_1 H_3 + 2 H_1 \zeta_3 + H_4 \\
& - 2 \bar{H}_1 \zeta_3 - \bar{H}_4] ,
\end{aligned} \tag{A.1.8}$$

A.1.6 Lyndon words of weight 5

$$\begin{aligned}
L_5^+ = & \frac{1}{4} [2 H_0 \bar{H}_{0,0,0,0} + 2 H_0 \bar{H}_{1,0,0,0} + 2 \bar{H}_0 H_{0,0,0,0} + 2 \bar{H}_0 H_{1,0,0,0} \\
& + 2 H_1 \bar{H}_{0,0,0,0} + 2 \bar{H}_1 H_{0,0,0,0} + 2 H_{0,0} \bar{H}_{0,0,0} + 2 H_{0,0} \bar{H}_{1,0,0} \\
& + 2 \bar{H}_{0,0} H_{0,0,0} + 2 \bar{H}_{0,0} H_{1,0,0} + 2 H_{1,0} \bar{H}_{0,0,0} + 2 \bar{H}_{1,0} H_{0,0,0} + 2 H_{0,0,0,0,0} \\
& + 2 H_{1,0,0,0,0} + 2 \bar{H}_{0,0,0,0,0} + 2 \bar{H}_{1,0,0,0,0} + 2 H_5 + 2 \bar{H}_5] ,
\end{aligned} \tag{A.1.9}$$

$$\begin{aligned}
L_{3,1,1}^+ = & \frac{1}{4} [H_5 + \bar{H}_5 + H_{4,0} + \bar{H}_{4,0} + H_{4,1} + \bar{H}_{4,1} + H_{3,2} + \bar{H}_{3,2} + H_{3,1,0} \\
& + H_{2,0,0,0} + \bar{H}_{2,0,0,0} + H_{2,1,0,0} + \bar{H}_{2,1,0,0} + H_{1,0,0,0,0} + \bar{H}_{1,0,0,0,0} + H_{1,2,0,0}
\end{aligned} \tag{A.1.10}$$

$$\begin{aligned}
& +\overline{H}_{1,2,0,0} + H_{1,1,0,0,0} + \overline{H}_{1,1,0,0,0} + 2 H_{0,0,0,0,0} + 2 \overline{H}_{0,0,0,0,0} + H_0 \overline{H}_4 \\
& + 2 H_{3,0,0} + 2 \overline{H}_{3,0,0} + 2 H_{3,1,1} + 2 \overline{H}_{3,1,1} + 2 H_{1,1,1,0,0} + 2 \overline{H}_{1,1,1,0,0} + 4 \zeta_5 \\
& + H_0 \overline{H}_{3,1} + H_0 \overline{H}_{2,0,0} + H_0 \overline{H}_{2,1,0} + H_0 \overline{H}_{1,0,0,0} + H_0 \overline{H}_{1,2,0} + H_0 \overline{H}_{1,1,0,0} \\
& + \overline{H}_0 H_4 + \overline{H}_0 H_{3,1} + \overline{H}_0 H_{2,0,0} + \overline{H}_0 H_{2,1,0} + \overline{H}_0 H_{1,0,0,0} + \overline{H}_0 H_{1,2,0} \\
& + \overline{H}_0 H_{1,1,0,0} + H_1 \overline{H}_{0,0,0,0} + H_1 \overline{H}_4 + H_1 \overline{H}_{3,0} + \overline{H}_1 H_{0,0,0,0} + \overline{H}_1 H_4 \\
& + \overline{H}_1 H_{3,0} + H_{0,0} \overline{H}_{2,0} + H_{0,0} \overline{H}_{2,1} + H_{0,0} \overline{H}_{1,0,0} + H_{0,0} \overline{H}_{1,2} + \overline{H}_{3,1,0} \\
& + H_{0,0} \overline{H}_{1,1,0} + \overline{H}_{0,0} H_{2,0} + \overline{H}_{0,0} H_{2,1} + \overline{H}_{0,0} H_{1,0,0} + \overline{H}_{0,0} H_{1,2} + \overline{H}_{0,0} H_{1,1,0} \\
& + H_2 \overline{H}_{0,0,0} + H_2 \overline{H}_3 + \overline{H}_2 H_{0,0,0} + \overline{H}_2 H_3 + H_{1,0} \overline{H}_{0,0,0} + H_{1,0} \overline{H}_3 \\
& + \overline{H}_{1,0} H_{0,0,0} + \overline{H}_{1,0} H_3 + H_{1,1} \overline{H}_{0,0,0} + \overline{H}_{1,1} H_{0,0,0} + 2 H_0 \overline{H}_{0,0,0,0} \\
& + 2 H_0 \overline{H}_{3,0} + 2 H_0 \overline{H}_{1,1,1,0} + 2 \overline{H}_0 H_{0,0,0,0} + 2 \overline{H}_0 H_{3,0} + 2 \overline{H}_0 H_{1,1,1,0} \\
& + 2 H_1 \overline{H}_{3,1} + 2 \overline{H}_1 H_{3,1} + 2 H_{0,0} \overline{H}_{0,0,0} + 2 H_{0,0} \overline{H}_3 + 2 H_{0,0} \overline{H}_{1,1,1} \\
& + 2 \overline{H}_{0,0} H_{0,0,0} + 2 \overline{H}_{0,0} H_3 + 2 \overline{H}_{0,0} H_{1,1,1} - 2 H_2 \zeta_3 - 2 \overline{H}_2 \zeta_3 - 2 H_{1,0} \zeta_3 \\
& - 2 \overline{H}_{1,0} \zeta_3 + 2 H_{1,1} \overline{H}_3 + 2 \overline{H}_{1,1} H_3 - 4 H_{1,1} \zeta_3 - 4 \overline{H}_{1,1} \zeta_3 \\
& - 2 H_0 \overline{H}_1 \zeta_3 - 2 \overline{H}_0 H_1 \zeta_3 \Big],
\end{aligned}$$

$$\begin{aligned}
L_{2,2,1}^+ &= \frac{1}{4} [H_5 + \overline{H}_5 + H_{4,1} + \overline{H}_{4,1} + H_{2,3} + \overline{H}_{2,3} + H_{1,0,0,0,0} + \overline{H}_{1,0,0,0,0} \quad (\text{A.1.11}) \\
& + H_{1,3,0} + \overline{H}_{1,3,0} + H_{1,1,0,0,0} + \overline{H}_{1,1,0,0,0} + 2 H_{0,0,0,0,0} + 2 \overline{H}_{0,0,0,0,0} \\
& + 2 H_{4,0} + 2 \overline{H}_{4,0} + 2 H_{2,0,0,0} + 2 \overline{H}_{2,0,0,0} + 2 H_{2,2,0} + 2 \overline{H}_{2,2,0} \\
& + 2 H_{2,2,1} + 2 \overline{H}_{2,2,1} + 2 H_{1,1,2,0} + 2 \overline{H}_{1,1,2,0} - 6 \zeta_5 + H_0 \overline{H}_{1,0,0,0} \\
& + H_0 \overline{H}_{1,3} + H_0 \overline{H}_{1,1,0,0} + \overline{H}_0 H_{1,0,0,0} + \overline{H}_0 H_{1,3} + \overline{H}_0 H_{1,1,0,0} + H_1 \overline{H}_{0,0,0,0} \\
& + H_1 \overline{H}_4 + H_1 \overline{H}_{2,0,0} + \overline{H}_1 H_{0,0,0,0} + \overline{H}_1 H_4 + \overline{H}_1 H_{2,0,0} \\
& + H_{0,0} \overline{H}_{1,0,0} + H_{0,0} \overline{H}_{1,1,0} + \overline{H}_{0,0} H_{1,0,0} + \overline{H}_{0,0} H_{1,1,0} + H_2 \overline{H}_{1,0,0} \\
& + \overline{H}_2 H_{1,0,0} + H_{1,0} \overline{H}_{0,0,0} + H_{1,0} \overline{H}_{2,0} + \overline{H}_{1,0} H_{0,0,0} + \overline{H}_{1,0} H_{2,0} \\
& + H_{1,1} \overline{H}_{0,0,0} + \overline{H}_{1,1} H_{0,0,0} + 2 H_0 \overline{H}_{0,0,0,0} + 2 H_0 \overline{H}_4 + 2 H_0 \overline{H}_{2,0,0} \\
& + 2 \overline{H}_0 H_4 + 2 \overline{H}_0 H_{2,0,0} + 2 \overline{H}_0 H_{2,2} + 2 \overline{H}_0 H_{1,1,2} + 2 H_1 \overline{H}_{2,2} \\
& + 2 \overline{H}_1 H_{2,2} + 2 H_0 \overline{H}_{2,2} + 2 H_0 \overline{H}_{1,1,2} + 2 \overline{H}_0 H_{0,0,0,0} + 2 H_{0,0} \overline{H}_{0,0,0}
\end{aligned}$$

$$\begin{aligned}
& +2 H_{0,0} \bar{H}_{2,0} + 2 \bar{H}_{0,0} H_{0,0,0} + 2 \bar{H}_{0,0} H_{2,0} + 2 H_2 \bar{H}_{0,0,0} + 2 H_2 \bar{H}_{2,0} \\
& +2 H_2 \bar{H}_{1,1,0} + 2 H_2 \zeta_3 + 2 \bar{H}_2 H_{0,0,0} + 2 \bar{H}_2 H_{2,0} + 2 \bar{H}_2 H_{1,1,0} + 2 \bar{H}_2 \zeta_3 \\
& +2 H_{1,1} \bar{H}_{2,0} + 2 \bar{H}_{1,1} H_{2,0} - 4 H_{0,0} \zeta_3 - 4 \bar{H}_{0,0} \zeta_3 + 4 H_{1,0} \zeta_3 + 4 \bar{H}_{1,0} \zeta_3 \\
& +8 H_{1,1} \zeta_3 + 8 \bar{H}_{1,1} \zeta_3 - 4 H_0 \bar{H}_0 \zeta_3 + 4 H_0 \bar{H}_1 \zeta_3 + 4 \bar{H}_0 H_1 \zeta_3 \Big],
\end{aligned}$$

$$\begin{aligned}
L_{4,1}^- = & \frac{1}{4} \Big[H_0 \bar{H}_{2,0,0} + H_0 \bar{H}_{1,0,0,0} + \bar{H}_0 H_{2,0,0} + \bar{H}_0 H_{1,0,0,0} + H_1 \bar{H}_{0,0,0,0} \quad (\text{A.1.12}) \\
& + \bar{H}_1 H_{0,0,0,0} + H_{0,0} \bar{H}_{2,0} + H_{0,0} \bar{H}_{1,0,0} + \bar{H}_{0,0} H_{2,0} + \bar{H}_{0,0} H_{1,0,0} \\
& + H_2 \bar{H}_{0,0,0} + \bar{H}_2 H_{0,0,0} + H_{1,0} \bar{H}_{0,0,0} + \bar{H}_{1,0} H_{0,0,0} + 2 H_0 \bar{H}_{0,0,0,0} \\
& + 2 H_0 \bar{H}_{1,1,0,0} + 2 \bar{H}_0 H_{0,0,0,0} + 2 \bar{H}_0 H_{1,1,0,0} + 2 H_{0,0} \bar{H}_{0,0,0} + 2 H_{0,0} \bar{H}_{1,1,0} \\
& + 2 \bar{H}_{0,0} H_{0,0,0} + 2 \bar{H}_{0,0} H_{1,1,0} + 2 H_{1,1} \bar{H}_{0,0,0} + 2 \bar{H}_{1,1} H_{0,0,0} \\
& - 4 H_{0,0} \zeta_3 - 4 H_{1,0} \zeta_3 + H_{4,0} + H_{2,0,0,0} + H_{1,0,0,0,0} + 2 H_{0,0,0,0,0} + 2 H_{4,1} \\
& - 4 \bar{H}_{0,0} \zeta_3 - 4 \bar{H}_{1,0} \zeta_3 + \bar{H}_{4,0} + \bar{H}_{2,0,0,0} + \bar{H}_{1,0,0,0,0} + 2 \bar{H}_{0,0,0,0,0} + 2 \bar{H}_{4,1} \\
& + 2 \bar{H}_{1,1,0,0,0} - 4 H_0 \bar{H}_0 \zeta_3 - 4 H_0 \bar{H}_1 \zeta_3 - 4 \bar{H}_0 H_1 \zeta_3 + H_0 \bar{H}_4 \\
& + 2 H_{1,1,0,0,0} + \bar{H}_0 H_4 + 2 H_1 \bar{H}_4 + 2 \bar{H}_1 H_4 + H_5 + \bar{H}_5 - 4 \zeta_5 \Big],
\end{aligned}$$

$$\begin{aligned}
L_{3,2}^- = & \frac{1}{4} \Big[H_0 \bar{H}_{1,0,0,0} + \bar{H}_0 H_{1,0,0,0} + H_1 \bar{H}_{0,0,0,0} + \bar{H}_1 H_{0,0,0,0} + H_{0,0} \bar{H}_{1,0,0,0} \quad (\text{A.1.13}) \\
& + \bar{H}_{0,0} H_{1,0,0} + H_{1,0} \bar{H}_{0,0,0} + \bar{H}_{1,0} H_{0,0,0} + 2 H_0 \bar{H}_{0,0,0,0} + 2 H_0 \bar{H}_{3,0} \\
& + 2 H_0 \bar{H}_{1,2,0} + 2 \bar{H}_0 H_{0,0,0,0} + 2 \bar{H}_0 H_{3,0} + 2 \bar{H}_0 H_{1,2,0} + 2 H_1 \bar{H}_{3,0} \\
& + 2 \bar{H}_1 H_{3,0} + 2 H_{0,0} \bar{H}_{0,0,0} + 2 H_{0,0} \bar{H}_3 + 2 H_{0,0} \bar{H}_{1,2} + 2 \bar{H}_{0,0} H_{0,0,0} \\
& + 2 \bar{H}_{0,0} H_3 + 2 \bar{H}_{0,0} H_{1,2} + 2 H_{1,0} \bar{H}_3 + 2 \bar{H}_{1,0} H_3 + 8 H_{0,0} \zeta_3 \\
& + 8 H_{1,0} \zeta_3 + H_{1,0,0,0,0} + 2 H_{0,0,0,0,0} + 2 H_{3,0,0} + 2 H_{3,2} + 2 H_{1,2,0,0} \\
& + 8 \bar{H}_{0,0} \zeta_3 + 8 \bar{H}_{1,0} \zeta_3 + \bar{H}_{1,0,0,0,0} + 2 \bar{H}_{0,0,0,0,0} + 2 \bar{H}_{3,0,0} + 2 \bar{H}_{3,2} \\
& + 2 \bar{H}_{1,2,0,0} + 8 H_0 \bar{H}_0 \zeta_3 + 8 H_0 \bar{H}_1 \zeta_3 + 8 \bar{H}_0 H_1 \zeta_3 + H_5 + \bar{H}_5 + 16 \zeta_5 \Big],
\end{aligned}$$

$$\begin{aligned}
L_{2,1,1,1}^- = & \frac{1}{4} \Big[H_5 + \bar{H}_5 + H_{4,1} + \bar{H}_{4,1} + H_{3,2} + \bar{H}_{3,2} + H_{3,1,1} + \bar{H}_{3,1,1} + H_{2,3} \quad (\text{A.1.14}) \\
& + H_{2,2,1} + \bar{H}_{2,2,1} + H_{2,1,2} + \bar{H}_{2,1,2} + H_{1,0,0,0,0} + \bar{H}_{1,0,0,0,0} + H_{1,3,0} + \bar{H}_{1,3,0} \\
& + H_{1,2,0,0} + \bar{H}_{1,2,0,0} + H_{1,2,1,0} + \bar{H}_{1,2,1,0} + H_{1,1,0,0,0} + \bar{H}_{1,1,0,0,0} + H_{1,1,2,0} \\
& + \bar{H}_{1,1,2,0} + H_{1,1,1,0,0} + \bar{H}_{1,1,1,0,0} + 2 H_{0,0,0,0,0} + 2 \bar{H}_{0,0,0,0,0} + 2 H_{4,0} + \bar{H}_{2,3}
\end{aligned}$$

$$\begin{aligned}
& +2\bar{H}_{4,0} + 2H_{3,0,0} + 2\bar{H}_{3,0,0} + 2H_{3,1,0} + 2\bar{H}_{3,1,0} + 2H_{2,0,0,0} + 2\bar{H}_{2,0,0,0} \\
& +2H_{2,2,0} + 2\bar{H}_{2,2,0} + 2H_{2,1,0,0} + 2\bar{H}_{2,1,0,0} + 2H_{2,1,1,0} + 2\bar{H}_{2,1,1,0} \\
& +2H_{2,1,1,1} + 2\bar{H}_{2,1,1,1} + 2H_{1,1,1,1,0} + 2\bar{H}_{1,1,1,1,0} - 4\zeta_5 + H_0\bar{H}_{1,0,0,0} \\
& +H_0\bar{H}_{1,3} + H_0\bar{H}_{1,2,0} + H_0\bar{H}_{1,2,1} + H_0\bar{H}_{1,1,0,0} + H_0\bar{H}_{1,1,2} + H_0\bar{H}_{1,1,1,0} \\
& +\bar{H}_0H_{1,0,0,0} + \bar{H}_0H_{1,3} + \bar{H}_0H_{1,2,0} + \bar{H}_0H_{1,2,1} + \bar{H}_0H_{1,1,0,0} + \bar{H}_0H_{1,1,2} \\
& +\bar{H}_0H_{1,1,1,0} + H_1\bar{H}_{0,0,0,0} + H_1\bar{H}_4 + H_1\bar{H}_{3,0} + H_1\bar{H}_{3,1} + H_1\bar{H}_{2,0,0} \\
& +H_1\bar{H}_{2,2} + H_1\bar{H}_{2,1,0} + \bar{H}_1H_{0,0,0,0} + \bar{H}_1H_4 + \bar{H}_1H_{3,0} + \bar{H}_1H_{3,1} \\
& +\bar{H}_1H_{2,0,0} + \bar{H}_1H_{2,2} + \bar{H}_1H_{2,1,0} + H_{0,0}\bar{H}_{1,0,0} + H_{0,0}\bar{H}_{1,2} + H_{0,0}\bar{H}_{1,1,0} \\
& +H_{0,0}\bar{H}_{1,1,1} + \bar{H}_{0,0}H_{1,0,0} + \bar{H}_{0,0}H_{1,2} + \bar{H}_{0,0}H_{1,1,0} + \bar{H}_{0,0}H_{1,1,1} \\
& +H_2\bar{H}_{1,0,0} + H_2\bar{H}_{1,2} + H_2\bar{H}_{1,1,0} + \bar{H}_2H_{1,0,0} + \bar{H}_2H_{1,2} + \bar{H}_2H_{1,1,0} \\
& +H_{1,0}\bar{H}_{0,0,0} + H_{1,0}\bar{H}_3 + H_{1,0}\bar{H}_{2,0} + H_{1,0}\bar{H}_{2,1} + \bar{H}_{1,0}H_{0,0,0} + \bar{H}_{1,0}H_3 \\
& +\bar{H}_{1,0}H_{2,0} + \bar{H}_{1,0}H_{2,1} + H_{1,1}\bar{H}_{0,0,0} + H_{1,1}\bar{H}_3 + H_{1,1}\bar{H}_{2,0} \\
& +\bar{H}_{1,1}H_{0,0,0} + \bar{H}_{1,1}H_3 + \bar{H}_{1,1}H_{2,0} + 2H_0\bar{H}_{0,0,0,0} + 2H_0\bar{H}_4 + 2H_0\bar{H}_{3,0} \\
& +2H_0\bar{H}_{3,1} + 2H_0\bar{H}_{2,0,0} + 2H_0\bar{H}_{2,2} + 2H_0\bar{H}_{2,1,0} + 2H_0\bar{H}_{2,1,1} \\
& +2H_0\bar{H}_{1,1,1,1} + 2\bar{H}_0H_{0,0,0,0} + 2\bar{H}_0H_4 + 2\bar{H}_0H_{3,0} + 2\bar{H}_0H_{3,1} \\
& +2\bar{H}_0H_{2,0,0} + 2\bar{H}_0H_{2,2} + 2\bar{H}_0H_{2,1,0} + 2\bar{H}_0H_{2,1,1} + 2\bar{H}_0H_{1,1,1,1} \\
& +2H_1\bar{H}_{2,1,1} + 2\bar{H}_1H_{2,1,1} + 2H_{0,0}\bar{H}_{0,0,0} + 2H_{0,0}\bar{H}_3 + 2H_{0,0}\bar{H}_{2,0} \\
& +2H_{0,0}\bar{H}_{2,1} + 2\bar{H}_{0,0}H_{0,0,0} + 2\bar{H}_{0,0}H_3 + 2\bar{H}_{0,0}H_{2,0} + 2\bar{H}_{0,0}H_{2,1} \\
& +2H_2\bar{H}_{0,0,0} + 2H_2\bar{H}_3 + 2H_2\bar{H}_{2,0} + 2H_2\bar{H}_{2,1} + 2H_2\bar{H}_{1,1,1} \\
& +2\bar{H}_2H_{0,0,0} + 2\bar{H}_2H_3 + 2\bar{H}_2H_{2,0} + 2\bar{H}_2H_{2,1} + 2\bar{H}_2H_{1,1,1} \\
& +2H_{1,1}\bar{H}_{2,1} - 2H_{1,1}\zeta_3 + 2\bar{H}_{1,1}H_{2,1} - 2\bar{H}_{1,1}\zeta_3].
\end{aligned}$$

A.1.7 Expression of Brown's SVHPLs in terms of the L^\pm functions

In this appendix we present the expression of Brown's SVHPLs corresponding to Lyndon words in terms of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ eigenfunctions $L_w^\pm(z)$.

$$\begin{aligned}
L_0 &= L_0^-, \\
L_1 &= L_1^+ - \frac{1}{2} L_0^-, \\
L_2 &= L_2^-, \\
L_3 &= L_3^+ - \frac{1}{12} [L_0^-]^3, \\
L_{2,1} &= -\frac{1}{4} L_1^+ [L_0^-]^2 + \frac{1}{2} L_3^+ + L_{2,1}^- + \zeta_3, \\
L_4 &= L_4^-, \\
L_{3,1} &= -\frac{1}{4} L_2^- [L_0^-]^2 + L_4^- + L_{3,1}^+, \\
L_{2,1,1} &= -\frac{1}{4} L_2^- L_0^- L_1^+ + \frac{1}{2} L_{3,1}^+ + L_{2,1,1}^-, \\
L_5 &= L_5^+ - \frac{1}{240} [L_0^-]^5, \\
L_{4,1} &= \frac{1}{48} L_1^+ [L_0^-]^4 - \frac{1}{4} L_3^+ [L_0^-]^2 + \frac{1}{2} [L_0^-]^2 \zeta_3 + \frac{3}{2} L_5^+ + L_{4,1}^- + \zeta_5, \\
L_{3,2} &= -\frac{1}{16} L_1^+ [L_0^-]^4 + \frac{1}{2} L_3^+ [L_0^-]^2 - \frac{7}{2} L_5^+ - [L_0^-]^2 \zeta_3 + L_{3,2}^- - 4 \zeta_5, \\
L_{3,1,1} &= \frac{1}{16} [L_0^-]^3 [L_1^+]^2 - \frac{1}{4} L_{2,1}^- [L_0^-]^2 + \frac{7}{960} [L_0^-]^5 - \frac{1}{4} L_0^- L_1^+ L_3^+ + \frac{1}{2} L_0^- L_1^+ \zeta_3 \\
&\quad + L_{4,1}^- + L_{3,1,1}^+, \\
L_{2,2,1} &= -\frac{3}{16} [L_0^-]^3 [L_1^+]^2 + \frac{1}{2} L_{2,1}^- [L_0^-]^2 - \frac{13}{960} [L_0^-]^5 + \frac{3}{4} L_0^- L_1^+ L_3^+ - \frac{1}{2} L_0^- L_1^+ \zeta_3 \\
&\quad - \frac{7}{2} L_{4,1}^- - \frac{1}{2} L_{3,2}^- + L_{2,2,1}^+, \\
L_{2,1,1,1} &= \frac{1}{48} [L_0^-]^2 [L_1^+]^3 - \frac{1}{192} L_1^+ [L_0^-]^4 + \frac{1}{16} L_3^+ [L_0^-]^2 - \frac{1}{8} [L_0^-]^2 \zeta_3 - \frac{1}{4} L_0^- L_{2,1}^- L_1^+ \\
&\quad - \frac{1}{4} L_5^+ + \frac{1}{2} L_{3,1,1}^+ + \frac{1}{2} \zeta_5 + L_{2,1,1,1}^-, \\
L_6 &= L_6^-, \\
L_{5,1} &= -\frac{1}{4} L_4^- [L_0^-]^2 + \frac{1}{48} L_2^- [L_0^-]^4 + 2 L_6^- + L_{5,1}^+, \\
L_{4,2} &= \frac{3}{4} L_4^- [L_0^-]^2 - \frac{1}{12} L_2^- [L_0^-]^4 - \frac{11}{2} L_6^- + L_{4,2}^+,
\end{aligned} \tag{A.1.15}$$

$$\begin{aligned}
L_{4,1,1} &= \frac{1}{16} L_2^- L_1^+ [L_0^-]^3 - \frac{1}{4} L_{3,1}^+ [L_0^-]^2 - \frac{1}{4} L_4^- L_0^- L_1^+ + \frac{1}{2} L_2^- L_0^- \zeta_3 + \frac{3}{2} L_{5,1}^+ + L_{4,1,1}^-, \\
L_{3,2,1} &= -\frac{3}{16} L_2^- L_1^+ [L_0^-]^3 + \frac{1}{2} L_{3,1}^+ [L_0^-]^2 + \frac{3}{4} L_4^- L_0^- L_1^+ - \frac{1}{2} L_2^- L_0^- \zeta_3 - \frac{7}{2} L_{5,1}^+ + L_{3,2,1}^-, \\
L_{3,1,2} &= -\frac{1}{4} L_2^- L_0^- L_3^+ - \frac{3}{2} L_2^- L_0^- \zeta_3 + L_{3,1,2}^- + 3 L_{5,1}^+ + L_{4,2}^+, \\
L_{3,1,1,1} &= \frac{1}{16} L_2^- [L_0^-]^2 [L_1^+]^2 + \frac{1}{4} L_4^- [L_0^-]^2 - \frac{5}{192} L_2^- [L_0^-]^4 - \frac{1}{4} L_{2,1,1}^- [L_0^-]^2 \\
&\quad - \frac{1}{4} L_0^- L_1^+ L_{3,1}^+ - L_6^- + L_{4,1,1}^- + L_{3,1,1,1}^+, \\
L_{2,2,1,1} &= -\frac{1}{4} L_2^- [L_0^-]^2 [L_1^+]^2 - \frac{3}{4} L_4^- [L_0^-]^2 + \frac{1}{12} L_2^- [L_0^-]^4 + \frac{3}{4} L_{2,1,1}^- [L_0^-]^2 + \frac{11}{4} L_6^- \\
&\quad + \frac{1}{4} L_2^- L_1^+ L_3^+ - \frac{1}{2} L_2^- L_1^+ \zeta_3 + \frac{3}{4} L_0^- L_1^+ L_{3,1}^+ - \frac{1}{2} L_{3,1,2}^- - 5 L_{4,1,1}^- - L_{3,2,1}^- + L_{2,2,1,1}^+, \\
L_{2,1,1,1,1} &= -\frac{5}{192} L_2^- L_1^+ [L_0^-]^3 + \frac{1}{16} L_{3,1}^+ [L_0^-]^2 + \frac{1}{48} L_2^- L_0^- [L_1^+]^3 + \frac{1}{8} L_4^- L_0^- L_1^+ \\
&\quad - \frac{1}{4} L_2^- L_0^- \zeta_3 - \frac{1}{4} L_0^- L_{2,1,1}^- L_1^+ - \frac{1}{4} L_{5,1}^+ + \frac{1}{2} L_{3,1,1,1}^+ + L_{2,1,1,1,1}^-.
\end{aligned} \tag{A.1.16}$$

A.2 Analytic continuation of harmonic sums

In this section we review the analytic continuation of multiple harmonic sums and the structural relations between them, as presented by Blümlein [54]. Multiple harmonic sums are defined by,

$$S_{a_1, \dots, a_n}(N) = \sum_{k_1=1}^N \sum_{k_2=1}^{k_1} \dots \sum_{k_n=1}^{k_{n-1}} \frac{\text{sgn}(a_1)^{k_1}}{k_1^{|a_1|}} \dots \frac{\text{sgn}(a_n)^{k_n}}{k_n^{|a_n|}}, \tag{A.2.1}$$

where the a_k are positive or negative integers, and N is a positive integer. For the cases in which we are interested, they are similar to the Euler-Zagier sums (1.3.10), except that the summation range differs slightly. They are related to Mellin transforms of real functions or distributions $f(x)$,

$$S_{a_1, \dots, a_n}(N) = \int_0^1 dx x^N f_{a_1, \dots, a_n} = \mathbf{M}[f_{a_1, \dots, a_n}(x)](N). \tag{A.2.2}$$

Typically $f(x)$ are HPLs weighted by factors of $1/(1 \pm x)$. To avoid singularities at $x = 1$, it is often useful to consider the $+$ -distribution,

$$\mathbf{M}[(f(x))_+](N) = \int_0^1 dx (x^N - 1) f(x). \quad (\text{A.2.3})$$

The weight $|w|$ of the harmonic sum is given by $|w| = \sum_{k=1}^n |a_k|$. The number of harmonic sums of weight w is equal to $2 \cdot 3^{|w|-1}$, but not all of them are independent. For example, they obey shuffle relations [176]. It is natural to ask whether these are the only relations they satisfy. In fact, it is known that in the special case $N \rightarrow \infty$, in which the sums reduce to multiple zeta values, many new relations emerge [65, 174, 177, 178]. In ref. [54], an analytic continuation of the harmonic sums was considered. It is defined by the integral representation, eq. (A.2.2), where N is allowed to take complex values. This allows for two new operations—differentiation and evaluation at fractional arguments—which generate new structural relations among the harmonic sums.

In the present work, harmonic sums with negative indices do not appear, so we will assume that $a_k > 0$. This assumption provides a considerable simplification. The derivative relations allow for the extraction of logarithmic factors,

$$\mathbf{M}[\log^l(x)f(x)](N) = \frac{d^l}{dN^l} \mathbf{M}[f(x)](N), \quad (\text{A.2.4})$$

which explains why the derivatives of the building blocks in section 1.6 generate SVHPLs. In ref. [54], all available relations are imposed, and the following are the irreducible functions through weight five:

weight 1

$$S_1(N) = \psi(N+1) + \gamma_E = \mathbf{M} \left[\left(\frac{1}{x-1} \right)_+ \right] (N) \quad (\text{A.2.5})$$

weight 3

$$F_4(N) = \mathbf{M} \left[\left(\frac{\text{Li}_2(x)}{1-x} \right)_+ \right] (N) \quad (\text{A.2.6})$$

weight 4

$$\begin{aligned}
F_{6a}(N) &= \mathbf{M} \left[\left(\frac{\text{Li}_3(x)}{1-x} \right)_+ \right] (N) \\
F_7(N) &= \mathbf{M} \left[\left(\frac{S_{1,2}(x)}{x-1} \right)_+ \right] (N)
\end{aligned} \tag{A.2.7}$$

weight 5

$$\begin{aligned}
F_9(N) &= \mathbf{M} \left[\left(\frac{\text{Li}_4(x)}{x-1} \right)_+ \right] (N) \\
F_{11}(N) &= \mathbf{M} \left[\left(\frac{S_{2,2}(x)}{x-1} \right)_+ \right] (N) \\
F_{13}(N) &= \mathbf{M} \left[\left(\frac{\text{Li}_2^2(x)}{x-1} \right)_+ \right] (N) \\
F_{17}(N) &= \mathbf{M} \left[\left(\frac{S_{1,3}(x)}{x-1} \right)_+ \right] (N)
\end{aligned} \tag{A.2.8}$$

There are no irreducible basis functions of weight two. These functions are meromorphic with poles at the negative integers. To use these functions in the integral transform (1.4.4), we need the expansions near the poles. Actually, we only need the expansions around zero, since the expansions around any integer can be obtained

from them using the recursion relations of ref. [54],

$$\begin{aligned}
\psi^{(n)}(1+z) &= \psi^{(n)}(z) + (-1)^n \frac{n!}{z^{n+1}} \\
F_4(z) &= F_4(z-1) - \frac{1}{z} \left[\zeta_2 - \frac{S_1(z)}{z} \right] \\
F_{6a}(z) &= F_{6a}(z-1) - \frac{\zeta_3}{z} + \frac{1}{z^2} \left[\zeta_2 - \frac{S_1(z)}{z} \right] \\
F_7(z) &= F_7(z-1) + \frac{\zeta_3}{z} - \frac{1}{2z^2} [S_1^2(z) + S_2(z)] \\
F_9(z) &= F_9(z-1) + \frac{\zeta_4}{z} - \frac{\zeta_3}{z^2} + \frac{\zeta_2}{z^3} - \frac{1}{z^4} S_1(z) \\
F_{11}(z) &= F_{11}(z-1) + \frac{\zeta_4}{4z} - \frac{\zeta_3}{z^2} + \frac{1}{2z^3} [S_1^2(z) + S_2(z)] \\
F_{13}(z) &= F_{13}(z-1) + \frac{\zeta_2^2}{z} - \frac{4\zeta_3}{z^2} - \frac{2\zeta_2}{z^2} S_1(z) + \frac{2S_{2,1}(z)}{z^2} + \frac{2}{z^3} [S_1^2(z) + S_2(z)] \\
F_{17}(z) &= F_{17}(z-1) + \frac{\zeta_4}{z} - \frac{1}{6z^2} [S_1^3(z) + 3S_1(z)S_2(z) + 2S_3(z)] .
\end{aligned} \tag{A.2.9}$$

The expansions around zero can be obtained from the integral representations. We find that, for $\delta \rightarrow 0$, the expansions can all be expressed simply in terms of multiple

zeta values,

$$\begin{aligned}
S_1(\delta) &= - \sum_{n=1}^{\infty} (-\delta)^n \zeta_{n+1} , \\
F_4(\delta) &= \sum_{n=1}^{\infty} (-\delta)^n \zeta_{n+1,2} , \\
F_{6a}(\delta) &= \sum_{n=1}^{\infty} (-\delta)^n \zeta_{n+1,3} , \\
F_7(\delta) &= - \sum_{n=1}^{\infty} (-\delta)^n \zeta_{n+1,2,1} , \\
F_9(\delta) &= - \sum_{n=1}^{\infty} (-\delta)^n \zeta_{n+1,4} , \\
F_{11}(\delta) &= - \sum_{n=1}^{\infty} (-\delta)^n \zeta_{n+1,3,1} , \\
F_{13}(\delta) &= - \sum_{n=1}^{\infty} (-\delta)^n (2\zeta_{n+1,2,2} + 4\zeta_{n+1,3,1}) , \\
F_{17}(\delta) &= - \sum_{n=1}^{\infty} (-\delta)^n \zeta_{n+1,2,1,1} .
\end{aligned} \tag{A.2.10}$$

These single-variable functions can be assembled to form two-variable functions of ν and n , such that their inverse Fourier-Mellin transforms produce sums of SVHPLs. This construction is not unique, because other building blocks could be added. We

choose to define the two-variable functions as,

$$\begin{aligned}
\tilde{F}_4 &= \text{sgn}(n) \left\{ F_4\left(i\nu + \frac{|n|}{2}\right) + F_4\left(-i\nu + \frac{|n|}{2}\right) - \frac{1}{4}D_\nu^2 E_{\nu,n} - \frac{1}{8}N^2 E_{\nu,n} - \frac{1}{2}V^2 E_{\nu,n} \right. \\
&\quad \left. + \frac{1}{2}\left(\psi_- + V\right)D_\nu E_{\nu,n} + \zeta_2 E_{\nu,n} - 4\zeta_3 \right\} + N \left\{ \frac{1}{2}V\psi_- + \frac{1}{2}\zeta_2 \right\}, \\
\tilde{F}_{6a} &= \text{sgn}(n) \left\{ F_{6a}\left(i\nu + \frac{|n|}{2}\right) - F_{6a}\left(-i\nu + \frac{|n|}{2}\right) - \frac{1}{12}D_\nu^3 E_{\nu,n} - \frac{3}{8}N^2 V E_{\nu,n} - \frac{1}{2}V^3 E_{\nu,n} \right. \\
&\quad \left. + \frac{1}{4}\left(\psi_- + V\right)D_\nu^2 E_{\nu,n} + \zeta_2 D_\nu E_{\nu,n} + \zeta_3 \psi_- \right\} \\
&\quad + N \left\{ \frac{1}{16} (N^2 + 12 V^2) \psi_- + \zeta_2 V \right\}, \\
\tilde{F}_7 &= F_7\left(i\nu + \frac{|n|}{2}\right) - F_7\left(-i\nu + \frac{|n|}{2}\right) - \frac{1}{2}\tilde{F}_{6a} + \frac{1}{2}V\tilde{F}_4 \\
&\quad - \left[\frac{1}{8}(\psi_-)^2 - \frac{1}{4}\psi'_+ + \frac{1}{2}\zeta_2 \right] D_\nu E_{\nu,n} \\
&\quad + \left[\frac{1}{2}\tilde{F}_4 + \frac{1}{16}N^2 E_{\nu,n} + \frac{1}{4}V^2 E_{\nu,n} - \frac{1}{4}V D_\nu E_{\nu,n} + \frac{1}{8}D_\nu^2 E_{\nu,n} - \zeta_3 \right] \psi_- + 5V\zeta_3 \\
&\quad + \text{sgn}(n)N \left\{ -\frac{1}{8}V E_{\nu,n}^2 - \frac{1}{2}V^3 - \frac{3}{32}VN^2 - \left[\frac{1}{8}(\psi_-)^2 - \frac{1}{4}\psi'_+ + \frac{1}{2}\zeta_2 \right] V \right\},
\end{aligned} \tag{A.2.11}$$

where

$$\begin{aligned}
\psi_- &\equiv \psi\left(1 + i\nu + \frac{|n|}{2}\right) - \psi\left(1 - i\nu + \frac{|n|}{2}\right), \\
\psi'_+ &\equiv \psi'\left(1 + i\nu + \frac{|n|}{2}\right) + \psi'\left(1 - i\nu + \frac{|n|}{2}\right).
\end{aligned} \tag{A.2.12}$$

A.2.1 The basis in (ν, n) space in terms of single-valued HPLs

In this appendix we present the analytic expressions for the basis of $\mathbb{Z}_2 \times \mathbb{Z}_2$ eigenfunctions in (ν, n) space in terms of single-valued HPLs in (w, w^*) space up to weight five. The $\mathbb{Z}_2 \times \mathbb{Z}_2$ acts on (w, w^*) space via conjugation and inversion, while it acts on (ν, n) space via $[n \leftrightarrow -n]$ and $[\nu \leftrightarrow -\nu, n \leftrightarrow -n]$. The eigenvalue under $\mathbb{Z}_2 \times \mathbb{Z}_2$ in (w, w^*) space will be referred to as *parity*.

Basis of weight 1 with parity $(+, +)$:

$$\mathcal{I}[1] = 2 L_1^+ . \quad (\text{A.2.13})$$

Basis of weight 1 with parity $(+, -)$:

$$\mathcal{I}[\delta_{0,n}] = L_0^- . \quad (\text{A.2.14})$$

Basis of weight 2 with parity $(+, +)$:

$$\mathcal{I}[E_{\nu,n}] = [L_1^+]^2 - \frac{1}{4} [L_0^-]^2 , \quad (\text{A.2.15})$$

$$\mathcal{I}[\delta_{0,n}/(i\nu)] = \frac{1}{2} [L_0^-]^2 . \quad (\text{A.2.16})$$

Basis of weight 2 with parity $(+, -)$:

$$\mathcal{I}[V] = -L_0^- L_1^+ . \quad (\text{A.2.17})$$

Basis of weight 2 with parity $(-, -)$:

$$\mathcal{I}[N] = 4 L_2^- . \quad (\text{A.2.18})$$

Basis of weight 3 with parity $(+, +)$:

$$\mathcal{I}[E_{\nu,n}^2] = \frac{2}{3} [L_1^+]^3 - L_3^+ , \quad (\text{A.2.19})$$

$$\mathcal{I}[N^2] = 12 L_3^+ - 2 L_1^+ [L_0^-]^2 , \quad (\text{A.2.20})$$

$$\mathcal{I}[V^2] = \frac{1}{2} L_1^+ [L_0^-]^2 - L_3^+ . \quad (\text{A.2.21})$$

Basis of weight 3 with parity $(+, -)$:

$$\mathcal{I}[V E_{\nu,n}] = \frac{1}{6} [L_0^-]^3 - 2 L_{2,1}^-, \quad (\text{A.2.22})$$

$$\mathcal{I}[D_\nu E_{\nu,n}] = -\frac{1}{12} [L_0^-]^3 - L_0^- [L_1^+]^2 + 4 L_{2,1}^-, \quad (\text{A.2.23})$$

$$\mathcal{I}[\delta_{0,n}/(i\nu)^2] = \frac{1}{6} [L_0^-]^3. \quad (\text{A.2.24})$$

Basis of weight 3 with parity $(-, +)$:

$$\mathcal{I}[N V] = -L_2^- L_0^-. \quad (\text{A.2.25})$$

Basis of weight 3 with parity $(-, -)$:

$$\mathcal{I}[N E_{\nu,n}] = 2 L_2^- L_1^+. \quad (\text{A.2.26})$$

Basis of weight 4 with parity $(+, +)$:

$$\begin{aligned} \mathcal{I}[E_{\nu,n}^3] &= \frac{1}{2} [L_2^-]^2 + \frac{1}{2} [L_0^-]^2 [L_1^+]^2 + \frac{7}{96} [L_0^-]^4 + \frac{1}{2} [L_1^+]^4 - \frac{3}{2} L_0^- L_{2,1}^- \\ &\quad - \frac{5}{2} L_1^+ L_3^+ - 3 L_1^+ \zeta_3, \end{aligned} \quad (\text{A.2.27})$$

$$\mathcal{I}[N^2 E_{\nu,n}] = \frac{1}{12} [L_0^-]^4 + 2 [L_2^-]^2 - 2 L_0^- L_{2,1}^- + 2 L_1^+ L_3^+ - 4 L_1^+ \zeta_3, \quad (\text{A.2.28})$$

$$\begin{aligned} \mathcal{I}[V^2 E_{\nu,n}] &= -\frac{1}{2} [L_2^-]^2 - \frac{1}{4} [L_0^-]^2 [L_1^+]^2 - \frac{1}{12} [L_0^-]^4 + \frac{3}{2} L_0^- L_{2,1}^- \\ &\quad + \frac{1}{2} L_1^+ L_3^+ - L_1^+ \zeta_3, \end{aligned} \quad (\text{A.2.29})$$

$$\begin{aligned} \mathcal{I}[V D_\nu E_{\nu,n}] &= \frac{3}{4} [L_0^-]^2 [L_1^+]^2 + \frac{1}{16} [L_0^-]^4 + [L_2^-]^2 - 2 L_0^- L_{2,1}^- - 2 L_1^+ L_3^+ \\ &\quad + 4 L_1^+ \zeta_3, \end{aligned} \quad (\text{A.2.30})$$

$$\mathcal{I}[D_\nu^2 E_{\nu,n}] = -\frac{1}{2} [L_0^-]^2 [L_1^+]^2 - \frac{1}{24} [L_0^-]^4 - 2 [L_2^-]^2 + 4 L_1^+ L_3^+ - 8 L_1^+ \zeta_3, \quad (\text{A.2.31})$$

$$\mathcal{I}[\delta_{0,n}/(i\nu)^3] = \frac{1}{24} [L_0^-]^4. \quad (\text{A.2.32})$$

Basis of weight 4 with parity $(+, -)$:

$$\mathcal{I}[V E_{\nu,n}^2] = \frac{1}{8} L_1^+ [L_0^-]^3 + \frac{1}{6} L_0^- [L_1^+]^3 - L_0^- \zeta_3 - 2 L_{2,1}^- L_1^+, \quad (\text{A.2.33})$$

$$\mathcal{I}[N^2 V] = \frac{1}{3} L_1^+ [L_0^-]^3 - 2 L_0^- L_3^+, \quad (\text{A.2.34})$$

$$\mathcal{I}[V^3] = \frac{1}{2} L_0^- L_3^+ - \frac{1}{6} L_1^+ [L_0^-]^3, \quad (\text{A.2.35})$$

$$\begin{aligned} \mathcal{I}[E_{\nu,n} D_\nu E_{\nu,n}] &= -\frac{1}{8} L_1^+ [L_0^-]^3 - \frac{1}{2} L_0^- [L_1^+]^3 + \frac{1}{2} L_0^- L_3^+ + L_0^- \zeta_3 \\ &\quad + 2 L_{2,1}^- L_1^+, \end{aligned} \quad (\text{A.2.36})$$

Basis of weight 4 with parity $(-, +)$:

$$\mathcal{I}[N V E_{\nu,n}] = -2 L_{3,1}^+, \quad (\text{A.2.37})$$

$$\mathcal{I}[N D_\nu E_{\nu,n}] = 8 L_{3,1}^+ - 2 L_2^- L_0^- L_1^+. \quad (\text{A.2.38})$$

Basis of weight 4 with parity $(-, -)$:

$$\mathcal{I}[\tilde{F}_4] = -\frac{1}{4} L_2^- [L_0^-]^2 + L_2^- [L_1^+]^2 + 4 L_4^- - 6 L_{2,1,1}^-, \quad (\text{A.2.39})$$

$$\mathcal{I}[N E_{\nu,n}^2] = \frac{1}{2} L_2^- [L_0^-]^2 - 6 L_4^- + 8 L_{2,1,1}^-, \quad (\text{A.2.40})$$

$$\mathcal{I}[N^3] = 40 L_4^- - 6 L_2^- [L_0^-]^2, \quad (\text{A.2.41})$$

$$\mathcal{I}[N V^2] = \frac{1}{2} L_2^- [L_0^-]^2 - 2 L_4^-. \quad (\text{A.2.42})$$

Basis of weight 5 with parity $(+, +)$:

$$\begin{aligned} \mathcal{I}[E_{\nu,n}^4] &= \frac{17}{96} L_1^+ [L_0^-]^4 - \frac{5}{4} L_3^+ [L_0^-]^2 + \frac{2}{5} [L_1^+]^5 + \frac{43}{4} L_5^+ \\ &\quad + [L_0^-]^2 [L_1^+]^3 + 4 [L_0^-]^2 \zeta_3 - 4 L_3^+ [L_1^+]^2 - 8 [L_1^+]^2 \zeta_3 \\ &\quad - 4 L_0^- L_{2,1}^- L_1^+ + 12 L_{3,1,1}^+ + 8 L_{2,2,1}^+, \end{aligned} \quad (\text{A.2.43})$$

$$\begin{aligned} \mathcal{I}[N^2 E_{\nu,n}^2] &= \frac{1}{3} [L_0^-]^2 [L_1^+]^3 - \frac{1}{24} L_1^+ [L_0^-]^4 + 4 L_1^+ [L_2^-]^2 + 3 L_3^+ [L_0^-]^2 \\ &\quad - 8 [L_0^-]^2 \zeta_3 - 25 L_5^+ - 24 L_{3,1,1}^+ - 16 L_{2,2,1}^+, \end{aligned} \quad (\text{A.2.44})$$

$$\mathcal{I}[N^4] = \frac{13}{6} L_1^+ [L_0^-]^4 - 20 L_3^+ [L_0^-]^2 + 140 L_5^+, \quad (\text{A.2.45})$$

$$\mathcal{I} [V^2 E_{\nu,n}^2] = -\frac{1}{12} [L_0^-]^2 [L_1^+]^3 - \frac{13}{96} L_1^+ [L_0^-]^4 + \frac{1}{4} L_3^+ [L_0^-]^2 - \frac{1}{4} L_5^+ \quad (\text{A.2.46})$$

$$- L_1^+ [L_2^-]^2 + 2 [L_0^-]^2 \zeta_3 + 10 L_{3,1,1}^+ + 4 L_{2,2,1}^+ - 4 \zeta_5,$$

$$\mathcal{I} [N^2 V^2] = -\frac{1}{8} L_1^+ [L_0^-]^4 + L_3^+ [L_0^-]^2 - 5 L_5^+, \quad (\text{A.2.47})$$

$$\mathcal{I} [V^4] = \frac{5}{96} L_1^+ [L_0^-]^4 - \frac{1}{4} L_3^+ [L_0^-]^2 + \frac{3}{4} L_5^+, \quad (\text{A.2.48})$$

$$\mathcal{I} [V E_{\nu,n} D_\nu E_{\nu,n}] = \frac{7}{48} L_1^+ [L_0^-]^4 - \frac{3}{4} L_3^+ [L_0^-]^2 - \frac{3}{2} [L_0^-]^2 \zeta_3 + \frac{7}{2} L_5^+ \quad (\text{A.2.49})$$

$$+ L_1^+ [L_2^-]^2 + L_0^- L_{2,1}^- L_1^+ - 12 L_{3,1,1}^+ - 4 L_{2,2,1}^+ + 6 \zeta_5,$$

$$\mathcal{I} [(D_\nu E_{\nu,n})^2] = \frac{3}{2} [L_0^-]^2 [L_1^+]^3 - \frac{1}{3} L_1^+ [L_0^-]^4 - 2 L_1^+ [L_2^-]^2 + 2 L_3^+ [L_0^-]^2 \quad (\text{A.2.50})$$

$$+ 2 [L_0^-]^2 \zeta_3 - 4 L_3^+ [L_1^+]^2 + 8 [L_1^+]^2 \zeta_3 - 8 L_0^- L_{2,1}^- L_1^+,$$

$$- 9 L_5^+ + 48 L_{3,1,1}^+ + 16 L_{2,2,1}^+ - 24 \zeta_5$$

$$\mathcal{I} [E_{\nu,n} D_\nu^2 E_{\nu,n}] = \frac{1}{6} L_1^+ [L_0^-]^4 - [L_0^-]^2 [L_1^+]^3 - L_3^+ [L_0^-]^2 + 4 L_3^+ [L_1^+]^2 + 2 L_5^+ \quad (\text{A.2.51})$$

$$- 8 [L_1^+]^2 \zeta_3 + 4 L_0^- L_{2,1}^- L_1^+ - 24 L_{3,1,1}^+ - 8 L_{2,2,1}^+ + 12 \zeta_5,$$

$$\mathcal{I} [N \tilde{F}_4] = \frac{1}{12} L_1^+ [L_0^-]^4 - \frac{7}{4} L_3^+ [L_0^-]^2 + \frac{7}{2} [L_0^-]^2 \zeta_3 - L_1^+ [L_2^-]^2 \quad (\text{A.2.52})$$

$$- L_0^- L_{2,1}^- L_1^+ + 15 L_5^+ + 12 L_{3,1,1}^+ + 8 L_{2,2,1}^+.$$

Basis of weight 5 with parity (+, -):

$$\mathcal{I} [\tilde{F}_7] = \frac{5}{8} L_0^- [L_2^-]^2 - \frac{11}{48} [L_0^-]^3 [L_1^+]^2 + \frac{1}{4} L_{2,1}^- [L_0^-]^2 + \frac{59}{3840} [L_0^-]^5 \quad (\text{A.2.53})$$

$$+ \frac{5}{48} L_0^- [L_1^+]^4 + \frac{3}{2} L_0^- L_1^+ L_3^+ - \frac{7}{2} L_{3,2}^- - L_{2,1}^- [L_1^+]^2$$

$$- 8 L_0^- L_1^+ \zeta_3 - 10 L_{4,1}^- + 7 L_{2,1,1,1}^-,$$

$$\mathcal{I} [V E_{\nu,n}^3] = \frac{1}{2} L_0^- [L_2^-]^2 + \frac{3}{16} [L_0^-]^3 [L_1^+]^2 + \frac{3}{4} L_{2,1}^- [L_0^-]^2 - \frac{1}{192} [L_0^-]^5 \quad (\text{A.2.54})$$

$$- \frac{1}{4} L_0^- L_1^+ L_3^+ + \frac{9}{2} L_0^- L_1^+ \zeta_3 - \frac{9}{2} L_{3,2}^- - 6 L_{4,1}^- - 12 L_{2,1,1,1}^-,$$

$$\mathcal{I} [N^2 V E_{\nu,n}] = -\frac{1}{4} [L_0^-]^3 [L_1^+]^2 - \frac{1}{48} [L_0^-]^5 + L_{2,1}^- [L_0^-]^2 + L_0^- L_1^+ L_3^+ \quad (\text{A.2.55})$$

$$- 2 L_0^- L_1^+ \zeta_3 - 8 L_{4,1}^- - 2 L_{3,2}^-,$$

$$\mathcal{I} [V^3 E_{\nu,n}] = \frac{3}{16} [L_0^-]^3 [L_1^+]^2 - \frac{3}{4} L_{2,1}^- [L_0^-]^2 + \frac{23}{960} [L_0^-]^5 - \frac{3}{4} L_0^- L_1^+ L_3^+ \quad (\text{A.2.56})$$

$$\begin{aligned}
& + \frac{3}{2} L_0^- L_1^+ \zeta_3 + \frac{3}{2} L_{3,2}^- + 4 L_{4,1}^-, \\
\mathcal{I} [E_{\nu,n}^2 D_\nu E_{\nu,n}] &= -\frac{1}{2} L_0^- [L_2^-]^2 - \frac{7}{24} [L_0^-]^3 [L_1^+]^2 - \frac{1}{48} [L_0^-]^5 - \frac{1}{6} L_0^- [L_1^+]^4 \quad (\text{A.2.57}) \\
& + L_0^- L_1^+ L_3^+ - 2 L_0^- L_1^+ \zeta_3 + 4 L_{4,1}^- + 3 L_{3,2}^- + 8 L_{2,1,1,1}^-,
\end{aligned}$$

$$\begin{aligned}
\mathcal{I} [N^2 D_\nu E_{\nu,n}] &= \frac{3}{2} [L_0^-]^3 [L_1^+]^2 + \frac{1}{24} [L_0^-]^5 - 2 L_0^- [L_2^-]^2 - 4 L_{2,1}^- [L_0^-]^2 \quad (\text{A.2.58}) \\
& - 8 L_0^- L_1^+ L_3^+ + 16 L_0^- L_1^+ \zeta_3 + 48 L_{4,1}^- + 12 L_{3,2}^-,
\end{aligned}$$

$$\begin{aligned}
\mathcal{I} [V^2 D_\nu E_{\nu,n}] &= \frac{1}{2} L_0^- [L_2^-]^2 - \frac{3}{8} [L_0^-]^3 [L_1^+]^2 - \frac{1}{480} [L_0^-]^5 + L_{2,1}^- [L_0^-]^2 \quad (\text{A.2.59}) \\
& + 2 L_0^- L_1^+ L_3^+ - 4 L_0^- L_1^+ \zeta_3 - 12 L_{4,1}^- - 5 L_{3,2}^-,
\end{aligned}$$

$$\begin{aligned}
\mathcal{I} [V D_\nu^2 E_{\nu,n}] &= -\frac{1}{15} [L_0^-]^5 - 2 L_0^- [L_2^-]^2 - 2 L_0^- L_1^+ L_3^+ + 4 L_0^- L_1^+ \zeta_3 \quad (\text{A.2.60}) \\
& + 24 L_{4,1}^- + 12 L_{3,2}^-,
\end{aligned}$$

$$\begin{aligned}
\mathcal{I} [D_\nu^3 E_{\nu,n}] &= \frac{1}{2} [L_0^-]^3 [L_1^+]^2 + \frac{7}{40} [L_0^-]^5 + 6 L_0^- [L_2^-]^2 - 48 L_{4,1}^- \quad (\text{A.2.61}) \\
& - 24 L_{3,2}^-,
\end{aligned}$$

$$\mathcal{I} [\delta_{0,n}/(i\nu)^4] = \frac{1}{120} [L_0^-]^5. \quad (\text{A.2.62})$$

Basis of weight 5 with parity $(-, +)$:

$$\mathcal{I} [\tilde{F}_{6a}] = \frac{1}{12} L_2^- [L_0^-]^3 - L_4^- L_0^- + L_2^- L_{2,1}^- - L_1^+ L_{3,1}^+, \quad (\text{A.2.63})$$

$$\begin{aligned}
\mathcal{I} [V \tilde{F}_4] &= \frac{1}{48} L_2^- [L_0^-]^3 - \frac{1}{2} L_2^- L_0^- [L_1^+]^2 - \frac{3}{4} L_4^- L_0^- - L_2^- L_{2,1}^- \quad (\text{A.2.64}) \\
& + 3 L_0^- L_{2,1,1}^- + L_1^+ L_{3,1}^+,
\end{aligned}$$

$$\begin{aligned}
\mathcal{I} [N V E_{\nu,n}^2] &= -\frac{1}{48} L_2^- [L_0^-]^3 + \frac{1}{2} L_2^- L_0^- [L_1^+]^2 + \frac{3}{4} L_4^- L_0^- - 2 L_0^- L_{2,1,1}^- \quad (\text{A.2.65}) \\
& - 2 L_1^+ L_{3,1}^+,
\end{aligned}$$

$$\mathcal{I} [N^3 V] = \frac{3}{4} L_2^- [L_0^-]^3 - 5 L_4^- L_0^-, \quad (\text{A.2.66})$$

$$\mathcal{I} [N V^3] = \frac{3}{4} L_4^- L_0^- - \frac{7}{48} L_2^- [L_0^-]^3, \quad (\text{A.2.67})$$

$$\mathcal{I} [N E_{\nu,n} D_\nu E_{\nu,n}] = -\frac{5}{24} L_2^- [L_0^-]^3 + \frac{3}{2} L_4^- L_0^- - L_2^- L_0^- [L_1^+]^2 + 4 L_1^+ L_{3,1}^+. \quad (\text{A.2.68})$$

Basis of weight 5 with parity $(-, -)$:

$$\begin{aligned} \mathcal{I} [N E_{\nu,n}^3] &= \frac{5}{8} L_2^- L_1^+ [L_0^-]^2 - \frac{15}{2} L_4^- L_1^+ - \frac{1}{2} L_2^- L_3^+ - L_2^- [L_1^+]^3 \\ &\quad + 12 L_{2,1,1}^- L_1^+ \end{aligned} \quad (\text{A.2.69})$$

$$\begin{aligned} \mathcal{I} [E_{\nu,n} N^3] &= -\frac{1}{2} L_2^- L_1^+ [L_0^-]^2 + 2 L_4^- L_1^+ + 6 L_2^- L_3^+ - 16 L_2^- \zeta_3 \\ &\quad - 4 L_0^- L_{3,1}^+, \end{aligned} \quad (\text{A.2.70})$$

$$\mathcal{I} [E_{\nu,n} N V^2] = -\frac{1}{8} L_2^- L_1^+ [L_0^-]^2 + \frac{1}{2} L_4^- L_1^+ - \frac{1}{2} L_2^- L_3^+ + L_0^- L_{3,1}^+, \quad (\text{A.2.71})$$

$$\mathcal{I} [N V D_\nu E_{\nu,n}] = \frac{3}{4} L_2^- L_1^+ [L_0^-]^2 - 3 L_4^- L_1^+ + L_2^- L_3^+ + 4 L_2^- \zeta_3 - 2 L_0^- L_{3,1}^+ \quad (\text{A.2.72})$$

$$\mathcal{I} [N D_\nu^2 E_{\nu,n}] = -L_2^- L_1^+ [L_0^-]^2 + 12 L_4^- L_1^+ - 4 L_2^- L_3^+ - 16 L_2^- \zeta_3, \quad (\text{A.2.73})$$

$$\begin{aligned} \mathcal{I} [E_{\nu,n} \tilde{F}_4] &= \frac{1}{8} L_2^- L_1^+ [L_0^-]^2 + \frac{2}{3} L_2^- [L_1^+]^3 + \frac{1}{2} L_4^- L_1^+ + \frac{1}{2} L_2^- L_3^+ \\ &\quad - \frac{1}{2} L_0^- L_{3,1}^+ - 2 L_2^- \zeta_3 - 4 L_{2,1,1}^- L_1^+. \end{aligned} \quad (\text{A.2.74})$$

Appendix B

Leading singularities and off-shell conformal integrals

B.1 Asymptotic expansions of the Easy and Hard integrals

In this appendix we collect the asymptotic expansions of the different orientations of the Easy and Hard integrals in terms of harmonic polylogarithms. The results for $E_{14;23}$ and $H_{12;34}$ were already presented in section 3.3. The results for the other orientations are given below.

$$\begin{aligned} x_{13}^2 x_{24}^2 E_{12;34} = & \log^3 u \left[-\frac{1}{3x^2} (2H_{1,2} + H_{1,1,1}) + \frac{1}{3x} (H_{1,2} + H_{1,1,1}) \right] \\ & + \log^2 u \left[\frac{2}{x^2} (2H_{2,2} + H_{2,1,1} + 2H_{1,3} + H_{1,1,2}) \right. \\ & - \frac{1}{2x} \left(-4H_{2,2} - 3H_{2,1,1} - 4H_{1,3} - H_{1,2,1} - 4H_{1,1,2} \right) \Big] \\ & + \log u \left[\frac{1}{x^2} \left(-16H_{3,2} - 8H_{3,1,1} - 16H_{2,3} - 8H_{2,1,2} - 8H_{1,4} + 4H_{1,3,1} \right. \right. \\ & - 4H_{1,2,2} - H_{1,2,1,1} - 4H_{1,1,3} + 2H_{1,1,2,1} - H_{1,1,1,2} \\ & + \frac{1}{x} \left(8H_{3,2} + 5H_{3,1,1} + 8H_{2,3} + H_{2,2,1} + 6H_{2,1,2} + 4H_{1,4} - H_{1,3,1} \right. \\ & \left. \left. + 5H_{1,2,2} + H_{1,2,1,1} + 4H_{1,1,3} - 2H_{1,1,2,1} + H_{1,1,1,2} \right) \right] \end{aligned} \quad (\text{B.1.1})$$

$$\begin{aligned}
& + \frac{1}{x^2} \left(4\zeta_3 H_{1,2} + 2\zeta_3 H_{1,1,1} + 32H_{4,2} + 16H_{4,1,1} + 32 H_{3,3} + 16H_{3,1,2} \right. \\
& + 16H_{2,4} - 8H_{2,3,1} + 8H_{2,2,2} + 2 H_{2,2,1,1} + 8H_{2,1,3} - 4H_{2,1,2,1} + 2H_{2,1,1,2} \\
& - 8H_{1,4,1} + 4 H_{1,3,2} + 4H_{1,3,1,1} + 4H_{1,2,3} - 2H_{1,2,2,1} + 2H_{1,2,1,2} - 4 H_{1,1,3,1} \\
& + H_{1,1,2,1,1} - H_{1,1,1,2,1} \Big) + \frac{1}{x} \left(-4\zeta_3 H_{2,1} - 6\zeta_3 H_{1,2} - 2\zeta_3 H_{1,1,1} - 16 H_{4,2} \right. \\
& - 10H_{4,1,1} - 16H_{3,3} - 10H_{3,1,2} - 8H_{2,4} + 4H_{2,3,1} - 8 H_{2,2,2} - 2H_{2,2,1,1} \\
& - 6H_{2,1,3} + 4H_{2,1,2,1} - 2H_{2,1,1,2} + 2 H_{1,4,1} - 6H_{1,3,2} - 4H_{1,3,1,1} - 6H_{1,2,3} \\
& + 2H_{1,2,2,1} - 2H_{1,2,1,2} + 4H_{1,1,3,1} - H_{1,1,2,1,1} + H_{1,1,1,2,1} - 8\zeta_3 H_3 \\
& \left. + 20\zeta_5 H_1 \right) + \mathcal{O}(u) ,
\end{aligned}$$

$$\begin{aligned}
x_{13}^2 x_{24}^2 E_{13;24} &= \frac{\log u}{x} \left(H_{2,2,1} - H_{2,1,2} + H_{1,3,1} - H_{1,2,1,1} - H_{1,1,3} + H_{1,1,2,1} - 6 \zeta_3 H_2 \right) \\
&+ \frac{1}{x} \left(4\zeta_3 H_{2,1} - 2\zeta_3 H_{1,2} - 2H_{3,2,1} + 2H_{3,1,2} - 2H_{2,3,1} + H_{2,2,1,1} + 2H_{2,1,3} \right. \\
&- 2H_{2,1,2,1} + H_{2,1,1,2} - 4H_{1,4,1} + 3H_{1,3,1,1} + H_{1,2,1,2} + 4H_{1,1,4} - 2H_{1,1,3,1} \\
&- H_{1,1,2,2} - H_{1,1,2,1,1} - H_{1,1,1,3} + H_{1,1,1,2,1} + 12\zeta_3 H_3 \Big) + \mathcal{O}(u) , \quad (\text{B.1.2})
\end{aligned}$$

$$\begin{aligned}
x_{13}^4 x_{24}^4 H_{13;24} &= \log^3 u \left[\frac{1}{3x^2} \left(2H_{2,1} - H_{1,2} - H_{1,1,1} \right) + \frac{1}{3(1-x)x} \left(H_{2,1} - H_3 \right) \right] \quad (\text{B.1.3}) \\
&+ \log^2 u \left[\frac{1}{x^2} \left(-4H_{3,1} - 2H_{2,2} + 2H_{1,3} + 2H_{1,2,1} + 2H_{1,1,2} \right) \right. \\
&+ \frac{1}{(1-x)x} \left(-2H_{3,1} - H_{2,2} - H_{2,1,1} - H_{1,3} + H_{1,2,1} + 4H_4 \right) \Big] \\
&+ \log u \left[\frac{1}{x^2} \left(16H_{3,2} + 8H_{3,1,1} + 8H_{2,3} - 8H_{2,2,1} - 4H_{1,4} - 12H_{1,3,1} \right. \right. \\
&- 4H_{1,2,2} + 2H_{1,2,1,1} - 4H_{1,1,3} - 2H_{1,1,1,2} \Big) + \frac{1}{(1-x)x} \left(4H_{4,1} + 4H_{3,2} \right. \\
&+ 6H_{3,1,1} + 4H_{2,3} + 2H_{2,1,2} + 8H_{1,4} - 4H_{1,3,1} - 2H_{1,2,2} - 2H_{1,2,1,1} \\
&- 2H_{1,1,3} + 2H_{1,1,2,1} - 20H_5 \Big) \Big] + \frac{1}{x^2} \left(32\zeta_3 H_{2,1} - 16\zeta_3 H_{1,2} - 16\zeta_3 H_{1,1,1} \right. \\
&+ 64H_{5,1} - 32H_{4,2} - 32H_{4,1,1} - 24H_{3,3} + 16H_{3,2,1} - 16H_{3,1,2} - 24H_{2,4} \\
&+ 40H_{2,3,1} - 4H_{2,2,1,1} - 8H_{2,1,3} + 4H_{2,1,1,2} + 40H_{1,4,1} + 4H_{1,3,2}
\end{aligned}$$

$$\begin{aligned}
& - 8H_{1,3,1,1} - 4H_{1,2,3} + 4H_{1,2,2,1} - 4H_{1,2,1,2} + 8H_{1,1,1,3} \Big) \\
& + \frac{1}{(1-x)x} \Big(16\zeta_3 H_{2,1} - 4H_{4,2} - 12H_{4,1,1} - 4H_{3,3} - 12H_{3,2,1} - 8H_{3,1,2} \\
& - 12H_{2,4} + 4H_{2,3,1} + 2H_{2,2,1,1} - 4H_{2,1,2,1} + 2H_{2,1,1,2} - 20H_{1,5} + 4H_{1,4,1} \\
& + 4H_{1,3,2} + 6H_{1,3,1,1} + 4H_{1,2,3} + 2H_{1,2,1,2} + 8H_{1,1,4} - 4H_{1,1,3,1} - 2H_{1,1,2,2} \\
& - 2H_{1,1,2,1,1} - 2H_{1,1,1,3} + 2H_{1,1,1,2,1} - 16\zeta_3 H_3 + 40H_6 \Big) + \mathcal{O}(u), \\
\\
x_{13}^4 x_{24}^4 H_{14;23} &= \frac{\log^3 u}{3x} \left[\frac{1}{x} \left(2H_{2,1} - H_{1,2} + 2H_{1,1,1} \right) - 2H_{2,1} - H_{1,2} - 2H_{1,1,1} - H_3 \right] \\
& + \log^2 u \left[-\frac{2}{x^2} \left(2H_{3,1} + H_{2,2} - H_{1,3} + 2H_{1,2,1} + 2H_{1,1,2} \right) \right. \quad (\text{B.1.4}) \\
& + \frac{4}{x} \left(H_{3,1} + H_{2,2} + H_{1,3} + H_{1,2,1} + H_{1,1,2} + H_4 \right) \Big] \\
& + \log u \left[\frac{4}{x^2} \left(4H_{3,2} - 4H_{3,1,1} + 2H_{2,3} + 4H_{2,1,2} - H_{1,4} + 2H_{1,3,1} + 4H_{1,2,2} \right. \right. \\
& - 2H_{1,2,1,1} + 4H_{1,1,3} + 2H_{1,1,1,2} \Big) + \frac{4}{x} \left(2H_{4,1} + 4H_{3,2} - 2H_{3,1,1} + 4H_{2,3} \right. \\
& + 2H_{2,1,2} + 5H_{1,4} + 2H_{1,3,1} + 4H_{1,2,2} - 2H_{1,2,1,1} + 4H_{1,1,3} + 2H_{1,1,1,2} \\
& + 5H_5 \Big) \Big] + \frac{8}{x^2} \left(4\zeta_3 H_{2,1} - 2\zeta_3 H_{1,2} + 4\zeta_3 H_{1,1,1} + 8H_{5,1} - 4H_{4,2} + 8H_{4,1,1} \right. \\
& - 6H_{3,3} + 4H_{3,2,1} - 4H_{3,1,2} - 3H_{2,4} + 2H_{2,3,1} - 4H_{2,2,2} + 2H_{2,2,1,1} \\
& - 6H_{2,1,3} - 2H_{2,1,1,2} + 2H_{1,4,1} - 3H_{1,3,2} + 4H_{1,3,1,1} - 5H_{1,2,3} + 2H_{1,2,2,1} \\
& - 2H_{1,2,1,2} - 4H_{1,1,4} - 2H_{1,1,2,2} - 2H_{1,1,1,3} \Big) + \frac{8}{x} \left(-4\zeta_3 H_{2,1} - 2\zeta_3 H_{1,2} \right. \\
& - 4\zeta_3 H_{1,1,1} + 3H_{4,2} - 2H_{4,1,1} + 3H_{3,3} - 2H_{3,2,1} + 4H_{2,4} + 2H_{2,2,2} \\
& + 2H_{2,1,3} + 5H_{1,5} + 3H_{1,3,2} - 2H_{1,3,1,1} + 3H_{1,2,3} - 2H_{1,2,2,1} + 4H_{1,1,4} \\
& + 2H_{1,1,2,2} + 2H_{1,1,1,3} - 2\zeta_3 H_3 + 5H_6 \Big) + \mathcal{O}(u),
\end{aligned}$$

B.2 An integral formula for the Hard integral

We want to find an integral formula for pure functions which involve $x - \bar{x}$ in the symbol as well as $x, \bar{x}, 1 - x, 1 - \bar{x}$. We are interested in single-valued functions, i.e.

ones obeying the constraints on the discontinuities,

$$[\text{disc}_x - \text{disc}_{\bar{x}}]f(x, \bar{x}) = 0, \quad [\text{disc}_{1-x} - \text{disc}_{1-\bar{x}}]f(x, \bar{x}) = 0. \quad (\text{B.2.1})$$

and with no other discontinuities.

It will be sufficient for us to consider functions whose symbols have final letters drawn from a restricted set of letters,

$$\mathcal{S}(F) = \mathcal{S}(X) \otimes \frac{x}{\bar{x}} + \mathcal{S}(Y) \otimes \frac{1-x}{1-\bar{x}} + \mathcal{S}(Z) \otimes (x - \bar{x}). \quad (\text{B.2.2})$$

where X, Y, Z are single-valued functions of x, \bar{x} .

We will suppose also that the function F obeys $F(x, x) = 0$, as required to remove the poles at $x = \bar{x}$ present in the leading singularities of the conformal integrals. We therefore take $Z(x, x) = 0$ also. If F has a definite parity under $x \leftrightarrow \bar{x}$ then X and Y have the opposite parity while Z has the same parity.

The functions X, Y and Z are not independent of each other. Integrability (i.e. $d^2F = 0$) imposes the following restrictions,

$$dX \wedge d \log \frac{x}{\bar{x}} + dY \wedge d \log \frac{1-x}{1-\bar{x}} + dZ \wedge d \log(x - \bar{x}) = 0. \quad (\text{B.2.3})$$

We may then define the derivative of F w.r.t x to be

$$\partial_x F(x, \bar{x}) = \frac{X}{x} - \frac{Y}{1-x} + \frac{Z}{x - \bar{x}}, \quad (\text{B.2.4})$$

so that

$$F(x, \bar{x}) = \int_{\bar{x}}^x dt \left[\frac{X(t, \bar{x})}{t} - \frac{Y(t, \bar{x})}{1-t} + \frac{Z(t, \bar{x})}{t - \bar{x}} \right]. \quad (\text{B.2.5})$$

A trivial example is the Bloch-Wigner dilogarithm function, defined via,

$$F_2(x, \bar{x}) = \log x \bar{x} (H_1(x) - H_1(\bar{x})) - 2(H_2(x) - H_2(\bar{x})). \quad (\text{B.2.6})$$

It has a symbol of the form (B.2.2) where

$$X_1 = \log(1-x)(1-\bar{x}), \quad Y_1 = -\log x\bar{x} \quad Z_1 = 0. \quad (\text{B.2.7})$$

Thus we can write the integral formula (B.2.5) for F_2 .

B.2.1 Limits

We want to be able to calculate the limits of the functions to compare with the asymptotic expressions obtained in section 3.3. The formula (B.2.5) allows us to calculate the limit $\bar{x} \rightarrow 0$ (which means dropping any power suppressed terms in this limit). We may commute the limit and integration

$$\lim_{\bar{x} \rightarrow 0} F(x, \bar{x}) = \int_{\bar{x}}^x dt \lim_{\bar{x} \rightarrow 0} \left[\frac{X(t, \bar{x})}{t} - \frac{Y(t, \bar{x})}{1-t} + \frac{Z(t, \bar{x})}{t} \right]. \quad (\text{B.2.8})$$

In the second and third terms one may also set the lower limit of integration to zero. directly. In the first one should take care that contributions from $X(t, \bar{x})$ which do not vanish as $t \rightarrow 0$ produce extra logarithms of \bar{x} , beyond those explicitly appearing in the limit of X , as the lower limit approaches zero.

B.2.2 First non-trivial example (weight three)

The first example of a single-valued function whose symbol involves $x - \bar{x}$ is at weight three [106]. There is exactly one such function at this weight, i.e. all single-valued functions can be written in terms of this one and single-valued functions constructed from single-variable HPLs with arguments x and \bar{x} only. It obeys $F_3(x, \bar{x}) = -F_3(\bar{x}, x)$. The symbol takes the form (B.2.2) with

$$\begin{aligned} X_2 &= -\log(x\bar{x})(H_1(x) + H_1(\bar{x})) + \frac{1}{2}(H_1(x) + H_1(\bar{x}))^2, \\ Y_2 &= -\frac{1}{2}\log^2(x\bar{x}) + \log(x\bar{x})(H_1(x) + H_1(\bar{x})), \\ Z_2 &= 2\log x\bar{x}(H_1(x) - H_1(\bar{x})) - 4(H_2(x) - H_2(\bar{x})). \end{aligned} \quad (\text{B.2.9})$$

Note that X_2, Y_2 and Z_2 are single-valued and that Z_2 is proportional to the Bloch-Wigner dilogarithm (it is the only antisymmetric weight-two single-valued function so it had to be). They obey the integrability condition (B.2.3) so we can write the integral formula (B.2.5) to define the function F_3 .

We have constructed a single-valued function with a given symbol, but in fact this function is uniquely defined since there is no antisymmetric function of weight one which is single-valued which could be multiplied by ζ_2 and added to our result. Moreover, since it is antisymmetric in x and \bar{x} , we cannot add a constant term proportional to ζ_3 .

Looking at the limit $\bar{x} \rightarrow 0$ we find, following the discussion above,

$$\begin{aligned} \lim_{\bar{x} \rightarrow 0} F_3(x, \bar{x}) = & \frac{1}{2} \log^2 \bar{x} H_1(x) + \log \bar{x} (H_2(x) + H_{1,0}(x) - H_{1,1}(x)) \\ & - 3H_3(x) - H_{1,2}(x) + H_{2,0}(x) + H_{2,1}(x) + H_{1,0,0}(x) - H_{1,1,0}(x) \end{aligned} \quad (\text{B.2.10})$$

Starting from the original symbol for F_3 and taking the limit $\bar{x} \rightarrow 0$ we see that the above formula indeed correctly captures the limit.

B.2.3 Weight five example

We now give an example directly analogous to the weight-three example above but at weight five. The example we are interested in is symmetric $F_5(x, \bar{x}) = F_5(\bar{x}, x)$. It has a symbol of the canonical form (B.2.2) with

$$\begin{aligned} X_4(x, \bar{x}) &= (\mathcal{L}_{0,0,1,1} - \mathcal{L}_{1,1,0,0} - \mathcal{L}_{0,1,1,1} + \mathcal{L}_{1,1,1,0}), \\ Y_4(x, \bar{x}) &= (\mathcal{L}_{0,0,0,1} - \mathcal{L}_{1,0,0,0} - \mathcal{L}_{0,0,1,1} + \mathcal{L}_{1,1,0,0}), \\ Z_4(x, \bar{x}) &= (\mathcal{L}_{0,0,1,1} + \mathcal{L}_{1,1,0,0} - \mathcal{L}_{0,1,1,0} - \mathcal{L}_{1,0,0,1}). \end{aligned} \quad (\text{B.2.11})$$

The above functions are single-valued and obey the integrability condition and therefore define a single-valued function of two variables of weight five via the integral formula.

Taking the limit $\bar{x} \rightarrow 0$ we find

$$\begin{aligned}
\lim_{\bar{x} \rightarrow 0} F_5(x, \bar{x}) = & H_{1,1} \bar{H}_{0,0,0} + (H_{1,1,0} - H_{1,1,1}) \bar{H}_{0,0} \\
& + (-H_{3,1} + H_{2,1,1} + H_{1,1,0,0} - H_{1,1,1,0}) \bar{H}_0 \\
& - H_{1,4} - H_{2,3} + 2H_{4,1} + H_{1,3,1} - H_{3,1,0} - H_{3,1,1} \\
& + H_{2,1,1,0} + H_{1,1,0,0,0} - H_{1,1,1,0,0} + 2H_{1,1} \zeta_3. \tag{B.2.12}
\end{aligned}$$

This formula correctly captures the limit taken directly on the symbol of F_5 . This weight-five function plays a role in the construction of the Hard integral.

B.2.4 The function $H^{(a)}$ from the Hard integral

The function $H^{(a)}$ from the Hard integral is a weight-six symmetric function obeying the condition $H^{(a)}(x, x) = 0$. The symbol of $H^{(a)}$ is known but is not of the form (B.2.2). However, we can use shuffle relations to rewrite the symbol in terms of logarithms of u and v and functions which end with our preferred set of letters. We find the symbol can be represented by a function of the form

$$\begin{aligned}
H^{(a)}(1-x, 1-\bar{x}) &= (2H_{0,0}(u) + 4H_0(u)H_0(v) + 8H_{0,0}(v))(\mathcal{L}_{0,0,1,1} + \mathcal{L}_{1,1,0,0} - \mathcal{L}_{0,1,1,0} - \mathcal{L}_{1,0,0,1}) \\
&\quad - 8F_5(H_0(u) + 2H_0(v)) + F_6. \tag{B.2.13}
\end{aligned}$$

Here F_5 is the weight-five function defined in section B.2.3. The function F_6 is now one whose symbol is of the form (B.2.2), where the functions X_5, Y_5 and Z_5 take the form

$$\begin{aligned}
X_5 = & 20\mathcal{L}_{0,0,0,1,1} + 12\mathcal{L}_{0,0,1,1,0} - 32\mathcal{L}_{0,0,1,1,1} - 8\mathcal{L}_{0,1,0,1,1} - 12\mathcal{L}_{0,1,1,0,0} - 8\mathcal{L}_{0,1,1,0,1} \\
& + 16\mathcal{L}_{0,1,1,1,1} - 8\mathcal{L}_{1,0,0,1,1} + 8\mathcal{L}_{1,0,1,1,0} - 20\mathcal{L}_{1,1,0,0,0} + 8\mathcal{L}_{1,1,0,0,1} + 8\mathcal{L}_{1,1,0,1,0} \\
& + 32\mathcal{L}_{1,1,1,0,0} - 16\mathcal{L}_{1,1,1,1,0} - 16\mathcal{L}_{1,1} \zeta_3, \tag{B.2.14} \\
Y_5 = & 20\mathcal{L}_{0,0,0,0,1} - 32\mathcal{L}_{0,0,0,1,1} - 8\mathcal{L}_{0,0,1,1,0} + 16\mathcal{L}_{0,0,1,1,1} - 8\mathcal{L}_{0,1,0,0,1} + \mathcal{L}_{0,1,1,0,0} \\
& - 20\mathcal{L}_{1,0,0,0,0} + 8\mathcal{L}_{1,0,0,1,0} + 16\mathcal{L}_{1,0,0,1,1} + 8\mathcal{L}_{1,0,1,0,0} + 32\mathcal{L}_{1,1,0,0,0} - 16\mathcal{L}_{1,1,0,0,1}
\end{aligned}$$

$$-16\mathcal{L}_{1,1,1,0,0} - 16\mathcal{L}_{1,0}\zeta_3 + 64\mathcal{L}_{1,1}\zeta_3. \quad (\text{B.2.15})$$

$$Z_5 = 32F_5. \quad (\text{B.2.16})$$

Note that the ζ_3 terms have been chosen in such a way the the functions X_5, Y_5 and Z_5 obey the integrability condition (B.2.3). The integral formula for F_6 based on the above functions will give a single-valued function with the correct symbol, i.e. one such that $H^{(a)}$ defined in eq. (B.2.13) has the correct symbol and is single-valued.

We recall that the Hard integral takes the form

$$H_{14;23} = \frac{1}{x_{13}^4 x_{24}^4} \left[\frac{H^{(a)}(1-x, 1-\bar{x})}{(x-\bar{x})^2} + \frac{H^{(b)}(1-x, 1-\bar{x})}{(1-x\bar{x})(x-\bar{x})} \right]. \quad (\text{B.2.17})$$

Calculating the limit $\bar{x} \rightarrow 0$ we find that $H^{(a)}$ reproduces the terms proportional to $1/x^2$ in the limit exactly, including the zeta terms. Note that in this limit the contributions of $H^{(a)}$ and $H^{(b)}$ are distinguishable since the harmonic polylogarithms come with different powers of x . Since there are no functions of weight four or lower which are symmetric in x and \bar{x} and which vanish at $x = \bar{x}$ and which vanish in the limit $\bar{x} \rightarrow 0$, we conclude that $H^{(a)}$ defined in eq. (B.2.13) is indeed the function. Comparing numerically with the formula obtained in section 3.5 we indeed find agreement to at least five significant figures.

B.3 A symbol-level solution of the four-loop differential equation

In this appendix we sketch an alternative approach to the evaluation of the four-loop integral. More precisely, we will show how the function $I^{(4)}$ can be determined using symbols and the coproduct on multiple polylogarithms. We start from the differential equation (3.7.17), which we recall here for convenience,

$$\partial_x \partial_{\bar{x}} \hat{f}(x, \bar{x}) = -\frac{1}{(1-x\bar{x})x\bar{x}} E_1(x, \bar{x}) - \frac{1}{(1-x\bar{x})} E_2(x, \bar{x}), \quad (\text{B.3.1})$$

where we used the abbreviations $E_1(x, \bar{x}) = E(1 - x, 1 - \bar{x})$ and $E_2(x, \bar{x}) = E(1 - 1/x, 1 - 1/\bar{x})$. We now act with the symbol map \mathcal{S} on the differential equation, and we get

$$\partial_x \partial_{\bar{x}} \mathcal{S}[\hat{f}(x, \bar{x})] = -\frac{1}{(1 - x\bar{x})x\bar{x}} \mathcal{S}[E_1(x, \bar{x})] - \frac{1}{(1 - x\bar{x})} \mathcal{S}[E_2(x, \bar{x})], \quad (\text{B.3.2})$$

where the differential operators act on tensors only in the last entry, e.g.,

$$\partial_x [a_1 \otimes \dots \otimes a_n] = [\partial_x \log a_n] a_1 \otimes \dots \otimes a_{n-1}, \quad (\text{B.3.3})$$

and similarly for $\partial_{\bar{x}}$. It is easy to see that the tensor

$$S_1 = \mathcal{S}[E_1(x, \bar{x})] \otimes \left(1 - \frac{1}{x\bar{x}}\right) \otimes (x\bar{x}) + \mathcal{S}[E_2(x, \bar{x})] \otimes (1 - x\bar{x}) \otimes (x\bar{x}) \quad (\text{B.3.4})$$

solves the equation (B.3.2). However, S_1 is not integrable in the pair of entries (6,7), and so S_1 is not yet the symbol of a solution of the differential equation. In order to obtain an integrable solution, we need to add a solution to the homogeneous equation associated to eq. (B.3.2). The homogeneous solution can easily be obtained by writing down the most general tensor S_2 with entries drawn from the set $\{x, \bar{x}, 1 - x, 1 - \bar{x}, 1 - x\bar{x}\}$ that has the correct symmetries and satisfies the first entry condition and

$$\partial_x \partial_{\bar{x}} S_2 = 0. \quad (\text{B.3.5})$$

In addition, we may assume that S_2 satisfies the integrability condition in all factors of the tensor product except for the pair of entries (6,7), because S_1 satisfies this condition as well. The symbol of the solution of the differential equation is then given by $S_1 + S_2$, subject to the constraint that the sum is integrable. It turns out

that there is a unique solution, which can be written in the schematic form

$$\begin{aligned} \mathcal{S}[\hat{f}(x, \bar{x})] &= s_1^- \otimes u \otimes u + s_2^- \otimes v \otimes u + s_3^- \otimes \frac{1-x}{1-\bar{x}} \otimes \frac{x}{\bar{x}} + s_4^+ \otimes \frac{x}{\bar{x}} \otimes u \\ &\quad + s_5^+ \otimes u \otimes \frac{x}{\bar{x}} + s_6^+ \otimes \frac{1-x}{1-\bar{x}} \otimes u + s_7^+ \otimes v \otimes \frac{x}{\bar{x}} + s_8^- \otimes \frac{x}{\bar{x}} \otimes \frac{x}{\bar{x}} \\ &\quad + s_9^- \otimes (1-u) \otimes u, \end{aligned} \quad (\text{B.3.6})$$

where s_i^\pm are (integrable) tensor that have all their entries drawn from the set $\{x, \bar{x}, 1-x, 1-\bar{x}\}$ and the superscript refers to the parity under an exchange of x and \bar{x} .

The form (B.3.6) of the symbol of $\hat{f}(x, \bar{x})$ allows us to make the following more refined ansatz: as the s_i^\pm are symbols of SVHPLs, and using the fact that the symbol is the maximal iteration of the coproduct, we conclude that there are linear combinations $f_i^\pm(x, \bar{x})$ of SVHPLs of weight six (including products of zeta values and SVHPLs of lower weight) such that $\mathcal{S}[f_i^\pm(x, \bar{x})] = s_i^\pm$ and

$$\begin{aligned} \Delta_{6,1,1}[\hat{f}(x, \bar{x})] &= f_1^-(x, \bar{x}) \otimes \log u \otimes \log u + f_2^-(x, \bar{x}) \otimes \log v \otimes \log u \\ &\quad + f_3^-(x, \bar{x}) \otimes \log \frac{1-x}{1-\bar{x}} \otimes \log \frac{x}{\bar{x}} + f_4^+(x, \bar{x}) \otimes \log \frac{x}{\bar{x}} \otimes \log u \\ &\quad + f_5^+(x, \bar{x}) \otimes \log u \otimes \log \frac{x}{\bar{x}} + f_6^+(x, \bar{x}) \otimes \log \frac{1-x}{1-\bar{x}} \otimes \log u \\ &\quad + f_7^+(x, \bar{x}) \otimes \log v \otimes \log \frac{x}{\bar{x}} + f_8^-(x, \bar{x}) \otimes \log \frac{x}{\bar{x}} \otimes \log \frac{x}{\bar{x}} \\ &\quad + f_9^-(x, \bar{x}) \otimes \log(1-u) \otimes u. \end{aligned} \quad (\text{B.3.7})$$

The coefficients of the terms proportional to zeta values and SVHPLs of lower weight (which were not captured by the symbol) can easy be fixed by appealing to the differential equation, written in the form¹

$$(\text{id} \otimes \partial_x \otimes \partial_{\bar{x}}) \Delta_{6,1,1}[\hat{f}(x, \bar{x})] = -\frac{1}{(1-x\bar{x})x\bar{x}} E_1(x, \bar{x}) \otimes 1 \otimes 1 - \frac{1}{(1-x\bar{x})} E_2(x, \bar{x}) \otimes 1 \otimes 1. \quad (\text{B.3.8})$$

The expression (B.3.7) has the advantage that it captures more information about the function $\hat{f}(x, \bar{x})$ than the symbol alone. In particular, we can use eq. (B.3.7) to

¹We stress that differential operators act in the last factor of the coproduct, just like for the symbol.

derive an iterated integral representation for $\hat{f}(x, \bar{x})$ with respect to x only. To see how this works, first note that there must be functions $A^\pm(x, \bar{x})$, that are respectively even and odd under an exchange of x and \bar{x} , such that

$$\Delta_{7,1}[\hat{f}(x, \bar{x})] = A^-(x, \bar{x}) \otimes \log u + A^+(x, \bar{x}) \otimes \log \frac{x}{\bar{x}}. \quad (\text{B.3.9})$$

with

$$\begin{aligned} \Delta_{6,1}[A^-(x, \bar{x})] &= f_1^-(x, \bar{x}) \otimes \log u + f_2^-(x, \bar{x}) \otimes \log v + f_4^+(x, \bar{x}) \otimes \log \frac{x}{\bar{x}} \\ &\quad + f_6^+(x, \bar{x}) \otimes \log \frac{1-x}{1-\bar{x}} + f_9^-(x, \bar{x}) \otimes \log(1-u), \\ \Delta_{6,1}[A^+(x, \bar{x})] &= f_3^-(x, \bar{x}) \otimes \log \frac{1-x}{1-\bar{x}} + f_5^+(x, \bar{x}) \otimes \log u \\ &\quad + f_7^+(x, \bar{x}) \otimes \log v + f_8^-(x, \bar{x}) \otimes \log \frac{x}{\bar{x}}. \end{aligned} \quad (\text{B.3.10})$$

The (6,1) component of the coproduct of $A^+(x, \bar{x})$ does not involve $\log(1-u)$, and so it can entirely be expressed in terms of SVHPLs. We can thus easily obtain the result for $A^+(x, \bar{x})$ by writing down the most general linear combination of SVHPLs of weight seven that are even under an exchange of x and \bar{x} and fix the coefficients by requiring the (6,1) component of the coproduct of the linear combination to agree with eq. (B.3.10). In this way we can fix $A^+(x, \bar{x})$ up to zeta values of weight seven (which are integration constants of the original differential equation).

The coproduct of $A^-(x, \bar{x})$, however, does involve $\log(1-u)$, and so it cannot be expressed in terms of SVHPLs alone. We can nevertheless derive a first-order differential equation for $A^-(x, \bar{x})$. We find

$$\begin{aligned} \partial_x A^-(x, \bar{x}) &= \frac{1}{x} [f_1^-(x, \bar{x}) + f_4^+(x, \bar{x})] - \frac{1}{1-x} [f_2^-(x, \bar{x}) + f_6^+(x, \bar{x})] \\ &\quad - \frac{\bar{x}}{1-x\bar{x}} f_9^-(x, \bar{x}) \\ &\equiv K(x, \bar{x}). \end{aligned} \quad (\text{B.3.11})$$

The solution to this equation is

$$A^-(x, \bar{x}) = h(\bar{x}) + \int_{\bar{x}}^x dt K(t, \bar{x}), \quad (\text{B.3.12})$$

where $h(\bar{x})$ is an arbitrary function of \bar{x} . The integral can easily be performed in terms of multiple polylogarithms. Antisymmetry of $A^-(x, \bar{x})$ under an exchange of x and \bar{x} requires $h(\bar{x})$ to vanish identically, because

$$A^-(x, \bar{x}) = h(\bar{x}) + \int_{\bar{x}}^x dt \partial_t A^-(t, \bar{x}) = h(\bar{x}) + A^-(x, \bar{x}) - A^-(\bar{x}, \bar{x}) = h(\bar{x}) + A^-(x, \bar{x}). \quad (\text{B.3.13})$$

We thus obtain a unique solution for $A^-(x, \bar{x})$.

Having obtained the analytic expressions for $A^\pm(x, \bar{x})$ (up to the integration constants in $A^+(x, \bar{x})$), we can easily obtain a first-order differential equation for $\hat{f}(x, \bar{x})$,

$$\partial_x \hat{f}(x, \bar{x}) = \frac{1}{x} [A^-(x, \bar{x}) + A^+(x, \bar{x})]. \quad (\text{B.3.14})$$

The solution reads

$$\hat{f}(x, \bar{x}) = \int_{\bar{x}}^x \frac{dt}{t} [A^-(t, \bar{x}) + A^+(t, \bar{x})]. \quad (\text{B.3.15})$$

The integral can again easily be performed in terms of multiple polylogarithms and the antisymmetry of $\hat{f}(x, \bar{x})$ under an exchange of x and \bar{x} again excludes any arbitrary function of \bar{x} only. The solution to eq. (B.3.14) is however not yet unique, because of the integration constants in $A^+(x, \bar{x})$, and we are left with three free coefficients of the form,

$$(c_1 \zeta_7 + c_2 \zeta_5 \zeta_2 + c_3 \zeta_4 \zeta_3) \log \frac{x}{\bar{x}}. \quad (\text{B.3.16})$$

The free coefficients can be fixed using the requirement that $\hat{f}(x, \bar{x})$ be single-valued (see the discussion in section 3.7). Alternatively, they can be fixed by requiring that $\hat{f}(x, \bar{x})$ be odd under inversion of (x, \bar{x}) and vanish at $x = \bar{x}$. We checked that the resulting function agrees analytically with the result derived in section 3.7.

Appendix C

Hexagon functions and the three-loop remainder function

C.1 Multiple polylogarithms and the coproduct

C.1.1 Multiple polylogarithms

Multiple polylogarithms are a general class of multi-variable iterated integrals, of which logarithms, polylogarithms, harmonic polylogarithms, and various other iterated integrals are special cases. They are defined recursively by $G(z) = 1$, and,

$$G(a_1, \dots, a_n; z) = \int_0^z \frac{dt}{t - a_1} G(a_2, \dots, a_n; t), \quad G(\vec{0}_p; z) = \frac{\ln^p z}{p!}, \quad (\text{C.1.1})$$

where we have introduced the vector notation $\vec{a}_n = (\underbrace{a, \dots, a}_n)$.

For special values of the weight vector (a_1, \dots, a_n) , multiple polylogarithms reduce to simpler functions. For example, if $a \neq 0$,

$$G(\vec{0}_{p-1}, a; z) = -\text{Li}_p(z/a), \quad G(\vec{0}_p, \vec{a}_q; z) = (-1)^q S_{p,q}(z/a), \quad (\text{C.1.2})$$

where $S_{p,q}$ is the Nielsen polylogarithm. More generally, if $a_i \in \{-1, 0, 1\}$, then

$$G(a_1, \dots, a_n; z) = (-1)^{w_1} H_{a_1, \dots, a_n}(z), \quad (\text{C.1.3})$$

where w_1 is the number of a_i equal to one.

Multiple polylogarithms are not all algebraically independent. One set of relations, known as the *shuffle relations*, derive from the definition (C.1.1) in terms of iterated integrals,

$$G(w_1; z) G(w_2; z) = \sum_{w \in w_1 \amalg w_2} G(w; z), \quad (\text{C.1.4})$$

where $w_1 \amalg w_2$ is the set of mergers of the sequences w_1 and w_2 that preserve their relative ordering. Radford's theorem [161] allows one to solve all of the identities (C.1.4) simultaneously in terms of a restricted subset of multiple polylogarithms $\{G(l_w; z)\}$, where l_w is a *Lyndon word*. The Lyndon words are those words w such that for every decomposition into two words $w = \{u, v\}$, the left word is smaller (based on some ordering) than the right, i.e. $u < v$.

One may choose whichever ordering is convenient; for our purposes, we choose an ordering so that zero is smallest. In this case, no zeros appear on the right of a weight vector, except in the special case of the logarithm, $G(0; z) = \ln z$. Therefore, we may adopt a Lyndon basis and assume without loss of generality that $a_n \neq 0$ in $G(a_1, \dots, a_n, z)$. Referring to eq. (C.1.1), it is then possible to rescale all integration variables by a common factor and obtain the following identity,

$$G(c a_1, \dots, c a_n; c z) = G(a_1, \dots, a_n; z), \quad a_n \neq 0, c \neq 0. \quad (\text{C.1.5})$$

Specializing to the case $c = 1/z$, we see that the algebra of multiple polylogarithms is spanned by $\ln z$ and $G(a_1, \dots, a_n; 1)$ where $a_n \neq 0$. This observation allows us to establish a one-to-one correspondence between multiple polylogarithms and particular multiple nested sums, provided those sums converge. In particular, if for $|x_i| < 1$ we define,

$$\text{Li}_{m_1, \dots, m_k}(x_1, \dots, x_k) = \sum_{n_1 < n_2 < \dots < n_k} \frac{x_1^{n_1} x_2^{n_2} \dots x_k^{n_k}}{n_1^{m_1} n_2^{m_2} \dots n_k^{m_k}}, \quad (\text{C.1.6})$$

then,

$$\mathrm{Li}_{m_1, \dots, m_k}(x_1, \dots, x_k) = (-1)^k G\left(\underbrace{0, \dots, 0}_{m_k-1}, \frac{1}{x_k}, \dots, \underbrace{0, \dots, 0}_{m_1-1}, \frac{1}{x_1 \cdots x_k}; 1\right). \quad (\text{C.1.7})$$

Equation (C.1.7) is easily established by expanding the measure $dt/(t-a_i)$ in eq. (C.1.1) in a series and integrating. A convergent series expansion for $G(a_1, \dots, a_n; z)$ exists if $|z| \leq |a_i|$ for all i ; otherwise, the integral representation gives the proper analytic continuation.

The relation to multiple sums endows the space of multiple polylogarithms with some additional structure. In particular, the freedom to change summation variables in the multiple sums allows one to establish *shuffle* or *quasi-shuffle* relations,

$$\mathrm{Li}_{\vec{m}_1}(\vec{x})\mathrm{Li}_{\vec{m}_2}(\vec{y}) = \sum_{\vec{n}} \mathrm{Li}_{\vec{n}}(\vec{z}). \quad (\text{C.1.8})$$

The precise formula for \vec{n} and \vec{z} in terms of \vec{m}_1 , \vec{m}_2 , \vec{x} , and \vec{y} is rather cumbersome, but can be written explicitly; see, e.g., ref. [65]. For small depth, however, the shuffle relations are quite simple. For example,

$$\mathrm{Li}_a(x)\mathrm{Li}_b(y) = \mathrm{Li}_{a,b}(x, y) + \mathrm{Li}_{b,a}(y, x) + \mathrm{Li}_{a+b}(xy). \quad (\text{C.1.9})$$

Beyond the shuffle and stuffle identities, there are additional relations between multiple polylogarithms with transformed arguments and weight vectors. For example, one such class of identities follows from Hölder convolution [65],

$$G(a_1, \dots, a_n; 1) = \sum_{k=0}^n (-1)^k G\left(1 - a_k, \dots, 1 - a_1; 1 - \frac{1}{p}\right) G\left(a_{k+1}, \dots, a_n; \frac{1}{p}\right), \quad (\text{C.1.10})$$

which is valid for any nonzero p whenever $a_1 \neq 1$ and $a_n \neq 0$.

One way to study identities among multiple polylogarithms is via the symbol,

which is defined recursively as,

$$\begin{aligned} \mathcal{S}(G(a_{n-1}, \dots, a_1; a_n)) &= \sum_{i=1}^{n-1} \left[\mathcal{S}(G(a_{n-1}, \dots, \hat{a}_i, \dots, a_1; a_n)) \otimes (a_i - a_{i+1}) \right. \\ &\quad \left. - \mathcal{S}(G(a_{n-1}, \dots, \hat{a}_i, \dots, a_1; a_n)) \otimes (a_i - a_{i-1}) \right], \end{aligned} \quad (\text{C.1.11})$$

While the symbol has the nice property that all relations result from simple algebraic manipulations, it has the drawback that its kernel contains all transcendental constants. To obtain information about these constants, one needs some more powerful machinery.

C.1.2 The Hopf algebra of multiple polylogarithms

When equipped with the shuffle product (C.1.4), the space of multiple polylogarithms forms an algebra, graded by weight. In ref. [162], it was shown how to further equip the space with a coproduct so that it forms a bialgebra, and, moreover, with an antipode so that it forms a Hopf algebra. The weight of the multiple polylogarithms also defines a grading on the Hopf algebra. In the following we will let \mathcal{A} denote the Hopf algebra and \mathcal{A}_n the weight- n subspace, so that,

$$\mathcal{A} = \bigoplus_{n=0}^{\infty} \mathcal{A}_n. \quad (\text{C.1.12})$$

The coproduct is defined most naturally on a slight variant of eq. (C.1.1),

$$I(a_0; a_1, \dots, a_n; a_{n+1}) = \int_{a_0}^{a_{n+1}} \frac{dt}{t - a_n} I(a_0; a_1, \dots, a_{n-1}; t). \quad (\text{C.1.13})$$

The two definitions differ only in the ordering of indices and the choice of basepoint. However, as shown in ref. [64], it is possible to reexpress any multiple polylogarithm with a generic basepoint as a sum of terms with basepoint zero. This manipulation

is trivial at weight one, where we have,

$$I(a_0; a_1; a_2) = I(0; a_1; a_2) - I(0; a_1; a_0) = G(a_1; a_2) - G(a_1; a_0). \quad (\text{C.1.14})$$

To build up further such relations at higher weights, one must simply apply the lower-weight identity to the integrand in eq. (C.1.13). In this way, it is easy to convert between the two different notations for multiple polylogarithms.

The coproduct on multiple polylogarithms is given by [162],

$$\Delta(I(a_0; a_1, \dots, a_n; a_{n+1})) = \sum_{0 < i_1 < \dots < i_k = n} I(a_0; a_{i_1}, \dots, a_{i_k}; a_{n+1}) \otimes \left[\prod_{p=0}^k I(a_{i_p}; a_{i_p+1}, \dots, a_{i_{p+1}-1}; a_{i_{p+1}}) \right]. \quad (\text{C.1.15})$$

Strictly speaking, this definition is only valid when the a_i are nonzero and distinct; otherwise, one must introduce a regulator to avoid divergent integrals. We refer the reader to refs. [64, 162] for these technical details.

It is straightforward to check a number of important properties of the coproduct. First, it respects the grading of \mathcal{A} in the following sense. If $G_n \in \mathcal{A}_n$, then,

$$\Delta(G_n) = \sum_{p+q=n} \Delta_{p,q}(G_n), \quad (\text{C.1.16})$$

where $\Delta_{p,q} \in \mathcal{A}_p \otimes \mathcal{A}_q$. Next, if we extend multiplication to tensor products so that it acts on each component separately,

$$(a_1 \otimes a_2) \cdot (b_1 \otimes b_2) = (a_1 \cdot b_1) \otimes (a_2 \cdot b_2), \quad (\text{C.1.17})$$

one can verify the compatibility of the product and the coproduct,

$$\Delta(a \cdot b) = \Delta(a) \cdot \Delta(b). \quad (\text{C.1.18})$$

Finally, the coproduct is coassociative,

$$(\text{id} \otimes \Delta)\Delta = (\Delta \otimes \text{id})\Delta, \quad (\text{C.1.19})$$

meaning that one may iterate the coproduct in any order and always reach a unique result.

This last property allows one to unambiguously define components of the coproduct corresponding to all integer compositions of the weight. Consider $G_n \in \mathcal{A}_n$ and a particular integer composition of n , $\{w_1, \dots, w_k\}$, such that $w_i > 0$ and $\sum_{i=1}^k w_i = n$. The component of the coproduct corresponding to this composition, $\Delta_{w_1, \dots, w_k}(G_n)$, is defined as the unique element of the $(k-1)$ -fold iterated coproduct in the space $\mathcal{A}_{w_1} \otimes \dots \otimes \mathcal{A}_{w_k}$. For our purposes it is sufficient to consider $k=2$, although other components have been useful in other contexts.

Consider the weight- n function $f^{(n)}(z_1, \dots, z_m)$ of m complex variables z_1, \dots, z_m with symbol,

$$\mathcal{S}(f^{(n)}) = \sum_{i_1, \dots, i_n} c_{i_1, \dots, i_n} \phi_{i_1} \otimes \dots \otimes \phi_{i_n}. \quad (\text{C.1.20})$$

The monodromy of $f^{(n)}$ around the point $z_k = z_0$ is encoded by the first entry of the symbol,

$$\mathcal{S}(\mathcal{M}_{z_k=z_0} f^{(n)}) = \sum_{i_1, \dots, i_n} \mathcal{M}_{z_k=z_0}(\ln \phi_{i_1}) c_{i_1, \dots, i_n} \phi_{i_2} \otimes \dots \otimes \phi_{i_n}, \quad (\text{C.1.21})$$

where $\mathcal{M}_{z_k=z_0}(\ln \phi_{i_1})$ is defined in eq. (4.6.15), and we have ignored higher powers of $(2\pi i)$ (see section 4.6). Similarly, derivatives act on the last entry of the symbol,

$$\mathcal{S}\left(\frac{\partial}{\partial z_k} f^{(n)}\right) = \sum_{i_1, \dots, i_n} c_{i_1, \dots, i_n} \phi_{i_1} \otimes \dots \otimes \phi_{i_{n-1}} \left(\frac{\partial}{\partial z_k} \ln \phi_{i_n}\right). \quad (\text{C.1.22})$$

In the same way, the monodromy operator acts only the first component of the coproduct and the derivative operator only on the last component,

$$\begin{aligned}\Delta(\mathcal{M}_{z_k=z_0} f^{(n)}) &= (\mathcal{M}_{z_k=z_0} \otimes \text{id}) \Delta(f^{(n)}), \\ \Delta\left(\frac{\partial}{\partial z_k} f^{(n)}\right) &= \left(\text{id} \otimes \frac{\partial}{\partial z_k}\right) \Delta(f^{(n)}).\end{aligned}\tag{C.1.23}$$

One may trivially extend the definition of the coproduct to include odd ζ values,

$$\Delta(\zeta_{2n+1}) = 1 \otimes \zeta_{2n+1} + \zeta_{2n+1} \otimes 1 \tag{C.1.24}$$

but including even ζ values and factors of π is more subtle. It was argued in ref. [63,64] that it is consistent to define,

$$\Delta(\zeta_{2n}) = \zeta_{2n} \otimes 1 \quad \text{and} \quad \Delta(\pi) = \pi \otimes 1. \tag{C.1.25}$$

Equation (C.1.25) implies that powers of π are absent from all factors of the coproduct except for the first one. Finally, we remark that the symbol may be recovered from the maximally-iterated coproduct if we drop all factors of π ,

$$\mathcal{S} \equiv \Delta_{1,\dots,1} \bmod \pi. \tag{C.1.26}$$

C.2 Complete basis of hexagon functions through weight five

We present the basis of hexagon functions through weight five by providing their $\{n-1, 1\}$ coproduct components. For a hexagon function F of weight n , we write,

$$\Delta_{n-1,1}(F) \equiv \sum_{i=1}^3 F^{u_i} \otimes \ln u_i + F^{1-u_i} \otimes \ln(1-u_i) + F^{y_i} \otimes \ln y_i, \quad (\text{C.2.1})$$

where the nine functions $\{F^{u_i}, F^{1-u_i}, F^{y_i}\}$ are of weight $n-1$ and completely specify the $\{n-1, 1\}$ component of the coproduct. They also specify all of the first derivatives of F ,

$$\begin{aligned} \left. \frac{\partial F}{\partial u} \right|_{v,w} &= \frac{F^u}{u} - \frac{F^{1-u}}{1-u} + \frac{1-u-v-w}{u\sqrt{\Delta}} F^{y_u} + \frac{1-u-v+w}{(1-u)\sqrt{\Delta}} F^{y_v} \\ &\quad + \frac{1-u+v-w}{(1-u)\sqrt{\Delta}} F^{y_w}, \\ \sqrt{\Delta} y_u \left. \frac{\partial F}{\partial y_u} \right|_{y_v, y_w} &= (1-u)(1-v-w)F^u - u(1-v)F^v - u(1-w)F^w \\ &\quad - u(1-v-w)F^{1-u} + uv F^{1-v} + uw F^{1-w} + \sqrt{\Delta} F^{y_u}. \end{aligned} \quad (\text{C.2.2})$$

The other derivatives can be obtained from the cyclic images of eq. (C.2.2). These derivatives, in turn, define integral representations for the function. Generically, we define the function F by (see eq. (4.4.10)),

$$F(u, v, w) = F(1, 1, 1) - \sqrt{\Delta} \int_1^u \frac{du_t}{v_t[u(1-w) + (w-u)u_t]} \frac{\partial F}{\partial \ln y_v}(u_t, v_t, w_t), \quad (\text{C.2.3})$$

where,

$$v_t = 1 - \frac{(1-v)u_t(1-u_t)}{u(1-w) + (w-u)u_t}, \quad w_t = \frac{(1-u)wu_t}{u(1-w) + (w-u)u_t}. \quad (\text{C.2.4})$$

We choose $F(1, 1, 1) = 0$ for all functions except for the special case $\Omega^{(2)}(1, 1, 1) = -6\zeta_4$. Other integral representations of the function also exist, as discussed in section 4.4.1.

We remark that the hexagon functions $\tilde{\Phi}_6$, G , N and O are totally symmetric under exchange of all three arguments; $\Omega^{(2)}$ is symmetric under exchange of its first two arguments; F_1 is symmetric under exchange of its last two arguments; and H_1 , J_1 and K_1 are symmetric under exchange of their first and third arguments.

C.2.1 $\tilde{\Phi}_6$

The only parity-odd hexagon function of weight three is $\tilde{\Phi}_6$. We may write the $\{2, 1\}$ component of its coproduct as,

$$\begin{aligned} \Delta_{2,1}(\tilde{\Phi}_6) = & \tilde{\Phi}_6^u \otimes \ln u + \tilde{\Phi}_6^v \otimes \ln v + \tilde{\Phi}_6^w \otimes \ln w \\ & + \tilde{\Phi}_6^{1-u} \otimes \ln(1-u) + \tilde{\Phi}_6^{1-v} \otimes \ln(1-v) + \tilde{\Phi}_6^{1-w} \otimes \ln(1-w) \\ & + \tilde{\Phi}_6^{y_u} \otimes \ln y_u + \tilde{\Phi}_6^{y_v} \otimes \ln y_v + \tilde{\Phi}_6^{y_w} \otimes \ln y_w, \end{aligned} \quad (\text{C.2.5})$$

where

$$\tilde{\Phi}_6^u = \tilde{\Phi}_6^v = \tilde{\Phi}_6^w = \tilde{\Phi}_6^{1-u} = \tilde{\Phi}_6^{1-v} = \tilde{\Phi}_6^{1-w} = 0. \quad (\text{C.2.6})$$

Furthermore, $\tilde{\Phi}_6$ is totally symmetric, which implies,

$$\tilde{\Phi}_6^{y_v} = \tilde{\Phi}_6^{y_u}(v, w, u), \quad \text{and} \quad \tilde{\Phi}_6^{y_w} = \tilde{\Phi}_6^{y_u}(w, u, v). \quad (\text{C.2.7})$$

The one independent function, $\tilde{\Phi}_6^{y_u}$, may be identified with a finite, four-dimensional one-loop hexagon integral, $\Omega^{(1)}$, which is parity-even and of weight two,

$$\tilde{\Phi}_6^{y_u} = -\Omega^{(1)}(v, w, u) = -H_2^u - H_2^v - H_2^w - \ln v \ln w + 2\zeta_2. \quad (\text{C.2.8})$$

C.2.2 $\Omega^{(2)}$

Up to cyclic permutations, the only non-HPL parity-even hexagon function of weight three is $\Omega^{(2)}$. We may write the $\{3, 1\}$ component of its coproduct as,

$$\begin{aligned} \Delta_{3,1}(\Omega^{(2)}) &= \Omega^{(2),u} \otimes \ln u + \Omega^{(2),v} \otimes \ln v + \Omega^{(2),w} \otimes \ln w \\ &\quad + \Omega^{(2),1-u} \otimes \ln(1-u) + \Omega^{(2),1-v} \otimes \ln(1-v) + \Omega^{(2),1-w} \otimes \ln(1-w) \\ &\quad + \Omega^{(2),y_u} \otimes \ln y_u + \Omega^{(2),y_v} \otimes \ln y_v + \Omega^{(2),y_w} \otimes \ln y_w, \end{aligned} \tag{C.2.9}$$

where the vanishing components are

$$\Omega^{(2),w} = \Omega^{(2),1-w} = \Omega^{(2),y_w} = 0, \tag{C.2.10}$$

and the nonvanishing components obey,

$$\Omega^{(2),v} = -\Omega^{(2),1-v} = -\Omega^{(2),1-u}(u \leftrightarrow v) = \Omega^{(2),u}(u \leftrightarrow v) \quad \text{and} \quad \Omega^{(2),y_v} = \Omega^{(2),y_u}. \tag{C.2.11}$$

The two independent functions are

$$\Omega^{(2),y_u} = -\frac{1}{2}\tilde{\Phi}_6, \tag{C.2.12}$$

and

$$\begin{aligned} \Omega^{(2),u} &= H_3^u + H_{2,1}^v - H_{2,1}^w - \frac{1}{2} \ln(uw/v) (H_2^u + H_2^w - 2\zeta_2) + \frac{1}{2} \ln(uv/w) H_2^v \\ &\quad + \frac{1}{2} \ln u \ln v \ln(v/w). \end{aligned} \tag{C.2.13}$$

C.2.3 F_1

Up to cyclic permutations, the only parity-odd function of weight four is F_1 . We may write the $\{4, 1\}$ component of its coproduct as,

$$\begin{aligned} \Delta_{3,1}(F_1) = & F_1^u \otimes \ln u + F_1^v \otimes \ln v + F_1^w \otimes \ln w \\ & + F_1^{1-u} \otimes \ln(1-u) + F_1^{1-v} \otimes \ln(1-v) + F_1^{1-w} \otimes \ln(1-w) \\ & + F_1^{y_u} \otimes \ln y_u + F_1^{y_v} \otimes \ln y_v + F_1^{y_w} \otimes \ln y_w, \end{aligned} \quad (\text{C.2.14})$$

where

$$F_1^{y_w} = F_1^{y_v}(v \leftrightarrow w) \quad \text{and} \quad F_1^u = F_1^v = F_1^w = F_1^{1-v} = F_1^{1-w} = 0. \quad (\text{C.2.15})$$

Of the three independent functions, one is parity odd, $F_1^{1-u} = \tilde{\Phi}_6$, and two are parity even,

$$F_1^{y_u} = -2H_3^u + 2\zeta_3 \quad (\text{C.2.16})$$

and

$$F_1^{y_v} = -2H_3^u - 2H_{2,1}^w + \ln w \left(H_2^u - H_2^v - H_2^w + 2\zeta_2 \right) + 2\zeta_3. \quad (\text{C.2.17})$$

In ref. [71] the pure function entering the parity-odd part of the six-point NMHV ratio function was determined to be

$$\tilde{V} = \frac{1}{8}(\tilde{V}_X + \tilde{f}), \quad (\text{C.2.18})$$

where $\tilde{V}_X + \tilde{f}$ satisfied an integral of the form (4.4.10) with

$$\begin{aligned} \frac{\partial(\tilde{V}_X + \tilde{f})}{\partial \ln y_v} &= \tilde{Z}(u, v, w) \\ &= 2 \left[H_3^u - H_{2,1}^u - \ln u \left(H_2^u + H_2^v - 2\zeta_2 - \frac{1}{2} \ln^2 w \right) \right] - (u \leftrightarrow w). \end{aligned} \quad (\text{C.2.19})$$

This integral can be expressed in terms of F_1 and $\tilde{\Phi}_6$ as,

$$\tilde{V}_X + \tilde{f} = -F_1(u, v, w) + F_1(w, u, v) + \ln(u/w) \tilde{\Phi}_6(u, v, w). \quad (\text{C.2.20})$$

C.2.4 G

The $\{4, 1\}$ component of the coproduct of the parity-odd weight five function G can be written as,

$$\begin{aligned} \Delta_{4,1}(G) = & G^u \otimes \ln u + G^v \otimes \ln v + G^w \otimes \ln w \\ & + G^{1-u} \otimes \ln(1-u) + G^{1-v} \otimes \ln(1-v) + G^{1-w} \otimes \ln(1-w) \\ & + G^{y_u} \otimes \ln y_u + G^{y_v} \otimes \ln y_v + G^{y_w} \otimes \ln y_w, \end{aligned} \quad (\text{C.2.21})$$

where

$$G^u = G^v = G^w = G^{1-u} = G^{1-v} = G^{1-w} = 0. \quad (\text{C.2.22})$$

Furthermore, G is totally symmetric. In particular,

$$G^{y_v}(u, v, w) = G^{y_u}(v, w, u), \quad \text{and} \quad G^{y_w}(u, v, w) = G^{y_u}(w, u, v). \quad (\text{C.2.23})$$

Therefore, it suffices to specify the single independent function, G^{y_u} ,

$$\begin{aligned} G^{y_u} = & -2 \left(H_{3,1}^u + H_{3,1}^v + H_{3,1}^w - \ln w H_{2,1}^v - \ln v H_{2,1}^w \right) \\ & + \frac{1}{2} \left(H_2^u + H_2^v + H_2^w + \ln v \ln w \right)^2 - \frac{1}{2} \ln^2 v \ln^2 w - 4\zeta_4. \end{aligned} \quad (\text{C.2.24})$$

C.2.5 H_1

The function $H_1(u, v, w)$ is parity-odd and has weight five. We may write the $\{4, 1\}$ component of its coproduct as,

$$\begin{aligned} \Delta_{4,1}(H_1(u, v, w)) = & \hat{H}_1^u \otimes \ln u + \hat{H}_1^v \otimes \ln v + \hat{H}_1^w \otimes \ln w \\ & + H_1^{1-u} \otimes \ln(1-u) + H_1^{1-v} \otimes \ln(1-v) + H_1^{1-w} \otimes \ln(1-w) \\ & + H_1^{y_u} \otimes \ln y_u + H_1^{y_v} \otimes \ln y_v + H_1^{y_w} \otimes \ln y_w, \end{aligned} \quad (\text{C.2.25})$$

where we put a hat on \hat{H}_1^u , *etc.*, to avoid confusion with the HPLs with argument $1 - u$. The independent functions are \hat{H}_1^u , $\hat{H}_1^{y_u}$, and $\hat{H}_1^{y_v}$,

$$\begin{aligned}\hat{H}_1^u &= -\frac{1}{4}\left(F_1(u, v, w) - \ln u \tilde{\Phi}_6\right) - (u \leftrightarrow w), \\ \hat{H}_1^{y_u} &= \left[\frac{1}{2}(\Omega^{(2)}(v, w, u) + \Omega^{(2)}(w, u, v)) + \frac{1}{2}(H_4^u + H_4^v) - \frac{1}{2}(H_{3,1}^u - H_{3,1}^v) \right. \\ &\quad - \frac{3}{2}(H_{2,1,1}^u + H_{2,1,1}^v) - \left(\ln u + \frac{1}{2}\ln(w/v)\right)H_3^u - \frac{1}{2}\ln v H_3^v - \frac{1}{2}\ln(w/v)H_{2,1}^u \\ &\quad - \frac{1}{2}\ln v H_{2,1}^v - \frac{1}{4}((H_2^u)^2 + (H_2^v)^2) + \frac{1}{4}(\ln^2 u - \ln^2(w/v))H_2^u \\ &\quad \left. - \frac{1}{8}\ln^2 u \ln^2(w/v) - \zeta_2\left(H_2^u + \frac{1}{2}\ln^2 u\right) + 3\zeta_4\right] + (u \leftrightarrow w), \\ \hat{H}_1^{y_v} &= \Omega^{(2)}(w, u, v).\end{aligned}\tag{C.2.26}$$

Of the remaining functions, two vanish, $\hat{H}_1^v = \hat{H}_1^{1-v} = 0$, and the others are simply related,

$$\hat{H}_1^{1-u} = \hat{H}_1^w = -\hat{H}_1^{1-w} = -\hat{H}_1^u, \quad \text{and} \quad \hat{H}_1^{y_w} = \hat{H}_1^{y_u}.\tag{C.2.27}$$

C.2.6 J_1

We may write the $\{4, 1\}$ component of the coproduct of the parity-odd weight-five function $J_1(u, v, w)$ as,

$$\begin{aligned}\Delta_{4,1}(J_1(u, v, w)) &= J_1^u \otimes \ln u + J_1^v \otimes \ln v + J_1^w \otimes \ln w \\ &\quad + J_1^{1-u} \otimes \ln(1-u) + J_1^{1-v} \otimes \ln(1-v) + J_1^{1-w} \otimes \ln(1-w) \\ &\quad + J_1^{y_u} \otimes \ln y_u + J_1^{y_v} \otimes \ln y_v + J_1^{y_w} \otimes \ln y_w,\end{aligned}\tag{C.2.28}$$

where the independent functions are J_1^u , $J_1^{y_u}$, and $J_1^{y_v}$,

$$\begin{aligned}
J_1^u &= \left[-F_1(u, v, w) + \ln u \tilde{\Phi}_6 \right] - (u \leftrightarrow w), \\
J_1^{y_u} &= \left[-\Omega^{(2)}(w, u, v) - 6H_4^u + 2 \left(H_{3,1}^u - H_{3,1}^v + H_{2,1,1}^u + 2(2 \ln u - \ln(w/v)) H_3^u \right) + \frac{1}{2} (H_2^v)^2 \right. \\
&\quad + 2 \ln(w/v) H_{2,1}^u - \ln u (\ln u - 2 \ln(w/v)) H_2^u - \frac{1}{2} \ln^2(u/w) H_2^v - \frac{1}{3} \ln v \ln^3 u \\
&\quad + \frac{1}{4} \ln^2 u \ln^2 w + \zeta_2 \left(8H_2^u + 2H_2^v + \ln^2(u/w) + 4 \ln u \ln v \right) - 14 \zeta_4 + (u \leftrightarrow w) \Big] \\
&\quad - \ln(u/w) \left(4H_{2,1}^v + 2 \ln v H_2^v - \frac{1}{3} \ln v \ln^2(u/w) \right), \\
J_1^{y_v} &= \left[-4 \left(H_4^u - H_{3,1}^u + H_{3,1}^v + H_{2,1,1}^u - \ln u (H_3^u - H_{2,1}^u) \right) - 2 \ln^2 u H_2^u \right. \\
&\quad + \left(H_2^v - 2 \ln u \ln(u/w) \right) H_2^v - \frac{1}{3} \ln u \ln w \left(\ln^2(u/w) + \frac{1}{2} \ln u \ln w \right) \\
&\quad \left. + 8 \zeta_2 \left(H_2^u + \frac{1}{2} \ln^2 u \right) - 8 \zeta_4 \right] + (u \leftrightarrow w).
\end{aligned} \tag{C.2.29}$$

Of the remaining functions, two vanish, $J_1^v = J_1^{1-v} = 0$, and the others are simply related,

$$J_1^{1-u} = J_1^w = -J_1^{1-w} = -J_1^u, \quad \text{and} \quad J_1^{y_w} = J_1^{y_u}(u \leftrightarrow w). \tag{C.2.30}$$

C.2.7 K_1

The final parity-odd function of weight five is $K_1(u, v, w)$. We may write the $\{4, 1\}$ component of its coproduct as,

$$\begin{aligned}
\Delta_{4,1}(K_1(u, v, w)) &= K_1^u \otimes \ln u + K_1^v \otimes \ln v + K_1^w \otimes \ln w \\
&\quad + K_1^{1-u} \otimes \ln(1-u) + K_1^{1-v} \otimes \ln(1-v) + K_1^{1-w} \otimes \ln(1-w) \\
&\quad + K_1^{y_u} \otimes \ln y_u + K_1^{y_v} \otimes \ln y_v + K_1^{y_w} \otimes \ln y_w,
\end{aligned} \tag{C.2.31}$$

where the independent functions are K_1^u , $K_1^{y_u}$, and $K_1^{y_v}$,

$$\begin{aligned}
K_1^u &= -F_1(w, u, v) + \ln w \tilde{\Phi}_6, \\
K_1^{y_u} &= -2(H_{3,1}^u + H_{3,1}^v + H_{3,1}^w) - 2\ln(v/w)H_3^u + 2\ln u H_3^w + 2\ln v H_{2,1}^w + 2\ln(uw)H_{2,1}^v \\
&\quad + \frac{1}{2}(H_2^u + H_2^v + H_2^w - 2\zeta_2)^2 + (\ln u \ln(v/w) + \ln v \ln w)(H_2^u + H_2^v - 2\zeta_2) \\
&\quad - (\ln u \ln(vw) - \ln v \ln w)H_2^w - \ln u \ln v \ln^2 w - 2\zeta_3 \ln(uw/v) + \zeta_4, \\
K_1^{y_v} &= \left[-4H_{3,1}^u - 2\ln(u/w)H_3^u + 2\ln(uw)H_{2,1}^u + \ln^2 u H_2^u \right. \\
&\quad \left. + 2\left(H_2^u + \frac{1}{2}\ln^2 u\right)\left(H_2^v - \frac{1}{2}\ln^2 w - 2\zeta_2\right) + 3\zeta_4 \right] + (u \leftrightarrow w).
\end{aligned} \tag{C.2.32}$$

Of the remaining functions, two vanish, $K_1^v = K_1^{1-v} = 0$, and the others are simply related,

$$K_1^{1-u} = -K_1^u, \quad K_1^w = -K_1^{1-w} = K_1^u(u \leftrightarrow w) \quad \text{and} \quad K_1^{y_w} = K_1^{y_u}(u \leftrightarrow w). \tag{C.2.33}$$

C.2.8 M_1

The $\{4, 1\}$ component of the coproduct of the parity-even weight-five function M_1 can be written as,

$$\begin{aligned}
\Delta_{4,1}(M_1) &= M_1^u \otimes \ln u + M_1^v \otimes \ln v + M_1^w \otimes \ln w \\
&\quad + M_1^{1-u} \otimes \ln(1-u) + M_1^{1-v} \otimes \ln(1-v) + M_1^{1-w} \otimes \ln(1-w) \tag{C.2.34} \\
&\quad + M_1^{y_u} \otimes \ln y_u + M_1^{y_v} \otimes \ln y_v + M_1^{y_w} \otimes \ln y_w,
\end{aligned}$$

where,

$$M_1^{1-v} = -M_1^w, \quad \text{and} \quad M_1^u = M_1^v = M_1^{1-w} = M_1^{y_u} = M_1^{y_v} = 0. \tag{C.2.35}$$

The three independent functions consist of one parity-odd function,

$$M_1^{yw} = -F_1(u, v, w), \quad (\text{C.2.36})$$

and two parity even functions,

$$\begin{aligned} M_1^{1-u} = & \left[-\Omega^{(2)}(u, v, w) + 2 \ln v \left(H_3^u + H_{2,1}^u \right) + 2 \ln u H_{2,1}^v \right. \\ & - \left(H_2^u - \frac{1}{2} \ln^2 u \right) \left(H_2^v + \frac{1}{2} \ln^2 v \right) + \ln u \ln v \left(H_2^u + H_2^v + H_2^w - 2\zeta_2 \right) \\ & \left. + 2\zeta_3 \ln w - (v \leftrightarrow w) \right] + \Omega^{(2)}(v, w, u) + 2H_4^w \\ & + 2H_{3,1}^w - 6H_{2,1,1}^w - 2 \ln w \left(H_3^w + H_{2,1}^w \right) - \left(H_2^v + \frac{1}{2} \ln^2 v \right) \left(H_2^w + \frac{1}{2} \ln^2 w \right) \\ & - (H_2^w)^2 + \left(\ln^2(v/w) - 4\zeta_2 \right) H_2^u + 2\zeta_3 \ln u + 6\zeta_4, \end{aligned} \quad (\text{C.2.37})$$

and,

$$\begin{aligned} M_1^w = & -2 \left(H_{3,1}^u - H_{3,1}^v - H_{3,1}^w + \ln(uv/w) (H_3^u - \zeta_3) + \ln w H_{2,1}^v + \ln v H_{2,1}^w \right) \\ & - \frac{1}{2} \left(H_2^u - H_2^v - H_2^w - \ln v \ln w + 2\zeta_2 \right)^2 + \frac{1}{2} \ln^2 v \ln^2 w + 5\zeta_4. \end{aligned} \quad (\text{C.2.38})$$

C.2.9 N

The $\{4, 1\}$ component of the coproduct of the parity-even weight-five function N can be written as,

$$\begin{aligned} \Delta_{4,1}(N) = & N^u \otimes \ln u + N^v \otimes \ln v + N^w \otimes \ln w \\ & + N^{1-u} \otimes \ln(1-u) + N^{1-v} \otimes \ln(1-v) + N^{1-w} \otimes \ln(1-w) \\ & + N^{yu} \otimes \ln y_u + N^{yv} \otimes \ln y_v + N^{yw} \otimes \ln y_w, \end{aligned} \quad (\text{C.2.39})$$

where,

$$N^{1-u} = -N^u, \quad N^{1-v} = -N^v, \quad N^{1-w} = -N^w, \quad \text{and} \quad N^{y_u} = N^{y_v} = N^{y_w} = 0. \quad (\text{C.2.40})$$

Furthermore, N is totally symmetric. In particular,

$$N^v(u, v, w) = N^u(v, w, u), \quad \text{and} \quad N^w(u, v, w) = N^u(w, u, v). \quad (\text{C.2.41})$$

Therefore, it suffices to specify the single independent function, N^u ,

$$\begin{aligned} N^u = & \left[\Omega^{(2)}(v, w, u) + 2H_4^v + 2H_{3,1}^v - 6H_{2,1,1}^v - 2 \ln v \left(H_3^v + H_{2,1}^v \right) - (H_2^v)^2 \right. \\ & \left. - \left(H_2^v + \frac{1}{2} \ln^2 v \right) \left(H_2^w + \frac{1}{2} \ln^2 w \right) + 6\zeta_4 \right] + (v \leftrightarrow w). \end{aligned} \quad (\text{C.2.42})$$

C.2.10 O

The $\{4, 1\}$ component of the coproduct of the parity-even weight-five function O can be written as,

$$\begin{aligned} \Delta_{4,1}(O) = & O^u \otimes \ln u + O^v \otimes \ln v + O^w \otimes \ln w \\ & + O^{1-u} \otimes \ln(1-u) + O^{1-v} \otimes \ln(1-v) + O^{1-w} \otimes \ln(1-w) \\ & + O^{y_u} \otimes \ln y_u + O^{y_v} \otimes \ln y_v + O^{y_w} \otimes \ln y_w, \end{aligned} \quad (\text{C.2.43})$$

where

$$O^u = O^v = O^w = O^{y_u} = O^{y_v} = O^{y_w} = 0. \quad (\text{C.2.44})$$

Furthermore, O is totally symmetric. In particular,

$$O^{1-v}(u, v, w) = O^{1-u}(v, w, u), \quad \text{and} \quad O^{1-w}(u, v, w) = O^{1-u}(w, u, v). \quad (\text{C.2.45})$$

Therefore, it suffices to specify the single independent function, O^{1-u} ,

$$\begin{aligned}
O^{1-u} = & \left[-\Omega^{(2)}(u, v, w) + 2H_{3,1}^v + (3 \ln u - 2 \ln w) H_{2,1}^v + 2 \ln v H_{2,1}^u - \frac{1}{2}(H_2^v)^2 \right. \\
& + \ln u \ln v (H_2^u + H_2^v) + \ln(u/v) \ln w H_2^v + \frac{1}{2} \ln^2 v H_2^u - \frac{1}{2} \ln^2 w H_2^v \\
& \left. + \frac{1}{4} \ln^2 u \ln^2 v + (v \leftrightarrow w) \right] + \Omega^{(2)}(v, w, u) - 2H_2^v H_2^w - \ln v \ln w H_2^u \\
& - \frac{1}{4} \ln^2 v \ln^2 w + 2\zeta_2 \left(H_2^v + H_2^w - \ln u \ln(vw) + \ln v \ln w \right) - 6\zeta_4.
\end{aligned} \tag{C.2.46}$$

C.2.11 Q_{ep}

The $\{4, 1\}$ component of the coproduct of the parity-even weight-five function Q_{ep} can be written as,

$$\begin{aligned}
\Delta_{4,1}(Q_{\text{ep}}) = & Q_{\text{ep}}^u \otimes \ln u + Q_{\text{ep}}^v \otimes \ln v + Q_{\text{ep}}^w \otimes \ln w \\
& + Q_{\text{ep}}^{1-u} \otimes \ln(1-u) + Q_{\text{ep}}^{1-v} \otimes \ln(1-v) + Q_{\text{ep}}^{1-w} \otimes \ln(1-w) \quad (\text{C.2.47}) \\
& + Q_{\text{ep}}^{y_u} \otimes \ln y_u + Q_{\text{ep}}^{y_v} \otimes \ln y_v + Q_{\text{ep}}^{y_w} \otimes \ln y_w,
\end{aligned}$$

where,

$$Q_{\text{ep}}^{1-v} = -Q_{\text{ep}}^v, \quad Q_{\text{ep}}^{1-w} = -Q_{\text{ep}}^w, \quad Q_{\text{ep}}^{y_w} = Q_{\text{ep}}^{y_v} \quad \text{and} \quad Q_{\text{ep}}^u = Q_{\text{ep}}^{1-u} = Q_{\text{ep}}^{y_u} = 0. \tag{C.2.48}$$

The three independent functions consist of one parity-odd function, $Q_{\text{ep}}^{y_v}$, which is fairly simple,

$$Q_{\text{ep}}^{y_v} = \frac{1}{64} \left[F_1(u, v, w) + F_1(v, w, u) - 2F_1(w, u, v) + (\ln u - 3 \ln v) \tilde{\Phi}_6 \right],$$

and two parity-even functions, Q_{ep}^v and Q_{ep}^w , which are complicated by the presence of a large number of HPLs,

$$\begin{aligned}
Q_{\text{ep}}^v = & \frac{1}{32}\Omega^{(2)}(u, v, w) + \frac{1}{16}\Omega^{(2)}(v, w, u) + \frac{1}{32}H_4^u + \frac{3}{32}H_4^v + \frac{1}{16}H_4^w - \frac{3}{32}H_{3,1}^u \\
& - \frac{3}{32}H_{2,1,1}^u - \frac{9}{64}H_{2,1,1}^v - \frac{3}{16}H_{2,1,1}^w + \frac{1}{32}\ln u H_3^v - \frac{1}{16}\ln u H_3^w - \frac{3}{32}\ln u H_{2,1}^v \\
& + \frac{1}{16}\ln u H_{2,1}^w + \frac{1}{32}\ln v H_3^u - \frac{3}{32}\ln v H_3^v - \frac{7}{32}\ln v H_{2,1}^u + \frac{1}{16}\ln v H_{2,1}^w \\
& - \frac{1}{32}\ln w H_3^u - \frac{1}{32}\ln w H_3^v + \frac{3}{32}\ln w H_{2,1}^u + \frac{3}{32}\ln w H_{2,1}^v - \frac{1}{16}\ln w H_{2,1}^w \\
& + \frac{1}{32}(H_2^u)^2 - \frac{3}{128}(H_2^v)^2 - \frac{1}{64}H_2^v H_2^w + \frac{1}{64}(H_2^w)^2 + \frac{1}{64}\ln^2 u H_2^u \\
& + \frac{1}{64}\ln^2 u H_2^w - \frac{3}{32}\ln u \ln v H_2^u - \frac{3}{32}\ln u \ln v H_2^v - \frac{1}{32}\ln u \ln v H_2^w \\
& + \frac{1}{32}\ln u \ln w H_2^u + \frac{1}{32}\ln u \ln w H_2^w - \frac{1}{16}\ln^2 v H_2^u + \frac{3}{128}\ln^2 v H_2^v \\
& - \frac{1}{128}\ln^2 v H_2^w + \frac{1}{16}\ln v \ln w H_2^u + \frac{3}{32}\ln v \ln w H_2^v + \frac{1}{32}\ln v \ln w H_2^w \\
& - \frac{1}{128}\ln^2 w H_2^v - \frac{1}{128}\ln^2 u \ln^2 v + \frac{1}{64}\ln^2 u \ln v \ln w - \frac{3}{64}\ln u \ln^2 v \ln w \\
& + \frac{5}{256}\ln^2 v \ln^2 w - \zeta_2 \left(\frac{1}{8}H_2^u + \frac{11}{128}H_2^v + \frac{1}{16}H_2^w + \frac{1}{32}\ln^2 u - \frac{3}{16}\ln u \ln v \right. \\
& \left. + \frac{1}{16}\ln u \ln w - \frac{3}{128}\ln^2 v + \frac{3}{16}\ln v \ln w \right) + \frac{7}{32}\zeta_3 \ln v,
\end{aligned}
\tag{C.2.49}$$

$$\begin{aligned}
Q_{\text{ep}}^w = & -\frac{1}{32}\Omega^{(2)}(v, w, u) + \frac{1}{32}\Omega^{(2)}(w, u, v) + \frac{1}{32}H_4^u - \frac{1}{32}H_4^v + \frac{3}{32}H_{3,1}^u - \frac{3}{32}H_{3,1}^v \\
& - \frac{3}{32}H_{2,1,1}^u + \frac{3}{32}H_{2,1,1}^v + \frac{1}{32}\ln u H_3^v - \frac{1}{16}\ln u H_3^w - \frac{1}{32}\ln u H_{2,1}^v - \frac{1}{32}\ln v H_3^u \\
& + \frac{1}{16}\ln v H_3^w - \frac{3}{32}\ln v H_{2,1}^u + \frac{1}{8}\ln v H_{2,1}^v + \frac{1}{32}\ln w H_3^u - \frac{1}{64}\ln w H_3^v \\
& - \frac{1}{32}\ln w H_{2,1}^u + \frac{3}{64}\ln w H_{2,1}^v - \frac{1}{64}(H_2^u)^2 + \frac{1}{64}(H_2^v)^2 + \frac{1}{16}H_2^v H_2^w \\
& + \frac{1}{64}\ln^2 u H_2^u + \frac{1}{64}\ln^2 u H_2^v - \frac{1}{16}\ln u \ln v H_2^u - \frac{1}{16}\ln u \ln v H_2^v \\
& - \frac{1}{32}\ln u \ln w H_2^v + \frac{3}{64}\ln^2 v H_2^u + \frac{3}{64}\ln^2 v H_2^v + \frac{1}{32}\ln^2 v H_2^w \\
& - \frac{1}{32}\ln v \ln w H_2^u + \frac{3}{64}\ln v \ln w H_2^v - \frac{1}{64}\ln^2 w H_2^u + \frac{1}{64}\ln^2 w H_2^v \\
& + \frac{1}{64}\ln^2 u \ln v \ln w - \frac{1}{128}\ln^2 u \ln^2 w - \frac{3}{64}\ln u \ln^2 v \ln w + \frac{3}{128}\ln^3 v \ln w \\
& + \frac{1}{128}\ln^2 v \ln^2 w + \zeta_2 \left(\frac{1}{16}H_2^u - \frac{1}{16}H_2^v + \frac{1}{128}\ln^2 v \ln^2 w - \frac{1}{16}H_2^w \right. \\
& \left. - \frac{1}{32}\ln^2 u + \frac{1}{8}\ln u \ln v - \frac{3}{32}\ln^2 v \right) - \frac{1}{16}\zeta_3 \ln w.
\end{aligned} \tag{C.2.50}$$

C.2.12 Relation involving M_1 and Q_{ep}

There is one linear relation between the six permutations of M_1 and the six permutations of Q_{ep} . The linear combination involves the totally antisymmetric linear combination of the S_3 permutations of both M_1 and Q_{ep} . It can be written as,

$$\left[\left(M_1(u, v, w) - \frac{64}{3}Q_{\text{ep}}(u, v, w) + 2\ln u \Omega^{(2)}(u, v, w) + E_{\text{rat}}(u, v) \right) - (u \leftrightarrow v) \right] + \text{cycl.} = 0, \tag{C.2.51}$$

where $E_{\text{rat}}(u, v)$ is constructed purely from ordinary HPLs,

$$\begin{aligned}
E_{\text{rat}}(u, v) = & \left(H_2^v + \frac{1}{2}\ln^2 v \right) \left(\frac{5}{3}(H_3^u + H_{2,1}^u) + \frac{1}{3}\ln u H_2^u - \frac{1}{2}\ln^3 u \right) \\
& - 4H_2^v \left(2H_{2,1}^u + \ln u H_2^u \right) \\
& - 2\ln v \left(H_4^u + 5H_{3,1}^u - 3H_{2,1,1}^u - \frac{1}{2}(H_2^u)^2 + \ln u (H_3^u - H_{2,1}^u) + 4\zeta_2 H_2^u \right).
\end{aligned} \tag{C.2.52}$$

Because of this relation, the images of M_1 and Q_{ep} under the S_3 symmetry group together provide only 11, not 12, of the 13 non-HPL basis functions for \mathcal{H}_5^+ . The totally symmetric functions N and O provide the remaining two basis elements.

C.3 Coproduct of R_{ep}

We may write the $\{5, 1\}$ component of the coproduct of the parity-even weight six-function R_{ep} as,

$$\begin{aligned} \Delta_{5,1}(R_{\text{ep}}) &= R_{\text{ep}}^u \otimes \ln u + R_{\text{ep}}^v \otimes \ln v + R_{\text{ep}}^w \otimes \ln w \\ &\quad + R_{\text{ep}}^{1-u} \otimes \ln(1-u) + R_{\text{ep}}^{1-v} \otimes \ln(1-v) + R_{\text{ep}}^{1-w} \otimes \ln(1-w) \\ &\quad + R_{\text{ep}}^{y_u} \otimes \ln y_u + R_{\text{ep}}^{y_v} \otimes \ln y_v + R_{\text{ep}}^{y_w} \otimes \ln y_w, \end{aligned} \quad (\text{C.3.1})$$

where,

$$\begin{aligned} R_{\text{ep}}^v &= -R_{\text{ep}}^{1-v} = -R_{\text{ep}}^{1-u}(u \leftrightarrow v) = R_{\text{ep}}^u(u \leftrightarrow v), \\ R_{\text{ep}}^{y_v} &= R_{\text{ep}}^{y_u}, \quad \text{and} \quad R_{\text{ep}}^w = R_{\text{ep}}^{1-w} = R_{\text{ep}}^{y_w} = 0. \end{aligned} \quad (\text{C.3.2})$$

The two independent functions may be written as,

$$\begin{aligned} R_{\text{ep}}^{y_u} &= \frac{1}{32} \left\{ -H_1(u, v, w) - 3H_1(v, w, u) - H_1(w, u, v) \right. \\ &\quad + \frac{3}{4} (J_1(u, v, w) + J_1(v, w, u) + J_1(w, u, v)) \\ &\quad + \left[-4(H_2^u + H_2^v) - \ln^2 u - \ln^2 v + \ln^2 w \right. \\ &\quad \left. \left. + 2 \left(\ln u \ln v - (\ln u + \ln v) \ln w \right) + 22\zeta_2 \right] \tilde{\Phi}_6 \right\}, \end{aligned} \quad (\text{C.3.3})$$

and,

$$\begin{aligned} R_{\text{ep}}^u &= -\frac{1}{3} \left(2(Q_{\text{ep}}(u, v, w) - Q_{\text{ep}}(u, w, v) + Q_{\text{ep}}(v, w, u)) + Q_{\text{ep}}(v, u, w) - 3Q_{\text{ep}}(w, v, u) \right) \\ &\quad + \frac{1}{32} \left[M_1(u, v, w) - M_1(v, u, w) + \left(5(\ln u - \ln v) + 4 \ln w \right) \Omega^{(2)}(u, v, w) \right. \\ &\quad \left. - (3 \ln u + \ln v - 2 \ln w) \Omega^{(2)}(v, w, u) - (\ln u + 3 \ln v - 4 \ln w) \Omega^{(2)}(w, u, v) \right] \\ &\quad + R_{\text{ep, rat}}^u, \end{aligned} \quad (\text{C.3.4})$$

where,

$$\begin{aligned}
R_{\text{ep, rat}}^u = & \frac{1}{32} \left\{ 24H_5^u - 14(H_{4,1}^u - H_{4,1}^v) - 16H_{4,1}^w + \frac{5}{2}H_{3,2}^u + \frac{11}{2}H_{3,2}^v - 8H_{3,2}^w + 42H_{3,1,1}^u \right. \\
& + 24H_{3,1,1}^v + 6H_{3,1,1}^w + \frac{13}{2}H_{2,2,1}^u + \frac{15}{2}H_{2,2,1}^v + 2H_{2,2,1}^w - 36H_{2,1,1,1}^u - 36H_{2,1,1,1}^v + 24H_{2,1,1,1}^w \\
& + \left(\frac{15}{2}H_{2,1}^v - 5H_3^u + \frac{1}{2}H_{2,1}^u - \frac{1}{3}H_3^w - \frac{1}{2}H_3^v - \frac{31}{3}H_{2,1}^w \right) H_2^u + \left(-\frac{5}{3}H_3^w + \frac{7}{2}H_{2,1}^v - \frac{5}{3}H_{2,1}^w \right. \\
& - 3H_3^v + 4H_{2,1}^u - 14H_3^u \Big) H_2^v + \left(-\frac{7}{6}H_3^u - \frac{7}{3}H_{2,1}^v + 4H_3^w + \frac{5}{3}H_3^v + \frac{17}{6}H_{2,1}^u \right) H_2^w \\
& + \left(-14H_4^u + 16H_4^v + 19H_{3,1}^u - 2(H_{3,1}^v + H_{3,1}^w) - \frac{57}{2}H_{2,1,1}^u - 24(H_{2,1,1}^v - H_{2,1,1}^w) + \frac{1}{4}(H_2^u)^2 \right. \\
& - \frac{5}{2}(H_2^v)^2 + \frac{3}{2}(H_2^w)^2 + 6H_2^u H_2^v - \frac{17}{6}H_2^u H_2^w - 4H_2^v H_2^w \Big) \ln u + \left(-10H_4^u - 8(H_4^w + H_4^v) \right. \\
& - 4H_{3,1}^u + 3H_{3,1}^v + 2H_{3,1}^w + 6H_{2,1,1}^u - \frac{3}{2}H_{2,1,1}^v + \frac{11}{2}(H_2^u)^2 + \frac{19}{4}(H_2^v)^2 + \frac{1}{2}(H_2^w)^2 \\
& + \frac{17}{2}H_2^u H_2^v + 4H_2^u H_2^w + \frac{7}{3}H_2^v H_2^w \Big) \ln v + (10(H_4^u + H_4^w) + 8H_4^v + 6H_{3,1}^u - 8H_{3,1}^v + 2H_{3,1}^w \\
& - 6(H_{2,1,1}^u + H_{2,1,1}^w) - 6(H_2^u)^2 - 5(H_2^v)^2 - 2(H_2^w)^2 - 8H_2^u H_2^v - \frac{17}{3}H_2^u H_2^w - \frac{1}{3}H_2^v H_2^w \Big) \ln w \\
& + \left(\frac{1}{2}H_3^u + \frac{3}{4}H_3^v + \frac{5}{6}H_3^w - 6H_{2,1}^u - \frac{21}{4}H_{2,1}^v + \frac{35}{6}H_{2,1}^w \right) \ln^2 u + \left(-7H_3^u + \frac{13}{2}H_3^v + \frac{1}{6}H_3^w \right. \\
& + 4H_{2,1}^u + 2H_{2,1}^v - \frac{11}{6}H_{2,1}^w \Big) \ln^2 v + \left(-\frac{7}{12}H_3^u + \frac{11}{6}H_3^v - 7H_3^w + \frac{17}{12}H_{2,1}^u - \frac{1}{6}H_{2,1}^v \right) \ln^2 w \\
& + \left(6H_3^u - 14H_3^v - 2H_3^w + 4H_{2,1}^v - 2H_{2,1}^w \right) \ln u \ln v - 2 \left(3H_3^u - H_3^w + H_3^v - H_{2,1}^w \right) \ln u \ln w \\
& + \left(-10H_3^v + 6H_3^w - 2H_{2,1}^u + 4H_{2,1}^v - 2H_{2,1}^w \right) \ln v \ln w + \left(\frac{1}{4}H_2^u - \frac{5}{2}H_2^v + \frac{3}{4}H_2^w \right) \ln^3 u \\
& + \left(\frac{7}{4}H_2^u - \frac{1}{4}H_2^v + H_2^w \right) \ln^3 v + \frac{1}{2} \left(H_2^u + H_2^v + 4H_2^w \right) \ln^3 w - \left(\frac{1}{2}H_2^w + H_2^u - \frac{3}{4}H_2^v \right) \ln^2 u \ln v \\
& + \left(\frac{9}{2}H_2^u + 6H_2^v - \frac{3}{2}H_2^w \right) \ln u \ln^2 v + \left(-\frac{5}{6}H_2^w + H_2^u - H_2^v \right) \ln^2 u \ln w \\
& + \left(-\frac{11}{12}H_2^u - \frac{1}{2}H_2^v - H_2^w \right) \ln u \ln^2 w + \left(-\frac{1}{6}H_2^w + 2H_2^v \right) \ln^2 v \ln w \\
& + \left(-\frac{5}{2}H_2^u - 3H_2^w - \frac{4}{3}H_2^v \right) \ln v \ln^2 w - 2(H_2^u + H_2^v - H_2^w) \ln u \ln v \ln w \\
& + \frac{3}{8} \ln^3 u \ln^2 w - \frac{3}{4} \ln^2 u \ln^3 w + \ln^2 u \ln^2 v \ln w - \frac{7}{4} \ln^2 u \ln v \ln^2 w - \frac{7}{4} \ln u \ln^2 v \ln^2 w \\
& + 2 \ln u \ln v \ln^3 w - \frac{5}{4} \ln^3 u \ln^2 v + \frac{7}{8} \ln^2 u \ln^3 v + \frac{1}{2} \ln^3 v \ln^2 w - \frac{3}{4} \ln^2 v \ln^3 w
\end{aligned}$$

$$\begin{aligned}
& +\zeta_2 \left[\frac{33}{4} H_3^u - \frac{9}{4} H_3^v + 2H_3^w + H_{2,1}^u - 17H_{2,1}^v + 24H_{2,1}^w + \left(14H_2^w + \frac{7}{4} H_2^u - 10H_2^v \right) \ln u \right. \\
& \quad + \left(-6H_2^w - 18H_2^u - \frac{47}{4} H_2^v \right) \ln v + \left(8H_2^v + 6H_2^w + 20H_2^u \right) \ln w - \frac{1}{4} \ln^3 u + \frac{1}{4} \ln^3 v \\
& \quad - 4 \ln^3 w + 2 \ln^2 u \ln v - 12 \ln u \ln^2 v - 2 \ln w \ln^2 u + 2 \ln u \ln^2 w - 4 \ln^2 v \ln w \\
& \quad \left. + 6 \ln v \ln^2 w + 12 \ln u \ln v \ln w \right] \\
& +\zeta_3 \left[7H_2^u - 5H_2^v - 2H_2^w + \frac{3}{2} \ln^2 u - \frac{1}{2} \ln^2 v - \ln^2 w \right] \\
& +\zeta_4 \left[14 \ln u + 50 \ln v - 44 \ln w \right] \Big\}.
\end{aligned}$$

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