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Determining the closed forms of the $O(a_s^3)$ anomalous dimensions and Wilson coefficients from Mellin moments by means of computer algebra

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Abstract

Single scale quantities, as anomalous dimensions and hard scattering cross sections, in renormalizable Quantum Field Theories are found to obey difference equations of finite order in Mellin space. It is often easier to calculate fixed moments for these quantities compared to a direct attempt to derive them in terms of harmonic sums and their generalizations involving the Mellin parameter N. Starting from a sufficiently large number of given moments, we establish linear recurrence relations of lowest possible order with polynomial coefficients of usually high degree. Then these recurrence equations are solved in terms of d'Alembertian solutions where the involved nested sums are represented in optimal nested depth. Given this representation, it is then an easy task to express the result in terms of harmonic sums. In this process we compactify the result such that no algebraic relations occur among the sums involved. We demonstrate the method for the QCD unpolarized anomalous dimensions and massless Wilson coefficients to 3–loop order treating the contributions for individual color coefficients. For the most complicated subproblem 5114 moments were needed in order to produce a recurrence of order 35 whose coefficients have degrees up to 938. About four months of CPU time were needed to establish and solve the recurrences for the anomalous dimensions and Wilson coefficients on a 2 GHz machine requiring less than 10 GB of memory. No algorithm is known yet to provide such a high number of moments for 3–loop quantities. Yet the method presented shows that it is possible to establish and solve recurrences of rather large order and degree, occurring in physics problems, uniquely, fast and reliably with computer algebra.

1 Introduction

Precision predictions for observables in Elementary Particle Physics require the calculation of the corresponding Feynman diagrams, the number of which grows fast with the order in the coupling constant being considered. According to the relevant number of different ratios of Lorentz invariants or scales involved one may group these observables into 0-scale, 1-scale, 2-scale etc processes. In renormalizable Quantum Field Theories the radiative corrections to the couplings, masses and external fields are examples for 0-scale quantities [1]. Anomalous dimensions and hard scattering cross sections, as the Wilson coefficients for light and heavy flavors (for $Q^2 \gg m_H^2$) in deeply inelastic scattering, are single scale quantities, cf. [2–6]. Also the sub-system cross sections for the Drell-Yan process and the cross section for hadronic Higgs-boson production in the heavy mass limit for the top–quark belong to this class. Mellin moments for single scale quantities $f(x)$,

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

are 0-scale quantities again for $N \in \mathbf{N}$ [7–10]. Here x usually denotes a fraction of Lorentz-invariants the support of which is or can be extended to $[0,1]$. In the lower order in perturbation theory 0-scale quantities can be expressed as linear combinations of specific numbers over $\mathbf{Q}$ which are multiple ζ-values [11],

$$\zeta_{a_1,\ldots,a_n} = \sum_{k=1}^{\infty} \frac{\text{sign}(a_1)^k}{k^{|a_1|}} S_{a_2,\ldots,a_n}(k), \quad a_i \in \mathbf{Z} \setminus \{0\}$$

at the beginning, with possible extensions in higher orders, which occur in both massive and massless calculations [12]. The 1-scale quantities can be expressed in terms of finite harmonic sums [13, 14]

$$S_{a_1,\ldots,a_n}(N) = \sum_{k=1}^{N} \frac{\text{sign}(a_1)^k}{k^{|a_1|}} S_{a_2,\ldots,a_n}(k), \quad S_\emptyset = 1, \quad a_i \in \mathbf{Z} \setminus \{0\}$$

and rational functions of the Mellin variable N at lower orders in perturbation theory. At higher orders one expects to find generalizations of harmonic sums. Much less is known on the function-spaces spanning 2- and higher scale processes. The Mellin-transformation (1) is empirically found to yield considerable structural simplifications of 1-scale processes, cf. [15]. In massless processes this is partly due to the factorization properties, but it seems to hold to an even wider extent. Corresponding diagonalizations for processes with a higher number of scales depend on their respective main symmetries, which may not even be fixed by just the number of scales.

In the present paper we study single scale processes and represent them in Mellin space. In order to apply our method under consideration, we shall assume the case that $\mathbf{M}[f(x)](N)$ can be found as the solution of a linear recurrence equation

$$a_0(N)F(N) + a_1(N)F(N+1) + \cdots + a_l(N)F(N+l) = 0, \tag{2}$$

with polynomial coefficients $a_k(N)$.

There is no general proof that the k-loop contributions to a 1-scale observable have to obey such a recurrence. On the other hand, it is known that all single scale processes having been calculated so far do, cf. [2–5, 15]. This is due to the fact that the corresponding observables are found as linear combinations of nested harmonic sums. The single harmonic sums obey

$$F(N+1) - F(N) = \frac{\text{sign}(a)^{N+1}}{(N+1)^{|a|}}.$$

Exploiting holonomic closure properties [16] one obtains higher order difference equations for polynomial expressions in terms of nested harmonic sums.

If a suitably large number of moments $\mathbf{M}[f(x)](N)$ is known, then a recurrence of the form (2) can be found automatically, see Section 2. Once a recurrence of some order l is found, this recurrence together with the first l moments specifies uniquely all the moments $\mathbf{M}[f(x)](N)$ for nonnegative integers N. Finally, we activate the summation package Sigma [17] and solve the recurrence (2) in terms of generalized harmonic sums. In particular, using the underlying summation theory of $\Pi\Sigma$-difference fields [18–20] or exploiting the algebraic relations [21], a closed form for $\mathbf{M}[f(x)](N)$ in terms of an algebraically independent basis of harmonic sums can be computed.

We emphasize that Eq. (2) covers a much wider class in which more general recurrent quantities can represent the corresponding observables. In particular, our general recurrence solver for d'Alembertian solutions [22–24] finds any solution that can be expressed in terms of indefinite nested sums and products. In even higher order or massive calculations further functions may contribute, which could be only found in this way.

The Mellin-moments of the unpolarized 3–loop splitting functions and Wilson coefficients for deep–inelastic scattering are more easily calculated [7–10] than the complete expressions, cf. [3–5]. In the present paper we investigate whether the exact formulae up to the unpolarized 3–loop anomalous dimensions and Wilson coefficients [3–5] can be found establishing and solving difference equations (2) for the Mellin moments of these quantities, without further assumptions.[1]

We consider the various color contributions to these quantities separately and try to find the complete result from a minimal number of moments. As input we apply the moments calculated from the exact solution [3–5].

The paper is organized as follows. In Section 2 we describe how the difference equations of the form (2) are found by just using a finite number of starting points of $F(N)$. In Section 3 the algorithms are outlined that can solve these recurrences in the setting of difference fields. They lead directly to the corresponding mathematical structures. These are nested harmonic sums in the present case. In course of the solution we compactify the results applying the algebraic relations to the harmonic sums [21]. [2] The results are discussed in Section 4. Our method applies in the same way to all other single scale processes of similar complexity, cf. [6, 15]. Section 5 contains the conclusions. In the appendix we present a compactified form of the non-singlet 3–loop anomalous dimensions, which is automatically provided in the formalism by Sigma. The corresponding expressions for the other anomalous dimensions and Wilson coefficients to 3-loop order are presented in Mathematica and FORM codes attached.

[1]Approximate reconstruction methods based on special ansatzes were discussed in the literature e.g. in [7, 25] to obtain first numerical estimates from a low number of moments, see also [26]. We also remind that the description of QCD-evolution relating fixed integer moment information to orthogonal polynomials is an old topic [27]; see also [28].

[2]Further compactifications can be obtained using the structural relations, cf. [29, 30].

2 Finding a Recurrence Equation

Suppose we are given a finite array of rational numbers,

$$q_1,\ q_2,\ \ldots,\ q_K\ ,$$

which are the first terms of a certain infinite sequence $F(N)$, i.e., $F(1) = q_1$, $F(2) = q_2$, etc. Let us assume that $F(N)$ satisfies a recurrence of type

$$\sum_{k=0}^{l}\Bigl(\sum_{i=0}^{d} c_{i,k}N^i\Bigr)F(N+k) = 0\ , \tag{3}$$

which we would like to deduce from the given numbers q_i $(i = 1, \ldots, K)$. In a strict sense, this is not possible without knowing how the sequence continues for $N > K$. One thing we can do is to determine the recurrence equations satisfied by the data we are given. Any recurrence for $F(N)$ must certainly be among those.

To find the recurrence equations of $F(N)$ valid for the first terms, the simplest way to proceed is by making an ansatz with undetermined coefficients. Let us fix an order $l \in \mathbf{N}$ and a degree $d \in \mathbf{N}$ and consider the generic recurrence (3), where the $c_{i,k}$ are indeterminates. For each specific choice $N = 1, 2, \ldots, K - l$, we can evaluate the ansatz, because we know all the values of $F(N + k)$ in this range, and we obtain a system of $K - l$ homogeneous linear equations for $(l + 1)(d + 1)$ unknowns $c_{i,j}$.

If $K - l > (l + 1)(d + 1)$, this system is under-determined and is thus guaranteed to have nontrivial solutions. All these solutions will be valid recurrences for $F(N)$ for $N = 1, \ldots, K - l$, but they will most typically fail to hold beyond. If, on the other hand, $K - l \leq (l + 1)(d + 1)$, then the system is overdetermined and nontrivial solutions are not to be expected. But at least recurrence equations valid for all N, if there are any, must appear among the solutions. We therefore expect in this case that the solution set will precisely consist of the recurrences of $F(N)$ of order l and degree d valid for all N.

As an example, let us consider the contribution to the gluon splitting function $\propto C_A$ at leading order, $P_{gg}^{(0)}(N)$. The first 20 terms, starting with $N = 3$, of the sequence $F(N)$ are

$$\frac{14}{5},\ \frac{21}{5},\ \frac{181}{35},\ \frac{83}{14},\ \frac{4129}{630},\ \frac{319}{45},\ \frac{26186}{3465},\ \frac{18421}{2310},\ \frac{752327}{90090},\ \frac{71203}{8190},\ \frac{811637}{90090},\ \frac{128911}{13860},\ \frac{29321129}{3063060},$$
$$\frac{2508266}{255255},\ \frac{292886261}{29099070},\ \frac{7045513}{684684},\ \frac{611259269}{58198140},\ \frac{1561447}{145860},\ \frac{4862237357}{446185740},\ \frac{988808455}{89237148}\ .$$

Making an ansatz for a recurrence of order 3 with polynomial coefficients of degree 3 leads to an overdetermined homogeneous linear system with 16 unknowns and 17 equations. Despite of being overdetermined and dense, this system has two linearly independent solutions. Using bounds for the absolute value of determinants depending on the size of a matrix and the bit size of its coefficients, one can very roughly estimate the probability for this to happen "by coincidence" to about 10^{-65}. And in fact, it did not happen by coincidence. The solutions to the system correspond to the two recurrence equations

$$\begin{aligned}&(7N^3 + 113N^2 + 494N + 592)F(N) - (12N^3 + 233N^2 + 1289N + 2156)F(N + 1)\\&\quad + (3N^3 + 118N^2 + 1021N + 2476)F(N + 2) + (2N^3 + 2N^2 - 226N - 912)F(N + 3) = 0\end{aligned} \tag{4}$$

and

$$\begin{aligned}&(4N^3 + 64N^2 + 278N + 332)F(N) - (7N^3 + 134N^2 + 735N + 1222)F(N + 1)\\&\quad + (2N^3 + 71N^2 + 595N + 1418)F(N + 2) + (N^3 - N^2 - 138N - 528)F(N + 3) = 0,\end{aligned} \tag{5}$$

which both are valid for all $N \geq 1$. If we had found that the linear system did not have a nontrivial solution, then we could have concluded that the sequence $F(N)$ would *definitely* (i.e. without any uncertainty) not satisfy a recurrence of order 3 and degree 3. It might then still have satisfied recurrences with larger order or degree, but more terms of the sequence had to be known for detecting those.

The method of determining (potential) recurrence equations for sequences as just described is not new. It is known to the experimental mathematics community as *automated guessing* and is frequently applied in the study of combinatorial sequences. Standard software packages for generating functions such as gfun [16] for Maple or GeneratingFunctions.m [31] for Mathematica provide functions which take as input a finite array of numbers, thought of as the first terms of some infinite sequence, and produce as output recurrence equations that are, with high probability, satisfied by the infinite sequence.

These packages apply the method described above more or less literally, and this is perfectly sufficient for small examples. But if thousands of terms of a sequence are needed, there is no way to get the linear systems solved using rational number arithmetic. Even worse, already for medium sized problems from our collection, the size of the linear system exceeds by far typical memory capacities of 16–64Gb. For the big problem $C^{(3)}_{2,q,C_F^3}(N)$, it would require approximately 11Tb of memory to represent the corresponding linear system explicitly. It is thus evident that computations with rational numbers are not feasible. Instead, we use arithmetic in finite fields together with Chinese remaindering and rational reconstruction [32–34]. Modulo a word size prime, the size of the biggest systems reduces to a few Gb, a size which easily fits on our architecture. And modulo a word size prime, such a system can be solved within no more than a few hours of computation time by Mathematica.

The modular results for several distinct primes $p_1, p_2, \ldots$ can be combined by Chinese remaindering to a modular result whose coefficients are correct modulo the product $p_1 p_2 \ldots$. If the bit size of this product exceeds twice the maximum bit size appearing in the rational solution, then the exact rational number coefficients can be recovered from the modular images by rational reconstruction [32–34]. The number of primes needed (and thus the overall runtime) is therefore proportional to the bit size of the coefficients in the final output.

The final output is a recurrence equation for $F(N)$. But the recurrence equation satisfied by a sequence $F(N)$ is not unique: if a sequence satisfies a recurrence equation at all, then it satisfies a variety of linearly independent recurrence equations. The bit size of the rational number coefficients in these recurrence equations may vary dramatically. In order to minimize the number of primes needed for the computation of the rational numbers in the recurrence, it seems preferable to compute on a recurrence whose coefficients are as small as possible in terms of bit size. According to our experience, this recurrence happens to be the (unique) recurrence whose order l is minimal among all the recurrence equations satisfied by $F(N)$. We have no explanation for this, but it seems to be a general phenomenon, as it can also be observed in certain combinatorial applications [35].

Also the number of unknowns for the linear system may vary dramatically among the possible recurrence equations for $F(N)$, and it seems preferable to compute on a recurrence where the number of unknowns is as small as possible. Small linear systems are not only preferable because of efficiency, but also because the number of unknowns in the linear system determines the number of initial terms q_i that have to be known a priori in order to detect the recurrence. According to our experience, the size of the linear system is minimized when the order l and the degree d are approximately balanced.

Unfortunately, it seems that the recurrence with *minimal* (in terms of bit size) rational number coefficients has the *maximal* number of unknowns in the corresponding linear system, and vice versa. But there is a way to combine the advantages of both at a reasonable computational cost. Consider the two recurrence equations (4) and (5) from the example of the gluon–gluon splitting function at leading order, $P_{gg,0}(N)$, quoted above. A recurrence of smaller order can be obtained from these by multiplying (4) by $(N^2 - 9N - 66)$ and (5) by $(2N^2 - 14N - 114)$, and then subtracting the results. The choice of the multipliers is such that the coefficient of $F(N+3)$ in the difference cancels: we obtain

$$\begin{aligned}
&(N^5 + 22N^4 + 189N^3 + 788N^2 + 1592N + 1224)F(N)\\
&- (2N^5 + 45N^4 + 396N^3 + 1701N^2 + 3580N + 2988)F(N+1)\\
&+ (N^5 + 23N^4 + 207N^3 + 913N^2 + 1988N + 1764)F(N+2) = 0.
\end{aligned}$$

The calculation just performed can be recognized as the first step in a difference operator version of the Euclidean algorithm [36]. Applied to two recurrence equations satisfied by a sequence $F(N)$, this algorithm yields their "greatest common (right) divisor", which is, with high probability, the minimal order recurrence satisfied by $F(N)$. In our example, the algorithm terminates in the next step, and indeed the sequence $F(N)$ of $P_{gg,0}(N)$ does not satisfy a recurrence of order less than two. Note that the linear system for finding the second order recurrence directly would have involved $(5+1)(2+1) = 18$ unknowns instead of the 16 unknowns we needed for finding the third order recurrences. For the big problem $C^{(3)}_{2,q,C_F^3}(N)$, a direct computation would require 33804 unknowns instead of the 5022 we actually used. We combine the advantage of a small linear system with the advantage of small coefficients in the output as follows. We first compute for several word size primes the solutions of a small linear system, but then instead of applying rational reconstruction to those, we compute, for each prime independently, their greatest common right divisor modulo this prime. We then apply rational reconstruction to recover the rational number coefficients of those.

In summary, we used the following procedure for finding the recurrence equations.

1. Choose a word size prime p.
2. Choose some bounds l and d and make an ansatz for a recurrence of order l and degree d. The linear system is constructed and solved modulo p only.
3. If there are no solutions, repeat step 2 with increased bounds l and d.
4. If there are solutions modulo p, compute their greatest common right divisor modulo p by the Euclidean algorithm for difference operators.
5. Repeat steps 1–4 until Chinese remaindering and rational reconstruction applied to the greatest common right divisors for the various primes yields a recurrence that matches the given data $q_1, q_2, \ldots, q_K$.
6. Return the reconstructed recurrence as the final result.

For the big problem $C^{(3)}_{2,q,C_F^3}(N)$, most of the computation time (about 53%) was spent in step 4. Solving the modular linear systems consumed about 28% of the time, and Chinese remaindering and rational reconstruction took about 18% of the time. The memory bottleneck is in step 2 where the linear system is constructed. The memory requirements for the other steps, if implemented well, are negligible.

For problems that are even bigger than those we considered, further improvements to the procedure are conceivable. First, there are asymptotically fast special purpose algorithms for step 2 available [37, 38]. These algorithms outperform the naive linear system approach we are taking for problem sizes where fast polynomial multiplication algorithms outperform classical algorithms. It is likely that their use would have already been beneficial for some of our problems. Second, a gain in efficiency might result from running the procedure on a different platform. We have done all our computations within Mathematica 6, but we expect that in particular step 4 might considerably benefit from a reimplementation in a computer algebra system providing high-performance polynomial arithmetic. Mathematica's modular arithmetic, on the other hand, appears to be quite competitive. Third, it might be worthwhile to run parts of the procedure in parallel. In particular, computations for distinct primes are completely independent from each other and can be done on different processors without any communication overhead. Observe that these steps dominate the runtime.

3 Solving the Recurrence Equations

After having obtained difference equations of high order and degree we will now discuss general, efficient algorithms by which these equations can be solved. *Given* a recurrence relation

$$a_0(N)F(N) + a_1(N)F(N+1) + \cdots + a_l(N)F(N+l) = q(N) \tag{6}$$

of order l, *find* all its solutions that can be expressed in terms of indefinite nested sums and products. Such solutions are also called d'Alembertian solutions [22–24], they form a subclass of Liouvillian solutions [39]. Note that such solutions cover as special cases, e.g., harmonic sums [13, 14] or generalized nested harmonic sums [40].

The solution to this problem consists of two parts.

1. First, compute all d'Alembertian solutions by factoring the recurrence as much as possible into linear right factors. Then each linear factor contributes to one extra solution. To be more precise, the ith factor yields a nested sum expression of depth $i-1$.

2. Second, simplify these nested sum solutions to closed form expressions, e.g., in terms of harmonic sums, that can be processed further in practical problem solving.

In general, the package Sigma [17] can solve these problems in the setting of $\Pi\Sigma$-difference fields [18, 41]. This means that the coefficients $a_0(N), \dots, a_l(N)$ and the inhomogeneous part $q(N)$ of (6) can be given as polynomial expressions in terms of indefinite nested sums and products.

For simplicity, we restrict ourself to the situation that the given coefficients $a_0(N), \dots, a_l(N)$ are polynomials in N and that the inhomogeneous part $q(N)$ is zero. In other words, we assume that we are given a recurrence of the form (2) or (3) that is produced, e.g., by the method described in the previous section.

3.1 Finding all d'Alembertian solutions

Subsequently, we present algorithms that find all d'Alembertian solutions of (2). Equivalently, we can say that we look for all d'Alembertian sequences which are annihilated by the linear operator

$$L := a_0(N) + a_1(N)\mathbf{S} + \cdots + a_l(N)\mathbf{S}^l, \tag{7}$$

which is understood to act on a sequence $F(N)$ via

$$(L \cdot F)(N) := a_0(N)F(N) + a_1(N)F(N+1) + \cdots + a_l(N)F(N+l).$$

We start as follows.

Step 1: Finding a product solution. First, we look for a solution of (7) which is of the form

$$T_0(N) = \prod_{i=\lambda}^{N} r(i) \tag{8}$$

for some rational function $r(i)$ in i. In Sigma this task can be carried out by executing a generalized version of algorithm [42] that works in general $\Pi\Sigma$-difference fields; for an alternative algorithm to find such hypergeometric terms we refer to [43].

If there does not exist such a product solution (8), then there is no d'Alembertian solution at all; see, e.g. [24, Theorem 4.5.5]. In this case, we just stop. Otherwise, we look for additional solutions as follows.

Step 2: Splitting off a linear right factor. By dividing the operator (7) from the right with the operator

$$\mathbf{S} - \frac{T_0(N+1)}{T_0(N)} = \mathbf{S} - r(N+1) \tag{9}$$

we arrive at an operator

$$L' := b_0(N) + b_1(N)\mathbf{S} + \cdots + b_{l-1}(N)\mathbf{S}^{l-1} \tag{10}$$

of order $l-1$ such that

$$\begin{aligned} L &= L'(\mathbf{S} - r(N+1)) \\ &= -r(N+1)b_0(N) + \big(b_0(N) - r(N+2)b_1(N)\big)\mathbf{S} + \cdots + \big(b_{l-1}(N) - r(N+l)b_l(N)\big)\mathbf{S}^l, \end{aligned}$$

i.e., $\mathbf{S} - r(N+1)$ is a linear right factor of L.

Step 3: Recursion. Now we continue by recursion and look for all d'Alembertian solutions for the operator L' with order $l-1$. Note that after at most $l-1$ steps we end up at a recurrence of order 1 whose d'Alembertian solution can be read off immediately.

Step 4: Combining the solutions. If we do not find any d'Alembertian solution for L', we just return the solution (8) for L.
Otherwise, let

$$t_1(N), \dots, t_k(N) \tag{11}$$

with $1 \leq k < l$ be the solutions of L' that we obtained after the recursion step. To this end, for $1 \leq j \leq k$ define

$$T_j(N) := T_0(N) \sum_{i=\lambda}^{N} \frac{t_j(i-1)}{T_0(i)} \tag{12}$$

for some properly chosen $\lambda \geq 0$ (i.e., $T_0(i)$ is nonzero for all i with $i \geq \lambda$). Then the final output of our algorithm is

$$T_0(N), T_1(N), \dots, T_k(N). \tag{13}$$

The following remarks are in place. By construction all the elements from (13) are solutions of (7): for each $1 \leq j < k$,

$$(\mathbf{S}-r(N+1)) \cdot T_j(N) = T_0(N+1)\sum_{i=\lambda}^{N+1}\frac{t_j(i-1)}{T_0(i)} - r(N+1)T_0(N)\sum_{i=\lambda}^{N}\frac{t_j(i-1)}{T_0(i)}$$
$$= r(N+1)T_0(N)\left(\sum_{i=\lambda}^{N}\frac{t_j(i-1)}{T_0(i)} + \frac{t_j(N)}{T_0(N+1)}\right) - r(N+1)T_0(N)\sum_{i=\lambda}^{N}\frac{t_j(i-1)}{T_0(i)} = t_j(N)$$

and hence

$$L \cdot T_j(N) = L' \cdot t_j(N) = 0.$$

But even more holds. The derived solutions (13) are linearly independent. In particular, any solution of L in terms of indefinite nested sums and products can be expressed as a linear combination of (13); see [39, Theorem 5.1] or [24, Proposition 4.5.2].

Summarizing, with the algorithm sketched above we can produce all d'Alembertian solutions of L, i.e., all solutions that are expressible in terms of indefinite nested sums and products.

We emphasize that the expensive part of the sketched method is the computation of the product solutions (8). The following improvements were crucial in order to solve the recurrences under consideration.

Improvement 1. If one finds several product solutions, say $P_1(N), \dots, P_u(N)$, one can produce immediately a recurrence L' like in (10), but with order $l-u$ instead of order $l-1$. Moreover, given all d'Alembertian solutions of this operator L', one gets all the solutions of the recurrence (7) without any further computations; see [24, Theorem 4.5.6].

Improvement 2. For the problems under consideration, it turns out that it suffices to search for product solutions (8) that can be written in the form

$$T_0(N) = \frac{p(N)}{q(N)} \quad \text{or} \quad T_0(N) = \frac{p(N)}{q(N)}(-1)^N \tag{14}$$

for polynomials $p(N)$ and $q(N)$. Therefore, we used optimized solvers [44] of Sigma which generalize the algorithm presented in [45]. In addition, arithmetic in finite fields is exploited in order to determine the solutions (14) effectively.

Improvement 3. In our applications, rather big factors from $t_j(i-1)$ and $T_0(i)$ cancel in the summand $\frac{t_j(i-1)}{T_0(i)}$ of (12); in particular, the usually irreducible factor $p(i)$ from (14) (N substituted with i) cancels. Hence it pays off to compute directly the summand expression $\frac{t_j(i-1)}{T_0(i)}$: Namely, instead of the operator (10) we continue with the operator

$$b_0(N) + r(N)b_1(N)\mathbf{S} + \dots + \left(\prod_{i=1}^{l-1} r(N+i)\right) b_{l-1}(N)\mathbf{S}^{l-1}, \tag{15}$$

and look for all its d'Alembertian solutions $t'_1(N), \dots, t'_k(N)$. Then by construction, the solutions of (6) can be given directly in the form

$$T_j(N) = T_0(N)\sum_{i=\lambda}^{N} t'_j(i). \tag{16}$$

Example 1 *As illustrative example we solve the difference equation for the $C_F N_F^2$-term of the unpolarized 3-loop splitting function $P_{gq,2}(N)$,*

$$F(N) = P_{gq,2,N_F^2 C_F}(N) \ .$$

Using the methods from the previous section, we generate the recurrence relation

$$a_0(N)F(N) + a_1(N)F(N+1) + a_2(N)F(N+2) + a_3(N)F(N+3) = 0 \ , \tag{17}$$

with

$$\begin{aligned}
a_0(N) &= (1-N)N(N+1)(N^6+15N^5+109N^4+485N^3+1358N^2+2216N+1616),\\
a_1(N) &= N(N+1)(3N^7+48N^6+366N^5+1740N^4+5527N^3+11576N^2+14652N+8592),\\
a_2(N) &= -(N+1)(3N^8+54N^7+457N^6+2441N^5+9064N^4+23613N^3\\
&\qquad +41180N^2+43172N+20768),\\
a_3(N) &= (N+4)^3(N^6+9N^5+49N^4+179N^3+422N^2+588N+368) \ .
\end{aligned}$$

Given this recurrence, we produce its d'Alembertian solutions as follows. First, Sigma *computes a rational solution, namely*

$$T_0(N) = \frac{N^2+N+2}{(N-1)N(N+1)}.$$

Now we can divide (17) *from the right by the operator* $\mathbf{S} - T_0(N+1)/T_0(N) = S - \frac{(N-1)\left(N^2+3N+4\right)}{(N+2)(N^2+N+2)}$. *Then the resulting recurrence of the operator* (15) *is*

$$b_0(N)G(N) + b_1(N)G(N+1) + b_2(N)G(N+2) = 0 \ , \tag{18}$$

with

$$\begin{aligned}
b_0(N) &= (N+1)(N+2)(N^2-N+2)(N^6+9N^5+49N^4+179N^3+422N^2+588N+368),\\
b_1(N) &= -(N+2)(2N^9+21N^8+124N^7+530N^6+1690N^5+3989N^4+6712N^3+7524N^2\\
&\qquad +5232N+2080),\\
b_2(N) &= (N^2+5N+8)(N^6+3N^5+19N^4+53N^3+104N^2+124N+64)(N+3)^2 \ .
\end{aligned}$$

Next, we proceed recursively and can compute the rational solution

$$P'(N) = \frac{N^4+4N^3+13N^2+22N+16}{(N-1)N(N+1)(N+2)\,(N^2+3N+4)}$$

of (18)*. Thus we divide* (18) *by the factor* $\mathbf{S} - \frac{P'(N+1)}{P'(N)}$ *which leads to the first order recurrence*

$$c_0(N)H(N) + c_1(N)H(N+1) = 0 \tag{19}$$

with

$$\begin{aligned}
c_0(N) &= -(N+1)(N^2+N+2)(N^4-4N^3+13N^2-14N+8)\\
&\qquad \times \left(N^6+3N^5+19N^4+53N^3+104N^2+124N+64\right),\\
c_1(N) &= (N+2)(N^2-N+2)(N^4+4N^3+13N^2+22N+16)\\
&\qquad \times (N^6-3N^5+19N^4-13N^3+44N^2+8N+8).
\end{aligned}$$

Here we can read off directly the solution

$$P''(N) = \frac{(N^2 - N + 2)\,(N^6 - 3N^5 + 19N^4 - 13N^3 + 44N^2 + 8N + 8)}{(N+1)\,(N^4 + 7N^2 + 4N + 4)\,(N^4 - 4N^3 + 13N^2 - 14N + 8)}.$$

Going back, we obtain besides $t_1(N) = P'(N)$ *the solution*

$$t_2(N) = P'(N)\sum_{j=1}^{N} P''(j) = \tfrac{N^4+7N^2+4N+4}{(N+1)(N^2-N+2)(N^2+N+2)} \sum_{j=1}^{N} \tfrac{\left(j^2-j+2\right)\left(j^6-3j^5+19j^4-13j^3+44j^2+8j+8\right)}{(j+1)(j^4+7j^2+4j+4)(j^4-4j^3+13j^2-14j+8)}$$

of (18). *Hence by* (16) *we obtain, besides* $T_0(N)$, *the solutions*

$$\begin{aligned} T_1(N) =& \frac{\left(N^2+N+2\right)\sum_{i=1}^{N}\frac{i^4+7i^2+4i+4}{(i+1)\,(i^2-i+2)\,(i^2+i+2)}}{(N-1)N(N+1)}, \\ T_2(n) =& \frac{\left(N^2+N+2\right)\sum_{i=1}^{N}\frac{\left(i^4+7i^2+4i+4\right)\sum_{j=1}^{i}\frac{\left(j^2-j+2\right)\left(j^6-3j^5+19j^4-13j^3+44j^2+8j+8\right)}{(j+1)(j^4+7j^2+4j+4)(j^4-4j^3+13j^2-14j+8)}}{(i+1)\,(i^2-i+2)\,(i^2+i+2)}}{(N-1)N(N+1)} \end{aligned} \tag{20}$$

for (17). *Since all three solutions* $T_0(N)$, $T_1(N)$ *and* $T_2(N)$ *are linearly independent over, say, the complex numbers, any solution* $F : \mathbf{N} \to \mathbf{C}$ *of* (17) *can be described as a linear combination*

$$F(N) = c_1T_0(N) + c_2T_1(N) + c_3T_2(N)$$

for $c_1, c_2, c_3 \in \mathbf{C}$. *The initial values* $F(3) = \frac{1267}{648}, F(4) = \frac{54731}{40500}, F(5) = \frac{20729}{20250}$ *imply*

$$P_{gq,2,N_F^2C_F}(N) = -\tfrac{32}{9}T_0(N) + \tfrac{64}{9}T_1(N) - \tfrac{8}{3}T_2(N). \tag{21}$$

For our concrete problems all the recurrences could be factored completely. Equivalently, for a recurrence of order d we found d linearly independent solutions $T_1(N), \dots, T_d(N)$ where the solution T_k with $1 \le k \le d$ can be given in the form

$$T_k(N) = s_0^N \frac{P_0(N)}{Q_0(N)} \sum_{i_1=1}^{N} s_1^{i_1}\frac{P_1(i_1)}{Q_1(i_1)} \sum_{i_2=1}^{i_1} s_2^{i_2}\frac{P_2(i_2)}{Q_2(i_2)} \cdots \sum_{i_k=1}^{i_{k-1}} s_k^{i_k}\frac{P_k(i_k)}{Q_k(i_k)} \tag{22}$$

where for $1 \le i \le k$ the P_i and Q_i are polynomials and $s_i \in \{-1, 1\}$.

Example 2 *For the* $C_AC_FN_F$*-term of the 3-loop non-singlet splitting function* $P^-_{NS,2}$ *we found a recurrence of order 7 which fills around five pages. The 7 linearly independent solutions can be computed within 10 seconds; the largest solution fills around three pages and has the form*

$$\sum_{i=6}^{N}\frac{P_1(i)}{Q_1(i)}\sum_{j=1}^{i}\frac{P_2(j)}{Q_2(j)}\sum_{k=5}^{j}\frac{P_3(k)}{Q_3(k)}\sum_{l=1}^{k}\frac{P_4(l)}{Q_4(l)}\sum_{r=1}^{l}\frac{P_5(r)}{Q_5(r)}\sum_{s=2}^{r}\frac{P_6(s)}{Q_6(s)} \tag{23}$$

where the irreducible polynomials $P_1, P_2, \dots, P_6$ *have the respective degrees 4, 8, 16, 28, 63, 69, and the denominators are of the form*

$$Q_1(s) = (s-1)^3 s(s+1)^3,$$

$$
\begin{aligned}
Q_2(r) =& \left(r^4 - 10r^3 + 29r^2 - 34r + 12\right)\left(r^4 - 6r^3 + 5r^2 - 2r - 2\right),\\
Q_3(l) =& \left(l^8 - 24l^7 + 215l^6 - 1017l^5 + 2866l^4 - 4975l^3 + 5146l^2 - 2812l + 576\right)\\
&\times \left(l^8 - 16l^7 + 75l^6 - 175l^5 + 236l^4 - 165l^3 - 4l^2 + 64l - 24\right),\\
Q_4(k) =& (k-4)(k-3)^2(k-2)^3(k-1)^3k^2\big(k^{10} - 38k^9 + 566k^8 - 4628k^7 + 23621k^6 - 79466k^5\\
&+ 178404k^4 - 261580k^3 + 235712k^2 - 114624k + 21600\big)\big(k^{10} - 28k^9 + 269k^8 - 1348k^7\\
&+ 4091k^6 - 7768k^5 + 8451k^4 - 3560k^3 - 1612k^2 + 1872k - 432\big),\\
Q_5(j) =& 2j^{20} - 795j^{19} + 40760j^{18} - 1036641j^{17} + 16752826j^{16} - 191239786j^{15} + 1632641752j^{14}\\
&- 10786299042j^{13} + 56334695030j^{12} - 235648109263j^{11} + 795075807544j^{10}\\
&- 2168602473357j^9 + 4771126881598j^8 - 8409573468828j^7 + 11731291260824j^6\\
&- 12705852943232j^5 + 10375981856560j^4 - 6104512549760j^3 + 2399836168064j^2\\
&- 547585520256j + 51445094400,\\
Q_6(i) =& (i-5)(i-1)i(i+1)\big(16i^{33} - 7192i^{32} + 673840i^{31} - 33108234i^{30} + 1069628658i^{29}\\
&+ \cdots + 16224508333715039232i - 11706508031797555200\big)\big(16i^{33} - 6664i^{32} + 452144i^{31}\\
&- 15699130i^{30} + \cdots + 6071537402380800i^2 - 670382971978752i + 32623028121600\big).
\end{aligned}
$$

Example 3 *The solution of the recurrence for the C_F^3-contribution to the unpolarized 3-loop Wilson coefficient for deeply inelastic scattering, $C^{(3)}_{2,q,C_F^3}(N)$, constituted the hardest problem to solve. We obtained a recurrence of order 35. Then our solver ran 25 hours and used 3 GB of memory to derive the 35 linearly independent solutions. In total, we needed only 478 instead of $\sum_{i=0}^{34} i = 595$ summation quantifiers in order to represent those solutions. This is possible due to the Improvement 1. For each of the summands around 20 MB of memory were used. In particular, in the summands the denominators have irreducible factors up to degree 1000; the integer coefficients of the polynomials were up to 700 decimal digits long.*

3.2 Simplification of d'Alembertian solutions

We consider the following problem: *Given* indefinite nested sum and product expressions, e.g., expressions of the form (22), *find* an alternative sum representation with the following properties:

1. All the involved sums are algebraically independent with each other.
2. The nested depth of the sum expressions is minimal.
3. In the summands the degree of the denominators is minimal.
4. The sums should be tuned in such a way that algorithms can perform this simplification as efficiently as possible.

In principal, this problem can be solved with Karr's summation algorithm [18] based on $\Pi\Sigma$-difference fields, if one knows explicitly the sum elements in which, e.g., the expression (22) should be expressed. For small examples such optimal sums with properties 1–3 from above might be guessed. In particular, if one has additional knowledge about the objects under consideration, a good sum representation might be known a priory. But if such additional knowledge is not available, Karr's algorithm is not applicable.

In order to overcome this restriction, the fourth named author has refined Karr's $\Pi\Sigma$-theory for symbolic summation [20, 46]. As a consequence, we can determine completely automatically such sum representations with the properties 1–4 from above; see [19, 47].

Example 4 *With* Sigma *we find the depth-optimal representation*

$$-\frac{4\left(N^2+N+2\right)}{3(N-1)N(N+1)}\left(\sum_{i=1}^{N}\frac{1}{i}\right)^2+\frac{8\left(8N^3+13N^2+27N+16\right)}{9(N-1)N(N+1)^2}\sum_{i=1}^{N}\frac{1}{i}$$
$$-\frac{8\left(4N^4+4N^3+23N^2+25N+8\right)}{9(N-1)N(N+1)^3}-\frac{4\left(N^2+N+2\right)}{3(N-1)N(N+1)}\sum_{i=1}^{N}\frac{1}{i^2}$$

of (23) *where the sums are given in* (20). *We can read off the harmonic sum representation*

$$-\frac{4\left(N^2+N+2\right)}{3(N-1)N(N+1)}S_1(N)^2+\frac{8\left(8N^3+13N^2+27N+16\right)}{9(N-1)N(N+1)^2}S_1(N)$$
$$-\frac{8\left(4N^4+4N^3+23N^2+25N+8\right)}{9(N-1)N(N+1)^3}-\frac{4\left(N^2+N+2\right)}{3(N-1)N(N+1)}S_2(N).$$

Example 5 *The sum expression for* $P^{-}_{NS,2,C_AC_FN_F}$ *containing in particular the 7-nested sum* (21) *can be simplified with* Sigma *to the depth-optimal representation*

$$P^{-}_{NS,2,C_AC_FN_F}=-\frac{2\left(1086N^7+3258N^6+2129N^5-288N^4-67N^3-206N^2-156N+144\right)}{27N^4(N+1)^3}$$
$$\frac{32\left(8N^4+33N^3+53N^2+25N+3\right)}{9N(N+1)^4}(-1)^N+\frac{16}{3}\sum_{i=1}^{N}\frac{1}{i^4}+\frac{32}{3}\sum_{i=1}^{N}\frac{(-1)^i}{i^4}$$
$$-\frac{16\left(10N^2+10N+3\right)}{9N(N+1)}\sum_{i=1}^{N}\frac{(-1)^i}{i^3}+\frac{1336}{27}\sum_{i=1}^{N}\frac{1}{i^2}-\frac{64\left(8N^2+8N+3\right)}{9N(N+1)}\sum_{i=1}^{N}\frac{(-1)^i}{i}$$
$$+\frac{16\left(4N^6+88N^5+314N^4+412N^3+201N^2+16N-12\right)}{9N^2(N+1)^2(N+2)^2}\sum_{i=1}^{N}\frac{(-1)^i}{i^2}$$
$$+\left(-\frac{8\left(14N^2+14N+3\right)}{3N(N+1)}-\frac{16}{3}\sum_{i=1}^{N}\frac{1}{i}\right)\sum_{i=1}^{N}\frac{1}{i^3}+\frac{64}{3}\sum_{i=1}^{N}\frac{\sum_{j=1}^{i}\frac{1}{j^3}}{i}+32\sum_{i=1}^{N}\frac{\sum_{j=1}^{i}\frac{(-1)^j}{j^2}}{(i+2)^2}$$
$$-\frac{32\left(22N^2+22N-3\right)}{9N(N+1)}\sum_{i=1}^{N}\frac{\sum_{j=1}^{i}\frac{(-1)^j}{j^2}}{i+2}+\left(\sum_{i=1}^{N}\frac{1}{i}\right)\left(\frac{32\left(2N^2+4N+1\right)}{3(N+1)^3}(-1)^N\right.$$
$$-\frac{4\left(65N^6+195N^5+195N^4+137N^3+36N^2+36N+18\right)}{27N^3(N+1)^3}+\frac{32}{3}\sum_{i=1}^{N}\frac{(-1)^i}{i^3}+\frac{128}{3}\sum_{i=1}^{N}\frac{(-1)^i}{i}$$
$$\left.+\frac{32\left(2N^3+2N^2-3N-2\right)}{3N(N+1)(N+2)}\sum_{i=1}^{N}\frac{(-1)^i}{i^2}-\frac{64}{3}\sum_{i=1}^{N}\frac{\sum_{j=1}^{i}\frac{(-1)^j}{j^2}}{i+2}\right)$$
$$-\frac{256}{3}\sum_{i=1}^{N}\frac{(-1)^i\sum_{j=1}^{i}\frac{1}{j}}{i}+\frac{128}{3}\sum_{i=1}^{N}\frac{\left(\sum_{j=1}^{i}\frac{(-1)^j}{j^2}\right)\left(\sum_{i=1}^{N}\frac{1}{j}\right)}{i+2}.$$

Finally, we use J. Ablinger's HarmonicSums *package [48]* [3], *which transforms this expression to*

[3] The package refers to algorithms and methods from [14, 21, 29, 30, 49, 50].

the harmonic sum notation:

$$\frac{64(-1)^N(4N+1)}{9(N+1)^4} - \frac{2\left(270N^7+810N^6-463N^5-1392N^4-211N^3-206N^2-156N+144\right)}{27N^4(N+1)^3}$$
$$+\frac{64}{3}S_{-4}(N)+S_{-3}(N)\left(\frac{32}{3}S_1(N)-\frac{16\left(10N^2+10N+3\right)}{9N(N+1)}\right)+\frac{32\left(10N^2+10N-3\right)}{9N(N+1)}S_{-2,1}(N)$$
$$+S_{-2}(N)\left(\frac{16\left(16N^2+10N-3\right)}{9N^2(N+1)^2}-\frac{320}{9}S_1(N)+\frac{64}{3}S_2(N)\right)-\frac{8\left(14N^2+14N+3\right)}{3N(N+1)}S_3(N)$$
$$+S_1(N)\Big(\frac{-4\left(209N^6+627N^5+627N^4+281N^3+36N^2+36N+18\right)}{27N^3(N+1)^3}+16S_3(N)+\frac{80}{3}S_4(N)$$
$$+\frac{1336}{27}S_2(N)+\frac{64}{3}S_{-2,1}(N)-\frac{32(-1)^N}{3(N+1)^3}\Big)-\frac{32}{3}S_{2,-2}(N)-\frac{64}{3}S_{3,1}(N)-\frac{128}{3}S_{-2,1,1}(N).$$

We emphasize that the harmonic sums in this expression are algebraically independent. The algebraic independence could be accomplished with the Sigma *package; out of convenience and efficiency we used the* HarmonicSums *package which contains among various other features the harmonic sum relations of [21].*

Example 6 *The derived sum expression of* $C^{(3)}_{2,q,C_F^3}$ *from Example 3 contains sums of the form* (22) *with depth* $k = 35$*. In around four days and 20 hours this expression could be simplified to an expression in terms of 65 sums that satisfy the properties 1–3 from above. Among them there are 47 sums with depth two; typical examples are*

$$\sum_{k=1}^{N}\frac{\left(\sum_{j=1}^{k}\frac{(-1)^j}{j^2}\right)\left(\sum_{j=1}^{k}\frac{1}{j}\right)^3}{k} \quad \text{and} \quad \sum_{k=1}^{N}\frac{\left(\sum_{j=1}^{k}\frac{1}{j^2}\right)\left(\sum_{j=1}^{k}\frac{(-1)^j}{j^2}\right)\sum_{j=1}^{k}\frac{1}{j}}{k}. \tag{24}$$

Only one sum of nested depth three has been used, namely

$$\sum_{k=1}^{N}\frac{\left(\sum_{j=1}^{k}\frac{(-1)^j}{j^2}\right)\sum_{j=1}^{k}\frac{\sum_{i=1}^{j}\frac{1}{i^2}}{j}}{k}.$$

We emphasize that these sums are constructed in such a way that the difference field algorithms [20] work most efficiently: The less nested the sums are, the more efficient our algorithms work. E.g., if we switch to harmonic sum notation with Ablinger's HarmonicSum *package, the first sum in* (24) *can be rewritten as*

$$S_{-3}(N)S_3(N)-S_{-2,1}(N)S_3(N)+S_{-2}(N)\left(\tfrac{1}{4}S_1(N)^4-\tfrac{3}{4}S_2(N)^2-\tfrac{3}{2}\,S_4(N)\right)$$
$$+S_{4,-2}(N)-3S_{-3,1,2}(N)-3S_{-3,2,1}(N)+3S_{-2}(N)S_{2,1,1}(N)-S_{3,1,-2}(N)$$
$$+6S_{-3,1,1,1}(N)+3S_{-2,1,1,2}(N)+3S_{-2,1,2,1}(N)-6S_{-2,1,1,1,1}(N);$$

the involved sums have nested depths up to five. With such representations the algorithms in Sigma *work much slower, or might even fail for our specific input due to time and memory limitations.*

4 3-Loop Anomalous Dimensions and Wilson Coefficients

In the following we apply the method described in the previous section to unfold all the unpolarized QCD anomalous dimensions and Wilson coefficients to 3-loop order from a series of Mellin moments. This sequence is calculated using the relations given in [3–5] for the different quantities per color factor and factors given by ζ-values. We will need rather high Mellin moments N. The corresponding harmonic sums cannot be calculated by `summer` [14] directly, but have to be evaluated recursively,

$$S_{a_1,a_2,\ldots a_k}(N+1) = \frac{\mathrm{sign}(a_1)^{N+1}}{(N+1)^{|a_1|}} S_{a_2,\ldots a_k}(N+1) + S_{a_1,a_2,\ldots a_k}(N) \; . \tag{25}$$

We used a Maple code for this. The highest moment to be calculated is $N = 5114$ for the C_F^3–contribution to the 3-loop Wilson coefficient $C_{2,q}$. Its recursive computation requires roughly 3 GB of memory and 270 min computational time on a 2 GHz processor. It is given by a fraction with 13888 numerator and 13881 denominator digits. The set of moments has a size of 69 MB. The determination of most of the other inputs sets requires far less resources.

In Tables 1–3 we summarize the run parameters for the individual color- and ζ–contributions to the splitting functions and in Tables 4–8 to the Wilson coefficients in unpolarized deeply inelastic scattering up to 3–loop order. We specify the number of moments needed on input and the order, degree, and length of the recurrence derived. For the solution we compare the number of harmonic sums in Refs. [3–5] and in the present calculation. The computation times needed to establish and to solve the recurrences are also given.

To give some example for the rise of complexity for different orders in the coupling constant, we compare the C_A^k contributions to $P^{(k)}_{gg,C_A^{k+1}}$. In case of the anomalous dimensions the largest amount of moments needed is $n = 19$ for $P^{(0)}_{gg,C_A}(n)$, $n = 181$ for $P^{(1)}_{gg,C_A^2}(n)$, and $n = 1393$ for $P^{(2)}_{gg,C_A^3}(n)$. The order and degree of the recurrences found are exactly, resp. nearly, the same for $P^{(k),\pm}_{NS}(n)$. For the non-singlet anomalous dimensions and the singlet anomalous dimensions and $P^{(k)}_{gq,gg}(n)$ order and degree of the difference equation are larger than in case of $P^{(k)}_{qg}(n)$. The total computation time needed for all anomalous dimensions amount to less than 18 h. The largest number of harmonic sums contributing is 26. There are significant reductions in their number comparing to the representation given in the attachment to [3, 4].[4] It amounts to a factor of two or larger, except in case of the very small recurrences. In the non-singlet case $P^{(k),\pm}_{NS,C_F^3}(n)$ the number reduces from 68 to 26. A large reduction is obtained for $P^{(k),\pm}_{gg,C_A^3}(n)$ from 130 to 21 harmonic sums.

For the Wilson coefficients $C^{(3)}_{2,q,C_F^3}(n), C^{(3)}_{2,q,C_F^2C_A}(N)$ and $C^{(3)}_{2,q,C_FC_A^2}(n)$ four weeks of computation time is needed in each case requiring $\leq$ 10Gb on a 2 GHz processor. The number of necessary harmonic sums is 60, reducing from 290 in [5] for $C^{(3)}_{2,q,C_F^2C_A}$. This is the number of all harmonic sums not containing the index $\{-1\}$ up to weight $w = 6$ after algebraic reduction, cf. [30].

If one compares the number of harmonic sums obtained in the present calculation after the algebraic reduction yields groups characterized by clusters of 58-60, 26-29, 11-15 and cases with a number of sums below 10, up to very few exceptions. As this pattern is the same

[4] Here, the linear representation given in the text has been reduced already, following an idea of one of the present authors.

for quite different quantities, it may be related rather to the topology, but the color- or field-structure of the respective diagrams. This pattern is not seen counting the harmonic sums in the representation of Ref. [3–5].

In case of the smaller recurrences the time needed for their derivation is usually shorter than that for its solution. Conversely, for the larger recurrences the time required to establish them and the solution time behave roughly like 4(3):1. The total computation time amounted to 110.3 CPU days. Concerning the size of the different problems to be dealt with a naive fivefold parallelization was possible. Here we did not yet consider parallelization w.r.t. the number of primes N_p chosen, which would significantly reduce the computational time, of the C_F^3 term of $C_{2,q}^{(3)}$, with $N_p = 140$, discussed above and for other comparably large contributions.

In course of solving the recurrences we reduce the harmonic sums appearing algebraically, [21], and can express all results in terms of the following harmonics sums:

$$\begin{aligned}
&S_1\\
&S_2, S_{-2}\\
&S_3, S_{-3}\\
&S_{2,1}, S_{1,-2}\\
&S_4, S_{-4}\\
&S_{3,1}, S_{-3,1}, S_{2,-2}\\
&S_{2,1,1}, S_{-2,1,1}\\
&S_5, S_{-5}\\
&S_{4,1}, S_{-4,1}, S_{3,-2}, S_{3,2}, S_{-3,2}, S_{-3,-2}\\
&S_{3,1,1}, S_{-3,1,1}, S_{2,2,1}, S_{-2,1,-2}, S_{2,1,-2}, S_{-2,2,1}\\
&S_{2,1,1,1}, S_{-2,1,1,1}\\
&S_6, S_{-6}\\
&S_{5,1}, S_{-5,1}, S_{4,2}, S_{4,-2}, S_{-4,2}, S_{-4,-2}, S_{-3,3}\\
&S_{4,1,1}, S_{-4,1,1}, S_{3,2,1}, S_{2,3,1}, S_{-3,2,1}, S_{-3,1,2}, S_{-2,3,1}, S_{3,1,-2}, S_{-3,1,-2}, S_{-3,-2,1}, S_{-2,2,2}, S_{2,-2,-2}\\
&S_{3,1,1,1}, S_{-3,1,1,1}, S_{2,2,1,1}, S_{-2,-2,1,1}, S_{2,-2,1,1}, S_{-2,2,1,1}, S_{-2,1,1,2}\\
&S_{2,1,1,1,1}, S_{-2,1,1,1,1}\ .
\end{aligned}$$

The 3-loop Wilson coefficients require the complete set of possible functions up to $w = 6$. This representation can be further reduced using the structural relations [29, 30] to:

$$\begin{aligned}
&S_1\\
&S_{2,1}, S_{-2,1}\\
&S_{-3,1}\\
&S_{2,1,1}, S_{-2,1,1}\\
&S_{4,1}, S_{-4,1}\\
&S_{3,1,1}, S_{-3,1,1}, S_{2,2,1}, S_{-2,1,-2}, S_{2,1,-2}, S_{-2,2,1}\\
&S_{2,1,1,1}, S_{-2,1,1,1}\\
&S_{-5,1}\\
&S_{4,1,1}, S_{-4,1,1}, S_{3,2,1}, S_{2,3,1}, S_{-3,2,1}, S_{-3,1,2}, S_{-2,3,1}, S_{3,1,-2}, S_{-3,1,-2}, S_{-3,-2,1}, S_{-2,2,2}, S_{2,-2,-2}\\
&S_{3,1,1,1}, S_{-3,1,1,1}, S_{2,2,1,1}, S_{-2,-2,1,1}, S_{2,-2,1,1}, S_{-2,2,1,1}, S_{-2,1,1,2}\\
&S_{2,1,1,1,1}, S_{-2,1,1,1,1}\ .
\end{aligned}$$

In [29,30] we applied a slightly different basis referring to $S_{-2,2,-2}$ instead of $S_{2,-2,-2}$ and to $S_{2,-3,1}$ instead of $S_{-3,1,2}$, which is algebraically equivalent. These 38 functions can be represented by 35 basic Mellin transforms.

The ab-initio calculation of moments for the quantities considered in the present paper can be performed by codes like mincer and MATAD [51] available for physics calculations. Both the computational time and memory requests rise drastically going to higher values of N. In case of mincer both parameters increase by a factor of ~ 5 enlarging $N \rightarrow N+2$. Comparable, but slightly larger factors are obtained for MATAD. In the well–known leading order case, enough moments may be provided for our procedure. Already for some color projections of the next-to-leading order corrections, this is no longer the case, [53], since around 150 initial values are needed. For the 3-loop anomalous dimensions and Wilson coefficients $N = 16$ can be reached with computation times of the order of 0.5–1 CPU year, cf. [9]. The codes [51] still may be improved. However, the power–growth going to higher moments will basically remain due to the algorithms used. The method presented in this paper can therefore not be applied to whole color-factor contributions for the anomalous dimensions and Wilson coefficients at the 3–loop level. They may, however, be useful in solving medium-size problems. In view of constructing general methods suitable to evaluate single scale quantities, methods to evaluate the fixed moments for these quantities at far lower expenses have to be developed.

To illustrate the results of the present calculation, the non-singlet anomalous dimensions to $O(a_s^3)$ are given as an example in the appendix. The relations for all unpolarized anomalous dimensions and Wilson coefficients, separated according to the corresponding color- and ζ-value terms, are attached to this paper in FORM- and Mathematica files. The FORM-codes provide a check of our relations with the moments calculated in Ref. [7, 8].

5 Conclusions

We established a general algorithm to calculate the exact expression for single scale quantities from a finite, suitably large number of moments, which are zero scale quantities. The latter ones are much more easily calculable than single scale quantities. We applied the method to the anomalous dimensions and Wilson coefficients up to 3-loop order. Hereby we compactified their representation exploiting all algebraic relations between the harmonic sums. The 3-loop Wilson coefficients require the whole set of basic harmonic sums in the sub-algebra spanned by the index set to $w = 6$ without $i = -1$. A further compactification can be obtained using the structural relations between the harmonic sums. After algebraic reduction the number of the harmonic sums contributing clusters in several classes mainly determined by the topology of the graphs and widely independent of the color- and field structure of the respective contributions. The CPU time for the whole problem amounted to about four months using 2 GHz processors and $\lesssim$ 10 GB of memory were needed. The problem can be naively parallelized fivefold. The real computational time needed to establish the recurrences can be shortened further running Chinese remaindering in parallel.

To solve 3-loop problems for whole color factor contributions is not possible at present, since the number of required moments is too large for the methods available. Methods to evaluate the fixed moments for these quantities to high order at far lower expenses have still to be developed.

We established and solved the recurrences for all color resp. ζ-projections at once, which forms a rather voluminous problem. Yet we showed that rather large difference equations [order 35; degree ~ 1000], which occur for the most advanced problems in Quantum Field Theory, can be reliably and fast established and solved unconditionally.

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Table 1: Run parameters for the unfolding of the non-singlet anomalous dimensions

	number of terms needed	order of recurrence	degree of recurrence	total time [sec]	length of recurrence [kbyte]	number of harm. sums a [b]	solution time [sec]
$P_{NS,0}$	14	2	3	0.05	0.087	1 [1]	0.55
$P^-_{NS,1,C_F^2}$	142	5	31	3.32	4.666	6 [10]	7.45
$P^-_{NS,1,C_AC_F}$	109	4	24	1.91	2.834	6 [7]	6.28
$P^-_{NS,1,C_FN_F}$	24	2	7	0.13	0.271	2 [2]	0.92
$P^+_{NS,1,C_F^2}$	142	5	31	3.35	4.707	6 [10]	7.45
$P^+_{NS,1,C_AC_F}$	109	4	23	1.88	2.703	6 [7]	6.23
$P^+_{NS,1,C_FN_F}$	24	2	7	0.09	0.271	2 [2]	0.89
$P^-_{NS,2,C_F^3}$	1079	16	192	3152.19	529.802	26 [68]	1194.41
$P^-_{NS,2,C_F^3\zeta_3}$	48	3	11	0.49	0.643	1 [1]	1.56
$P^-_{NS,2,C_AC_F^2}$	974	15	181	1736.08	450.919	26 [62]	1194.41
$P^-_{NS,2,C_AC_F^2\zeta_3}$	48	3	11	0.53	0.643	1 [1]	1.53
$P^-_{NS,2,C_A^2C_F}$	749	12	147	1004.12	242.892	26 [62]	1100.88
$P^-_{NS,2,C_A^2C_F\zeta_3}$	48	3	11	0.56	0.643	1 [1]	1.56
$P^-_{NS,2,C_FN_F^2}$	39	2	11	0.31	0.369	3 [3]	1.20
$P^-_{NS,2,C_F^2N_F}$	377	8	68	76.34	33.946	11 [24]	72.22
$P^-_{NS,2,C_F^2N_F\zeta_3}$	14	2	3	0.12	0.101	1 [1]	0.53
$P^-_{NS,2,C_AC_FN_F}$	356	7	62	65.25	23.830	11 [20]	52.67
$P^-_{NS,2,C_AC_FN_F\zeta_3}$	14	2	3	0.12	0.101	1 [1]	0.55
$P^+_{NS,2,C_F^3}$	1079	16	192	4713.27	527.094	26[68]	1165.22
$P^+_{NS,2,C_F^3\zeta_3}$	48	3	11	0.55	0.643	1[1]	1.562
$P^+_{NS,2,C_AC_F^2}$	974	15	178	1715.03	442.031	26[62]	889.047
$P^+_{NS,2,C_AC_F^2\zeta_3}$	48	3	11	0.61	0.643	1[1]	1.531
$P^+_{NS,2,C_A^2C_F}$	749	12	146	991.22	240.325	26[50]	516.812
$P^+_{NS,2,C_A^2C_F\zeta_3}$	48	3	11	0.61	0.643	1[1]	1.593
$P^+_{NS,2,C_F^2N_F}$	377	8	69	111.38	33.872	11[24]	71.235
$P^+_{NS,2,C_F^2N_F\zeta_3}$	14	2	3	0.15	0.101	1[1]	0.531
$P^+_{NS,2,C_AC_FN_F}$	307	7	61	48.62	23.808	11[24]	71.235
$P^+_{NS,2,C_AC_FN_F\zeta_3}$	14	2	3	0.15	0.101	1[1]	0.547
$P^+_{NS,2,C_FN_F^2}$	39	2	11	0.40	0.369	3[3]	1.172
$P^-_{NS,2,N_Fd_{abc}}$	459	7	87	239.62	0.369	5 [20]	32.5

Table 2: Run parameters for the unfolding of the singlet anomalous dimensions

	number of terms needed	order of recurrence	degree of recurrence	total time [sec]	length of recurrence [kbyte]	number of harm. sums a [b]	solution time [sec]
$P^{PS}_{1,N_F C_F}$	24	1	8	0.19	0.204	0[0]	0.244
$P^{PS}_{2,N_F^2 C_F}$	109	3	26	6.32	1.891	2[8]	2.812
$P^{PS}_{2,N_F C_A C_F}$	566	9	115	425.44	100.414	7 [40]	111.52
$P^{PS}_{2,N_F C_A C_F \zeta_3}$	19	1	6	0.42	0.117	0[0]	0.204
$P^{PS}_{2,N_F C_F^2}$	237	5	50	32.75	0.117	4[24]	14.601
$P^{PS}_{2,N_F C_F^2 \zeta_3}$	19	1	6	0.41	12.163	0[0]	0.200
$P_{qg,0}$	11	1	3	0.02	0.061	0 [0]	0.16
$P_{qg,1,N_F C_A}$	120	4	29	3.31	3.769	3[8]	4.872
$P_{qg,1,N_F C_F}$	63	3	16	0.68	0.951	2[9]	2.008
$P_{qg,2,N_F^2 C_A}$	239	6	54	45.30	17.403	6[24]	21.993
$P_{qg,2,N_F^2 C_F}$	194	5	41	27.75	7.911	3[15]	8.021
$P_{qg,2,N_F C_A^2}$	1088	15	201	3321.46	557.535	13 [88]	848.85
$P_{qg,2,N_F C_A^2 \zeta_3}$	39	2	11	0.86	0.408	1[3]	0.932
$P_{qg,2,N_F C_A C_F}$	1049	15	194	3963.62	552.100	12 [84]	714.45
$P_{qg,2,N_F C_A C_F \zeta_3}$	39	2	11	1.02	0.409	1 [3]	0.93
$P_{qg,2,N_F C_F^2}$	849	12	143	1337.36	261.804	13 [66]	387.6
$P_{qg,2,N_F C_F^2 \zeta_3}$	17	1	5	0.29	0.093	0 [0]	0.15
$P_{gq,0}$	11	1	3	0.03	0.062	0 [0]	0.15
$P_{gq,1,C_F^2}$	63	3	16	0.72	0.869	2[6]	1.924
$P_{gq,1,C_F C_A}$	125	4	31	4.55	4.059	3[12]	5.068
$P_{gq,1,N_F C_F}$	24	2	6	0.18	0.192	1[3]	0.588
$P_{gq,2,C_F^3}$	703	11	114	927.82	162.320	13[59]	245.53
$P_{gq,2,C_F^3 \zeta_3}$	35	2	9	0.79	0.281	1[3]	0.776
$P_{gq,2,C_A^2 C_F}$	1088	15	203	3327.32	633.346	12 [93]	830.2
$P_{gq,2,C_A^2 C_F \zeta_3}$	35	2	9	0.81	0.281	1[3]	0.776
$P_{gq,2,C_A C_F^2}$	1087	15	193	3184.13	528.827	14 [75]	853.31
$P_{gq,2,C_A C_F^2 \zeta_3}$	35	2	9	0.86	0.281	1[3]	0.776
$P_{gq,2,N_F C_F^2}$	339	7	69	106.93	30.626	5[25]	33.586
$P_{gq,2,N_F C_F^2 \zeta_3}$	11	1	3	0.24	0.062	0[0]	0.152
$P_{gq,2,N_F C_A C_F}$	1087	15	194	3201.52	58.943	17[87]	714.51
$P_{gq,2,N_F C_A C_F \zeta_3}$	11	1	3	0.21	0.062	0[0]	0.156
$P_{gq,2,N_F^2 C_F}$	41	3	9	1.04	0.445	2[6]	1.216
$P_{gg,0}$	19	2	5	0.04	0.166	1 [1]	0.65
$P_{gg,1,C_A^2}$	181	5	45	12.07	9.053	6 [17]	11.62
$P_{gg,1,N_F C_A}$	29	2	9	0.23	0.395	1[1]	0.856
$P_{gg,1,N_F C_F}$	31	1	11	0.23	0.228	0[0]	0.240

Table 3: Run parameters for the unfolding of the singlet anomalous dimensions (continued)

	number of terms needed	order of recurrence	degree of recurrence	total time [sec]	length of recurrence [kbyte]	number of harm. sums a [b]	solution time [sec]
$P_{gg,2,C_A^3}$	1393	16	277	12432.80	1087.615	21 [130]	2419.04
$P_{gg,2,N_F C_F^2}$	439	8	88	237.82	57.291	7 [35]	55.52
$P_{gg,2,N_F C_F^2 \zeta_3}$	15	1	4	0.31	0.073	0[0]	0.156
$P_{gg,2,N_F C_A^2}$	782	11	148	1638.62	205.980	6 [31]	160.89
$P_{gg,2,N_F C_A^2 \zeta_3}$	29	2	9	0.66	0.308	1[1]	0.796
$P_{gg,2N_F C_A C_F}$	749	10	127	1169.37	146.921	7 [40]	128.37
$P_{gg,2N_F C_A C_F \zeta_3}$	29	2	9	0.72	0.305	1[1]	0.828
$P_{gg,2,N_F^2 C_A}$	55	2	17	4.53	0.979	1[4]	1.092
$P_{gg,2,N_F^2 C_F}$	109	3	26	6.74	2.483	2[12]	2.668

Table 4: Run parameters for the unfolding of the unpolarized pure-singlet Wilson Coefficients

	number of terms needed	order of recurrence	degree of recurrence	total time [sec]	length of recurrence [kbyte]	number of harm. sums a [b]	solution time [sec]
$C^{(2)}_{2,PS,C_F N_F}$	209	5	42	20.85	8.422	3[16]	7.70
$C^{(3)}_{2,PS,C_F^2 N_F}$	1847	19	334	41001.00	1989.043	14 [122]	2701.04
$C^{(3)}_{2,PS,C_F^2 N_F \zeta_3}$	65	2	20	0.69	1.124	1 [6]	0.92
$C^{(3)}_{2,PS,C_F^2 N_F \zeta_4}$	19	1	6	0.08	0.117	0 [0]	0.14
$C^{(3)}_{2,PS,C_F C_A N_F}$	2023	20	368	54873.80	2670.459	14 [126]	4589.31
$C^{(3)}_{2,PS,C_F C_A N_F \zeta_3}$	71	2	21	0.82	1.429	1 [6]	0.97
$C^{(3)}_{2,PS,C_F C_A N_F \zeta_4}$	19	1	6	0.08	0.117	0 [0]	0.14
$C^{(3)}_{2,PS,C_F N_F^2}$	479	8	103	629.05	75.646	5 [34]	53.28
$C^{(3)}_{2,PS,C_F N_F^2 \zeta_3}$	19	1	6	0.09	0.122	0 [0]	0.14
$C^{(2)}_{L,PS,C_F N_F}$	41	2	11	0.20	0.384	1[4]	0.88
$C^{(3)}_{L,PS,C_F^2 N_F}$	869	11	162	4411.20	250.352	8 [62]	163.17
$C^{(3)}_{L,PS,C_F^2 N_F \zeta_3}$	35	2	10	0.17	0.406	1 [5]	0.63
$C^{(3)}_{L,PS,C_F C_A N_F}$	840	11	153	2005.44	231.837	8 [64]	153.99
$C^{(3)}_{L,PS,C_F C_A N_F \zeta_3}$	35	2	10	0.17	0.403	1 [5]	0.59
$C^{(3)}_{L,PS,C_F N_F^2}$	224	5	52	72.64	12.440	3 [13]	9.87

Table 5: Run parameters for the unfolding of the unpolarized quarkonic Wilson Coefficients for the structure function $F_2(x, Q^2)$.

	number of terms needed	order of recurrence	degree of recurrence	total time [sec]	length of recurrence [kbyte]	number of harm. sums a [b]	solution time [sec]
$C^{(1)}_{2,q,C_F}$	31	3	6	0.26	0.429	2[3]	1.47
$C^{(2)}_{2,q,C_F^2}$	689	11	137	1134.10	177.806	13[39]	258.24
$C^{(2)}_{2,q,C_F^2\zeta_3}$	15	2	3	0.27	0.100	1[1]	0.54
$C^{(2)}_{2,q,C_AC_F}$	545	10	121	413.33	127.893	12[35]	178.73
$C_{2,q,C_AC_F\zeta_3}$	15	2	3	0.27	0.112	1[1]	0.55
C_{2,q,N_FC_F}	71	4	16	2.68	1.655	4[10]	3.95
$C^{(3)}_{2,q,C_F^3}$	5114	35	938	1.79×10^6	30394.173	58[289]	509242
$C^{(3)}_{2,q,C_F^3\zeta_3}$	284	8	64	31.02	32.363	6 [18]	27.60
$C^{(3)}_{2,q,C_F^3\zeta_4}$	65	3	11	2.62	0.163	1 [1]	1.47
$C^{(3)}_{2,q,C_F^3\zeta_5}$	19	2	5	0.08	0.163	1 [1]	0.47
$C^{(3)}_{2,q,C_F^2C_A}$	5059	35	930	1.69×10^6	30122.380	60 [290]	0.478×10^6
$C^{(3)}_{2,q,C_F^2C_A\zeta_3}$	284	8	64	34.00	33.400	7 [18]	28.53
$C^{(3)}_{2,q,C_F^2C_A\zeta_4}$	48	3	11	0.32	0.643	1[1]	1.01
$C^{(3)}_{2,q,C_F^2C_A\zeta_5}$	19	2	5	0.08	0.167	1 [1]	0.42
$C^{(3)}_{2,q,C_FC_A^2}$	4564	33	863	1.39×10^6	24567.518	60 [258]	0.349×10^6
$C^{(3)}_{2,q,C_FC_A^2\zeta_3}$	284	8	63	26.83	29.918	7 [17]	30.46
$C^{(3)}_{2,q,C_FC_A^2\zeta_4}$	48	3	11	0.32	0.643	1 [1]	1.01
$C^{(3)}_{2,q,C_FC_A^2\zeta_5}$	19	2	5	0.08	0.175	1 [1]	0.42
$C^{(3)}_{2,q,C_F^2N_F}$	1762	20	348	40237.45	2339.516	28 [107]	7548.56
$C^{(3)}_{2,q,C_F^2N_F\zeta_3}$	87	4	21	1.94	2.354	3 [5]	2.83
$C^{(3)}_{2,q,C_F^2N_F\zeta_4}$	15	2	3	0.07	0.101	1 [1]	0.34
$C^{(3)}_{2,q,C_FC_AN_F}$	1847	20	360	47661.64	2507.362	28 [111]	7525.89
$C^{(3)}_{2,q,C_FC_AN_F\zeta_3}$	89	4	24	2.47	2.935	3 [8]	3.19
$C^{(3)}_{2,q,C_FC_AN_F\zeta_4}$	15	2	3	0.06	0.101	1 [1]	0.34
$C^{(3)}_{2,q,C_FN_F^2}$	131	5	30	58.00	5.347	7 [22]	12.22
$C^{(3)}_{2,q,C_FN_F^2\zeta_3}$	15	2	3	0.06	0.101	1 [1]	0.38
$C^{(3)}_{2,q,dabc}$	1199	14	242	6583.27	738.498	15 [62]	841.24
$C^{(3)}_{2,q,dabc\zeta_3}$	109	4	25	2.33	3.164	2[7]	2.40
$C^{(3)}_{2,q,dabc\zeta_5}$	8	1	2	0.03	0.041	0[0]	0.10

Table 6: Run parameters for the unfolding of the unpolarized quarkonic Wilson Coefficients for the structure function $F_L(x, Q^2)$.

	number of terms needed	order of recurrence	degree of recurrence	total time [sec]	length of recurrence [kbyte]	number of harm. sums a [b]	solution time [sec]
$C^{(1)}_{L,q,C_F}$	5	1	1	0.02	0.033	0[0]	0.12
$C^{(2)}_{L,q,C_F^2}$	203	5	51	7.86	12.381	6[11]	17.21
$C^{(2)}_{L,q,C_F^2\zeta_3}$	5	1	1	0.02	0.033	0[0]	0/13
$C^{(2)}_{L,q,C_AC_F}$	159	4	43	4.32	7.624	5[8]	11.43
$C^{(2)}_{L,q,C_AC_F\zeta_3}$	5	1	1	0.02	0.033	0[0]	0.12
$C^{(2)}_{L,q,C_FN_F}$	19	2	4	0.05	0.134	1[6]	5.30
$C^{(3)}_{L,q,C_F^3}$	2419	22	472	110504.41	4555.679	27 [142]	19060.10
$C^{(3)}_{L,q,C_F^3\zeta_3}$	131	5	34	3.52	6.257	3 [10]	7.40
$C^{(3)}_{L,q,C_F^3\zeta_5}$	11	1	3	0.05	0.069	0 [0]	0.14
$C^{(3)}_{L,q,C_F^2C_A}$	2551	23	486	124064.39	5176.054	27 [144]	24614.00
$C^{(3)}_{L,q,C_F^2C_A\zeta_3}$	131	5	34	4.51	6.807	3 [10]	7.39
$C^{(3)}_{L,q,C_F^2C_A\zeta_5}$	11	1	3	0.05	0.069	0 [0]	0.14
$C^{(3)}_{L,q,C_FC_A^2}$	1803	18	344	42500.82	2064.227	27 [109]	6269.33
$C^{(3)}_{L,q,C_FC_A^2\zeta_3}$	131	5	31	3.50	5.463	2 [10]	6.32
$C^{(3)}_{L,q,C_FC_A^2\zeta_5}$	11	1	3	0.05	0.069	0 [0]	0.15
$C^{(3)}_{L,q,C_FC_AN_F}$	1014	14	203	4041.82	539.901	13 [58]	896.70
$C^{(3)}_{L,q,C_FC_AN_F\zeta_3}$	41	2	12	0.19	0.518	1 [5]	0.92
$C^{(3)}_{L,q,C_F^2N_F}$	959	13	188	3507.92	400.784	13 [51]	769.90
$C^{(3)}_{L,q,C_F^2N_F\zeta_3}$	29	2	8	0.15	6.257	1 [1]	0.85
$C^{(3)}_{L,q,C_FN_F^2}$	47	3	10	1.58	0.498	2 [4]	1.45
$C^{(3)}_{L,q,dabcN_F}$	989	12	184	3536.04	371.269	15[60]	384.00
$C^{(3)}_{L,q,dabcN_F\zeta_3}$	89	4	18	1.90	2.034	2 [7]	2.68
$C^{(3)}_{L,q,dabcN_F\zeta_5}$	5	1	1	0.02	0.033	0 [0]	0.12

Table 7: Run parameters for the unfolding of the unpolarized gluonic Wilson Coefficients for the structure function $F_2(x,Q^2)$.

	number of terms needed	order of recurrence	degree of recurrence	total time [sec]	length of recurrence [kbyte]	number of harm. sums a [b]	solution time [sec]
$C^{(1)}_{2,g,N_F}$	24	2	6	0.14	0.191	1[3]	0.72
$C^{(2)}_{2,g,N_F C_A}$	459	9	93	202.96	73.022	7[35]	70.77
$C^{(2)}_{2,g,N_F C_A \zeta_3}$	8	1	2	0.11	0.038	0[0]	0.14
$C^{(2)}_{2,g,N_F C_F}$	419	8	91	207.98	63.468	7[32]	59.78
$C^{(2)}_{2,g,N_F C_F \zeta_3}$	8	1	2	0.14	0.038	0[0]	0.14
$C^{(3)}_{2,g,C_F^2 N_F}$	3464	28	658	542132.00	11742.788	29 [228]	65721.40
$C^{(3)}_{2,g,C_F^2 N_F \zeta_3}$	181	6	42	25.30	12.171	3 [14]	7.67
$C^{(3)}_{2,g,C_F^2 N_F \zeta_4}$	17	1	5	0.23	0.093	0 [0]	0.12
$C^{(3)}_{2,g,C_F^2 N_F \zeta_5}$	11	1	3	0.20	0.067	0 [0]	0.15
$C^{(3)}_{2,g,C_A^2 N_F}$	4014	30	739	869580.00	16320.095	28 [261]	97289.30
$C^{(3)}_{2,g,C_A^2 N_F \zeta_3}$	194	6	44	42.39	13.263	3 [15]	8.01
$C^{(3)}_{2,g,C_A^2 N_F \zeta_4}$	39	2	11	0.74	0.408	1 [3]	0.67
$C^{(3)}_{2,g,C_A^2 N_F \zeta_5}$	11	1	3	0.17	0.063	0 [0]	0.13
$C^{(3)}_{2,g,C_F C_A N_F}$	4014	30	747	889246.00	16640.997	29 [264]	100830.00
$C^{(3)}_{2,g,C_F C_A N_F \zeta_3}$	194	6	43	41.81	12.999	3 [15]	7.90
$C^{(3)}_{2,g,C_F C_A N_F \zeta_4}$	39	2	11	0.61	0.409	1 [3]	0.66
$C^{(3)}_{2,g,C_F C_A N_F \zeta_5}$	11	1	3	0.17	0.068	0 [0]	0.11
$C^{(3)}_{2,g,C_F N_F^2}$	1553	16	285	22235.00	1181.805	13 [101]	1506.79
$C^{(3)}_{2,g,C_F N_F^2 \zeta_3}$	55	2	16	2.81	0.962	1 [3]	0.70
$C^{(3)}_{2,g,C_A N_F^2}$	1329	17	259	10692.80	1033.138	13 [96]	1162.99
$C^{(3)}_{2,g,C_A N_F^2 \zeta_3}$	39	2	11	2.48	0.666	1 [3]	0.70
$C^{(3)}_{2,g,dabcN_F}$	1403	15	282	13951.90	1048.336	19 [81]	2668.66
$C^{(3)}_{2,g,dabcN_f \zeta_3}$	142	5	37	8.54	7.177	2 [12]	6.74
$C^{(3)}_{2,g,dabcN_F \zeta_5}$	19	1	7	0.30	0.139	0 [0]	0.14

Table 8: Run parameters for the unfolding of the unpolarized gluonic Wilson Coefficients for the structure function $F_L(x, Q^2)$.

	number of terms needed	order of recurrence	degree of recurrence	total time [sec]	length of recurrence [kbyte]	number of harm. sums a [b]	solution time [sec]
$C_{L,g}^{(1)}$	5	1	1	0.02	0.033	0[0]	0.13
$C_{L,g,C_FN_F}^{(2)}$	153	4	38	4.15	5.941	2[6]	5.30
$C_{L,g,C_AN_F}^{(2)}$	109	4	25	1.31	2.731	3[10]	4.22
$C_{L,g,C_F^2N_F}^{(3)}$	1679	17	314	48496.50	1498.918	16 [100]	2019.46
$C_{L,g,C_F^2N_F\zeta_3}^{(3)}$	120	4	28	3.64	3.967	2 [8]	3.23
$C_{L,g,C_F^2N_F\zeta_5}^{(3)}$	5	1	1	0.02	0.033	0 [0]	0.09
$C_{L,g,C_A^2N_F}^{(3)}$	1671	17	302	29219.30	1392.205	16 [112]	2012.38
$C_{L,g,C_A^2N_F\zeta_3}^{(3)}$	109	4	24	2.46	3.007	2[8]	2.836
$C_{L,g,C_A^2N_F\zeta_5}^{(3)}$	5	1	1	0.03	0.033	0 [0]	0.11
$C_{L,g,C_FC_AN_F}^{(3)}$	1935	18	351	44671.90	2036.550	16 [116]	3510.31
$C_{L,g,C_FC_AN_F\zeta_3}^{(3)}$	120	4	28	4.43	4.154	2 [8]	3.10
$C_{L,g,C_FC_AN_F\zeta_5}^{(3)}$	5	1	1	0.03	0.033	0 [0]	0.11
$C_{L,g,C_FN_F^2}^{(3)}$	699	9	140	1350.09	140.949	6 [35]	108.69
$C_{L,g,C_FN_F^2\zeta_3}^{(3)}$	15	1	4	0.06	0.074	0 [0]	0.17
$C_{L,g,C_AN_F^2}^{(3)}$	419	8	90	526.25	57.569	6 [30]	47.40
$C_{L,g,C_AN_F^2\zeta_3}^{(3)}$	5	1	1	0.02	0.033	0 [0]	0.08
$C_{L,g,dabcN_F}^{(3)}$	1109	13	231	10155.40	618.402	18 [75]	1714.70
$C_{L,g,dabcN_F\zeta_3}^{(3)}$	129	5	27	2.18	3.858	2 [11]	4.09
$C_{L,g,dabcN_F\zeta_5}^{(3)}$	11	2	2	0.06	0.074	0 [0]	0.12

6 Appendix: The non-singlet anomalous dimensions

The non-singlet anomalous dimensions $P_{qq}^{(0)}$ and $P_{qq}^{k,\pm}(n)|_{k=1,2}$ are given by

$$
\begin{aligned}
P^0_{qq}(n) &= C_F\left[4S_1 - \frac{3n^2+3n+2}{n(n+1)}\right] && (26)\\
P^{1,-}_{qq}(n) &= C_F^2\Bigg[-\frac{3n^6+9n^5+9n^4-5n^3-24n^2-32n-24}{2n^3(n+1)^3} - 16S_{-3}\\
&\quad +S_{-2}\left(\frac{16}{n(n+1)} - 32S_1\right) + S_1\left(\frac{8(2n+1)}{n^2(n+1)^2} - 16S_2\right) + \frac{4\left(3n^2+3n+2\right)}{n(n+1)}S_2\\
&\quad -16S_3 + 32S_{-2,1} + \frac{16(-1)^n}{(n+1)^3}\Bigg]\\
&+ C_AC_F\Bigg[-\frac{51n^5+102n^4+655n^3+484n^2+12n+144}{18n^3(n+1)^2} + 8S_{-3} + \frac{268}{9}S_1\\
&\quad +S_{-2}\left(16S_1 - \frac{8}{n(n+1)}\right) - \frac{44}{3}S_2 + 8S_3 - 16S_{-2,1} - \frac{8(-1)^n}{(n+1)^3}\Bigg]\\
&+ C_FN_F\left[\frac{3n^4+6n^3+47n^2+20n-12}{9n^2(n+1)^2} - \frac{40}{9}S_1 + \frac{8}{3}S_2\right] && (27)\\
P^{1,+}_{qq}(n) &= C_F^2\Bigg[-\frac{3n^6+9n^5+9n^4+59n^3+40n^2+32n+8}{2n^3(n+1)^3} - 16S_{-3}\\
&\quad +S_{-2}\left(\frac{16}{n(n+1)} - 32S_1\right) + S_1\left(\frac{8(2n+1)}{n^2(n+1)^2} - 16S_2\right)\\
&\quad +\frac{4\left(3n^2+3n+2\right)}{n(n+1)}S_2 - 16S_3 + 32S_{-2,1} + \frac{16(-1)^n}{(n+1)^3}\Bigg]\\
&+ C_AC_F\Bigg[-\frac{51n^5+153n^4+757n^3+851n^2+208n-132}{18n^2(n+1)^3} + 8S_{-3} + \frac{268}{9}S_1\\
&\quad +S_{-2}\left(16S_1 - \frac{8}{n(n+1)}\right) - \frac{44}{3}S_2 + 8S_3 - 16S_{-2,1} - \frac{8(-1)^n}{(n+1)^3}\Bigg]\\
&+ C_FN_F\left[\frac{3n^4+6n^3+47n^2+20n-12}{9n^2(n+1)^2} - \frac{40}{9}S_1 + \frac{8}{3}S_2\right] && (28)\\
P^{2,-}_{qq}(n) &= C_F^3\Bigg\{\left(\frac{64}{n(n+1)} - 128S_1\right)S_{-2}^2 + \Bigg(\frac{16\left(3n^6+9n^5+9n^4+17n^3+6n^2+8n+2\right)}{n^3(n+1)^3}\\
&+ S_1\left(\frac{64\left(3n^2-n+1\right)}{n^2(n+1)^2} - 1408S_2\right) - \frac{64\left(3n^2+3n-11\right)S_2}{n(n+1)} + 1536S_3 + 128S_{-2,1}\\
&- 2304S_{2,1}\Bigg)S_{-2} - \frac{16\left(3n^2+3n+2\right)S_2^2}{n(n+1)} - \frac{P_1(n)}{2n^5(n+1)^5} - 576S_{-5}
\end{aligned}
$$

$$
\begin{aligned}
&+ \quad S_{-4}\left(-\frac{16\left(9n^2+9n-26\right)}{n(n+1)}-832S_1\right) \qquad (29)\\
&+ \quad S_{-3}\left(640S_1^2-\frac{32\left(3n^2+3n+20\right)S_1}{n(n+1)}+\frac{16\left(21n^2+17n+20\right)}{n^2(n+1)^2}-320S_{-2}-2240S_2\right)\\
&+ \quad (-1)^n\left(-\frac{48\left(2n^2-n+1\right)}{(n+1)^5}+\frac{128S_{-2}}{(n+1)^3}+\frac{96(5n+3)S_1}{(n+1)^4}-\frac{64S_2}{(n+1)^3}\right)\\
&+ \quad \frac{4\left(13n^4+26n^3+13n^2-16n-20\right)S_3}{n^2(n+1)^2}-\frac{16\left(15n^2+15n+2\right)S_4}{n(n+1)}-192S_5-832S_{-4,1}\\
&+ \quad \frac{896S_{-3,1}}{n(n+1)}+1152S_{-3,2}+S_1^2\left(-\frac{32\left(3n^2+3n+1\right)}{n^3(n+1)^3}-768S_{-2,1}\right)-\frac{32\left(15n^2+11n+16\right)S_{-2,1}}{n^2(n+1)^2}\\
&+ \quad S_2\left(\frac{2\left(3n^6+9n^5+9n^4+19n^3+12n^2-4n-16\right)}{n^3(n+1)^3}+64S_3+2176S_{-2,1}\right)\\
&+ \quad \frac{32\left(3n^2+3n-26\right)S_{2,-2}}{n(n+1)}-1472S_{3,-2}+\frac{64\left(3n^2+3n-2\right)S_{3,1}}{n(n+1)}+192S_{3,2}+192S_{4,1}\\
&+ \quad 2304S_{-3,1,1}+512S_{-2,1,-2}+\frac{384\left(n^2+n-4\right)S_{-2,1,1}}{n(n+1)}+S_1\Bigg(64S_2^2-\frac{64(2n+1)S_2}{n^2(n+1)^2}\\
&+ \quad \frac{4\left(22n^6+186n^5+167n^4-40n^3-115n^2-120n-44\right)}{n^4(n+1)^4}-192S_3+64S_4-1792S_{-3,1}\\
&- \quad \frac{192\left(n^2+n-4\right)S_{-2,1}}{n(n+1)}+1664S_{2,-2}+256S_{3,1}+3072S_{-2,1,1}\Bigg)+2304S_{-2,2,1}+2304S_{2,1,-2}\\
&- \quad 384S_{3,1,1}-4608S_{-2,1,1,1}\\
&+ \quad \left(C_F^3-\frac{3}{2}C_F^2C_A\right)\zeta_3\left[-\frac{24\left(5n^4+10n^3+9n^2+4n+4\right)}{n^2(n+1)^2}-192S_{-2}\right]\Bigg\}\\
&+ \quad C_AC_F^2\Bigg\{\left(256S_1-\frac{16\left(3n^2+3n+8\right)}{n(n+1)}\right)S_{-2}^2\\
&+ \quad \Bigg[-\frac{8\left(81n^6+243n^5-229n^4-389n^3-130n^2+228n+72\right)}{9n^3(n+1)^3}+\frac{32\left(31n^2+31n-81\right)S_2}{3n(n+1)}\\
&+ \quad S_1\left(1728S_2-\frac{32\left(134n^4+268n^3+215n^2+45n+54\right)}{9n^2(n+1)^2}\right)-1792S_3-192S_{-2,1}+2688S_{2,1}\Bigg]S_{-2}\\
&+ \quad \frac{176}{3}S_2^2-\frac{P_2(n)}{36n^5(n+1)^5}+672S_{-5}+S_{-4}\left(\frac{8\left(97n^2+97n-210\right)}{3n(n+1)}+1120S_1\right)\\
&+ \quad S_{-3}\Bigg(-576S_1^2+\frac{16\left(31n^2+31n+108\right)S_1}{3n(n+1)}-\frac{8\left(268n^4+536n^3+811n^2+507n+450\right)}{9n^2(n+1)^2}\\
&+ \quad 480S_{-2}+2656S_2\Bigg)+(-1)^n\Bigg(\frac{8\left(382n^2+41n-161\right)}{9(n+1)^5}-\frac{256S_{-2}}{(n+1)^3}-\frac{16(127n+121)S_1}{3(n+1)^4}\\
&+ \quad \frac{32S_2}{(n+1)^3}\Bigg)-\frac{8\left(385n^4+770n^3+427n^2+6n-126\right)S_3}{9n^2(n+1)^2}+\frac{8\left(151n^2+151n-30\right)S_4}{3n(n+1)}\\
&+ \quad 384S_5+864S_{-4,1}-\frac{960S_{-3,1}}{n(n+1)}-1344S_{-3,2}
\end{aligned}
$$

$$
\begin{aligned}
&+ S_2\left(\frac{2\left(453n^5+906n^4+1325n^3+488n^2-120n+144\right)}{9n^3(n+1)^2}-32S_3-2624S_{-2,1}\right)\\
&+ \frac{16\left(268n^4+536n^3+625n^2+321n+414\right)S_{-2,1}}{9n^2(n+1)^2}+S_1^2(128S_3+896S_{-2,1})\\
&- \frac{16\left(31n^2+31n-174\right)S_{2,-2}}{3n(n+1)}+1824S_{3,-2}-\frac{32\left(29n^2+29n-24\right)S_{3,1}}{3n(n+1)}-384S_{3,2}-384S_{4,1}\\
&- 2688S_{-3,1,1}-768S_{-2,1,-2}+S_1\left(-\frac{8\left(135n^6+731n^5+245n^4-617n^3-395n^2-309n-144\right)}{9n^4(n+1)^4}\right.\\
&- \frac{2144}{9}S_2+\frac{32\left(31n^2+31n-12\right)S_3}{3n(n+1)}+160S_4+1920S_{-3,1}+\frac{32\left(31n^2+31n-84\right)S_{-2,1}}{3n(n+1)}\\
&- \left.1856S_{2,-2}-512S_{3,1}-3584S_{-2,1,1}\right)-\frac{64\left(31n^2+31n-84\right)S_{-2,1,1}}{3n(n+1)}-2688S_{-2,2,1}-2688S_{2,1,-2}\\
&+ 768S_{3,1,1}+5376S_{-2,1,1,1}\Big\}\\
&+ C_A^2C_F\left[\left(\frac{24\left(n^2+n+2\right)}{n(n+1)}-96S_1\right)S_{-2}^2+\left(\frac{8\left(27n^6+81n^5-155n^4-271n^3-92n^2+78n+27\right)}{9n^3(n+1)^3}\right.\right.\\
&+ S_1\left(\frac{16\left(134n^4+268n^3+188n^2+54n+45\right)}{9n^2(n+1)^2}-512S_2\right)-\frac{32\left(11n^2+11n-24\right)S_2}{3n(n+1)}+512S_3\\
&+ \left.64S_{-2,1}-768S_{2,1}\right)S_{-2}+\frac{P_3(n)}{108n^5(n+1)^5}-192S_{-5}+S_{-4}\left(-\frac{8\left(35n^2+35n-66\right)}{3n(n+1)}-352S_1\right)\\
&+ (-1)^n\left(-\frac{16\left(82n^2+17n-47\right)}{9(n+1)^5}+\frac{96S_{-2}}{(n+1)^3}+\frac{16(41n+47)S_1}{3(n+1)^4}\right)\\
&+ S_{-3}\left(128S_1^2-\frac{16\left(11n^2+11n+24\right)S_1}{3n(n+1)}+\frac{8\left(134n^4+268n^3+311n^2+177n+135\right)}{9n^2(n+1)^2}\right.\\
&- \left.160S_{-2}-768S_2\right)+\frac{4\left(389n^4+778n^3+398n^2+9n-81\right)S_3}{9n^2(n+1)^2}-\frac{8\left(55n^2+55n-24\right)S_4}{3n(n+1)}\\
&- 160S_5-224S_{-4,1}+\frac{256S_{-3,1}}{n(n+1)}+384S_{-3,2}+S_1^2(-64S_3-256S_{-2,1})\\
&- \frac{16\left(134n^4+268n^3+245n^2+111n+135\right)S_{-2,1}}{9n^2(n+1)^2}+S_2\left(768S_{-2,1}-\frac{4172}{27}\right)\\
&+ \frac{16\left(11n^2+11n-48\right)S_{2,-2}}{3n(n+1)}-544S_{3,-2}+\frac{32\left(11n^2+11n-12\right)S_{3,1}}{3n(n+1)}\\
&+ 192S_{3,2}+192S_{4,1}+768S_{-3,1,1}+256S_{-2,1,-2}+\frac{64\left(11n^2+11n-24\right)S_{-2,1,1}}{3n(n+1)}\\
&+ S_1\left(\frac{2\left(245n^8+980n^7+1542n^6+1524n^5+851n^4+100n^3+36n^2+22n-6\right)}{3n^4(n+1)^4}\right.\\
&- \frac{8\left(11n^2+11n-8\right)S_3}{n(n+1)}-128S_4-512S_{-3,1}-\frac{32\left(11n^2+11n-24\right)S_{-2,1}}{3n(n+1)}\\
&+ \left.512S_{2,-2}+256S_{3,1}+1024S_{-2,1,1}\right)+768S_{-2,2,1}+768S_{2,1,-2,}-384S_{3,1,1}
\end{aligned}
$$

$$
\begin{aligned}
&- \quad 1536 S_{-2,1,1,1}\Bigg]\\
&+ \quad C_A^2 C_F \zeta_3 \left[-\frac{12\left(5n^4+10n^3+9n^2-4n-4\right)}{n^2(n+1)^2} - 96 S_{-2}\right]\\
&+ \quad C_F N_F^2 \left[\frac{51n^6+153n^5+57n^4+35n^3+96n^2+16n-24}{27n^3(n+1)^3} - \frac{16}{27}S_1 - \frac{80}{27}S_2 + \frac{16}{9}S_3\right]\\
&+ \quad C_F^2 N_F \Bigg[-\frac{32}{3}S_2^2 - \frac{4\left(15n^4+30n^3+79n^2+16n-24\right)S_2}{9n^2(n+1)^2}\\
&+ \quad \frac{207n^8+828n^7+1443n^6+1123n^5-38n^4-779n^3-632n^2+120}{9n^4(n+1)^4} - \frac{128}{3}S_{-4}\\
&+ \quad S_{-3}\left(\frac{32\left(10n^2+10n+3\right)}{9n(n+1)} - \frac{64}{3}S_1\right) + (-1)^n\left(\frac{64S_1}{3(n+1)^3} - \frac{128(4n+1)}{9(n+1)^4}\right)\\
&+ \quad S_{-2}\left(-\frac{32\left(16n^2+10n-3\right)}{9n^2(n+1)^2} + \frac{640}{9}S_1 - \frac{128}{3}S_2\right) + \frac{16\left(29n^2+29n+12\right)S_3}{9n(n+1)} - \frac{128}{3}S_4\\
&+ \quad S_1\left(-\frac{2\left(165n^5+330n^4+165n^3+160n^2-16n-96\right)}{9n^3(n+1)^2} + \frac{320}{9}S_2 - \frac{128}{3}S_3 - \frac{128}{3}S_{-2,1}\right)\\
&- \quad \frac{64\left(10n^2+10n-3\right)S_{-2,1}}{9n(n+1)} + \frac{64}{3}S_{2,-2} + \frac{64}{3}S_{3,1} + \frac{256}{3}S_{-2,1,1}\Bigg]\\
&+ \quad \left(C_F^2 - C_F C_A\right) N_F \zeta_3 \left[32 S_1 - \frac{8\left(3n^2+3n+2\right)}{n(n+1)}\right]\\
&+ \quad C_A C_F N_F \Bigg[-\frac{2\left(270\ n^7+810n^6-463n^5-1392n^4-211n^3-206n^2-156n+144\right)}{27n^4(n+1)^3}\\
&+ \quad \frac{64}{3}S_{-4} + S_{-3}\left(\frac{32}{3}S_1 - \frac{16\left(10n^2+10n+3\right)}{9n(n+1)}\right) + (-1)^n\left(\frac{64(4n+1)}{9(n+1)^4} - \frac{32S_1}{3(n+1)^3}\right)\\
&+ \quad \frac{1336}{27}S_2 + S_{-2}\left(\frac{16\left(16n^2+10n-3\right)}{9n^2(n+1)^2} - \frac{320}{9}S_1 + \frac{64}{3}S_2\right) - \frac{8\left(14n^2+14n+3\right)S_3}{3n(n+1)} + \frac{80}{3}S_4\\
&+ \quad \frac{32\left(10n^2+10n-3\right)S_{-2,1}}{9n(n+1)} + S_1\Bigg(-\frac{4\left(209n^6+627n^5+627n^4+281n^3+36n^2+36n+18\right)}{27n^3(n+1)^3}\\
&+ \quad 16S_3 + \frac{64}{3}S_{-2,1}\Bigg) - \frac{32}{3}S_{2,-2} - \frac{64}{3}S_{3,1} - \frac{128}{3}S_{-2,1,1}\Bigg]
\end{aligned}
\tag{30}
$$

$$
\begin{aligned}
P_{qq}^{2,+} \quad &= \quad C_F^3 \Bigg[\left(\frac{64}{n(n+1)} - 128 S_1\right) S_{-2}^2 + \Bigg(\frac{16\left(3n^6+9n^5+9n^4+n^3+2n^2+4n+2\right)}{n^3(n+1)^3}\\
&+ \quad S_1\left(-\frac{64\left(3n^2+7n+5\right)}{n^2(n+1)^2} - 1408 S_2\right) - \frac{64\left(3n^2+3n-11\right)S_2}{n(n+1)} + 1536 S_3 + 128 S_{-2,1}
\end{aligned}
$$

$$
\begin{aligned}
- & \left. 2304 S_{2,1} \right) S_{-2} - \frac{16\left(3n^2+3n+2\right) S_2^2}{n(n+1)} - \frac{P_4(n)}{2n^5(n+1)^5} - 576 S_{-5} \\
+ & S_{-4}\left(-\frac{16\left(9n^2+9n-26\right)}{n(n+1)} - 832 S_1\right) + S_{-3}\left(640 S_1^2 - \frac{32\left(3n^2+3n+20\right) S_1}{n(n+1)}\right. \\
+ & \left.\frac{16\left(9n^2+5n+8\right)}{n^2(n+1)^2} - 320 S_{-2} - 2240 S_2\right) + (-1)^n\left(\frac{16\left(2n^2+11n+1\right)}{(n+1)^5} + \frac{128 S_{-2}}{(n+1)^3}\right. \\
+ & \left.\frac{96(5n+3)S_1}{(n+1)^4} - \frac{64 S_2}{(n+1)^3}\right) + \frac{4\left(13n^4+26n^3+13n^2-16n-20\right) S_3}{n^2(n+1)^2} \\
- & \frac{16\left(15n^2+15n+2\right) S_4}{n(n+1)} - 192 S_5 - 832 S_{-4,1} + \frac{896 S_{-3,1}}{n(n+1)} + 1152 S_{-3,2} \\
+ & S_1^2\left(-\frac{32\left(3n^2+3n+1\right)}{n^3(n+1)^3} - 768 S_{-2,1}\right) - \frac{32\left(3n^2-n+4\right) S_{-2,1}}{n^2(n+1)^2} \\
+ & S_2\left(\frac{2\left(3n^6+9n^5+9n^4+83n^3+76n^2+60n+16\right)}{n^3(n+1)^3} + 64 S_3 + 2176 S_{-2,1}\right) \\
+ & \frac{32\left(3n^2+3n-26\right) S_{2,-2}}{n(n+1)} - 1472 S_{3,-2} + \frac{64\left(3n^2+3n-2\right) S_{3,1}}{n(n+1)} + 192 S_{3,2} + 192 S_{4,1} \\
+ & 2304 S_{-3,1,1} + 512 S_{-2,1,-2} + \frac{384\left(n^2+n-4\right) S_{-2,1,1}}{n(n+1)} + S_1\left(64 S_2^2 - \frac{64(2n+1)S_2}{n^2(n+1)^2}\right. \\
+ & \frac{4\left(22n^6-54n^5+23n^4+88n^3+197n^2+160n+52\right)}{n^4(n+1)^4} - 192 S_3 + 64 S_4 - 1792 S_{-3,1} \\
- & \left.\frac{192\left(n^2+n-4\right) S_{-2,1}}{n(n+1)} + 1664 S_{2,-2} + 256 S_{3,1} + 3072 S_{-2,1,1}\right) + 2304 S_{-2,2,1} \\
+ & \left. 2304 S_{2,1,-2} - 384 S_{3,1,1} - 4608 S_{-2,1,1,1} \right] \\
+ & C_F^3 \zeta_3 \left[-\frac{24\left(5n^4+10n^3+n^2-4n-4\right)}{n^2(n+1)^2} - 192 S_{-2}\right] \\
+ & C_A C_F^2 \left\{\left(256 S_1 - \frac{16\left(3n^2+3n+8\right)}{n(n+1)}\right) S_{-2}^2\right. \\
+ & \left(-\frac{8\left(81n^5+243n^4-337n^3-1181n^2-526n-60\right)}{9n^2(n+1)^3} + \frac{32\left(31n^2+31n-81\right) S_2}{3n(n+1)}\right. \\
+ & \left. S_1\left(1728 S_2 - \frac{32\left(134n^4+268n^3+89n^2-81n-72\right)}{9n^2(n+1)^2}\right) - 1792 S_3 - 192 S_{-2,1} + 2688 S_{2,1}\right) S_{-2} \\
+ & \frac{176}{3} S_2^2 - \frac{P_5(n)}{36n^4(n+1)^4} + 672 S_{-5} + S_{-4}\left(\frac{8\left(97n^2+97n-210\right)}{3n(n+1)} + 1120 S_1\right) \\
+ & S_{-3}\left(-576 S_1^2 + \frac{16\left(31n^2+31n+108\right) S_1}{3n(n+1)} - \frac{8\left(268n^4+536n^3+487n^2+183n+126\right)}{9n^2(n+1)^2}\right.
\end{aligned}
$$

$$
\begin{aligned}
+ &\quad 480S_{-2} + 2656S_2\Bigg) + (-1)^n \left(\frac{8(346n-125)}{9(n+1)^4} - \frac{256S_{-2}}{(n+1)^3} - \frac{16(103n+73)S_1}{3(n+1)^4} + \frac{32S_2}{(n+1)^3}\right) \\
- &\quad \frac{8\left(385n^4+770n^3+427n^2+6n-126\right)S_3}{9n^2(n+1)^2} + \frac{8\left(151n^2+151n-30\right)S_4}{3n(n+1)} + 384S_5 \\
+ &\quad 864S_{-4,1} - \frac{960S_{-3,1}}{n(n+1)} - 1344S_{-3,2} + S_2\Bigg(\frac{2\left(453n^5+1359n^4+2231n^3+1525n^2+80n-264\right)}{9n^2(n+1)^3} \\
- &\quad 32S_3 - 2624S_{-2,1}\Bigg) + \frac{16\left(268n^4+536n^3+301n^2-3n+90\right)S_{-2,1}}{9n^2(n+1)^2} + S_1^2(128S_3+896S_{-2,1}) \\
- &\quad \frac{16\left(31n^2+31n-174\right)S_{2,-2}}{3n(n+1)} + 1824S_{3,-2} - \frac{32\left(29n^2+29n-24\right)S_{3,1}}{3n(n+1)} - 384S_{3,2} - 384S_{4,1} \\
- &\quad 2688S_{-3,1,1} - 768S_{-2,1,-2} + S_1\Bigg(-\frac{8\left(135n^6-649n^5-1039n^4-569n^3+487n^2+621n+216\right)}{9n^4(n+1)^4} \\
- &\quad \frac{2144}{9}S_2 + \frac{32\left(31n^2+31n-12\right)S_3}{3n(n+1)} + 160S_4 + 1920S_{-3,1} + \frac{32\left(31n^2+31n-84\right)S_{-2,1}}{3n(n+1)} \\
- &\quad 1856S_{2,-2} - 512S_{3,1} - 3584S_{-2,1,1}\Bigg) - \frac{64\left(31n^2+31n-84\right)S_{-2,1,1,n}}{3n(n+1)} - 2688S_{-2,2,1} \\
- &\quad 2688S_{2,1,-2} + 768S_{3,1,1} + 5376S_{-2,1,1,1}\Bigg] \\
+ &\quad C_A C_F^2 \zeta_3\left[\frac{36\left(5n^4+10n^3+n^2-4n-4\right)}{n^2(n+1)^2} + 288S_{-2}\right] \\
+ &\quad C_A^2 C_F\left(\frac{24\left(n^2+n+2\right)}{n(n+1)} - 96S_1\right)S_{-2}^2 + \Bigg(\frac{8\left(27n^6+81n^5-209n^4-595n^3-272n^2-48n-9\right)}{9n^3(n+1)^3} \\
+ &\quad S_1\left(\frac{16\left(134n^4+268n^3+116n^2-18n-27\right)}{9n^2(n+1)^2} - 512S_2\right) - \frac{32\left(11n^2+11n-24\right)S_2}{3n(n+1)} + 512S_3 \\
+ &\quad 64S_{-2,1} - 768S_{2,1}\Bigg)S_{-2} + \frac{P_6(N)}{108n^3(n+1)^5} - 192S_{-5} + S_{-4}\left(-\frac{8\left(35n^2+35n-66\right)}{3n(n+1)} - 352S_1\right) \\
+ &\quad (-1)^n\left(-\frac{16\left(91n^2+80n-29\right)}{9(n+1)^5} + \frac{96S_{-2}}{(n+1)^3} + \frac{16(29n+23)S_1}{3(n+1)^4}\right) \\
+ &\quad S_{-3}\Bigg(128S_1^2 - \frac{16\left(11n^2+11n+24\right)S_1}{3n(n+1)} + \frac{8\left(134n^4+268n^3+203n^2+69n+27\right)}{9n^2(n+1)^2} \\
- &\quad 160S_{-2} - 768S_2\Bigg) + \frac{4\left(389n^4+778n^3+398n^2+9n-81\right)S_3}{9n^2(n+1)^2} - \frac{8\left(55n^2+55n-24\right)S_4}{3n(n+1)} \\
- &\quad 160S_5 - 224S_{-4,1} + \frac{256S_{-3,1}}{n(n+1)} + 384S_{-3,2} + S_1^2(-64S_3-256S_{-2,1}) \\
- &\quad \frac{16\left(134n^4+268n^3+137n^2+3n+27\right)S_{-2,1}}{9n^2(n+1)^2} + S_2\left(768S_{-2,1} - \frac{4172}{27}\right) \\
+ &\quad \frac{16\left(11n^2+11n-48\right)S_{2,-2}}{3n(n+1)} - 544S_{3,-2} + \frac{32\left(11n^2+11n-12\right)S_{3,1}}{3n(n+1)} + 192S_{3,2}
\end{aligned}
$$

$$
\begin{aligned}
&+ \quad 192S_{4,1} + 768S_{-3,1,1} + 256S_{-2,1,-2} + \frac{64\left(11n^2+11n-24\right)S_{-2,1,1}}{3n(n+1)} \\
&+ \quad S_1\Biggl(\frac{2\left(245n^8+980n^7+1542n^6+964n^5+211n^4-60n^3+156n^2+222n+90\right)}{3n^4(n+1)^4} \\
&- \quad \frac{8\left(11n^2+11n-8\right)S_3}{n(n+1)} - 128S_4 - 512S_{-3,1} \\
&- \quad \frac{32\left(11n^2+11n-24\right)S_{-2,1}}{3n(n+1)} + 512S_{2,-2} + 256S_{3,1} + 1024S_{-2,1,1}\Biggr) + 768S_{-2,2,1} \\
&+ \quad 768S_{2,1,-2} - 384S_{3,1,1} - 1536S_{-2,1,1,1}\Biggr\} \\
&+ \quad C_A^2C_F\zeta_3\left[-\frac{12\left(5n^4+10n^3+n^2-4n-4\right)}{n^2(n+1)^2} - 96S_{-2}\right] \\
&+ \quad C_F^2N_F\Biggl\{-\frac{32}{3}S_2^2 - \frac{4\left(15n^4+30n^3+79n^2+16n-24\right)S_2}{9n^2(n+1)^2} + \frac{P_7(n)}{9n^4(n+1)^4} - \frac{128}{3}S_{-4} \\
&+ \quad S_{-3}\left(\frac{32\left(10n^2+10n+3\right)}{9n(n+1)} - \frac{64}{3}S_1\right) + (-1)^n\left(\frac{64S_1}{3(n+1)^3} - \frac{128(4n+1)}{9(n+1)^4}\right) \\
&+ \quad S_{-2}\left(-\frac{32\left(16n^2+10n-3\right)}{9n^2(n+1)^2} + \frac{640}{9}S_1 - \frac{128}{3}S_2\right) + \frac{16\left(29n^2+29n+12\right)S_3}{9n(n+1)} - \frac{128}{3}S_4 \\
&+ \quad S_1\left(-\frac{2\left(165n^5+495n^4+495n^3+517n^2+336n+80\right)}{9n^2(n+1)^3} + \frac{320}{9}S_2 - \frac{128}{3}S_3 - \frac{128}{3}S_{-2,1}\right) \\
&- \quad \frac{64\left(10n^2+10n-3\right)S_{-2,1}}{9n(n+1)} + \frac{64}{3}S_{2,-2} + \frac{64}{3}S_{3,1} + \frac{256}{3}S_{-2,1,1}\Biggr\} \\
&+ \quad C_F^2N_F\zeta_3\left[32S_1 - \frac{8\left(3n^2+3n+2\right)}{n(n+1)}\right] \\
&+ \quad C_FN_F^2\left[\frac{51n^6+153n^5+57n^4+35n^3+96n^2+16n-24}{27n^3(n+1)^3} - \frac{16}{27}S_1 - \frac{80}{27}S_2 + \frac{16}{9}S_3\right] \\
&+ \quad C_AC_FN_F\Biggl[-\frac{2\left(270n^7+1080n^6+383n^5-979n^4-571n^3+507n^2+106n-132\right)}{27n^3(n+1)^4} \\
&+ \quad \frac{64}{3}S_{-4} + S_{-3}\left(\frac{32}{3}S_1 - \frac{16\left(10n^2+10n+3\right)}{9n(n+1)}\right) + (-1)^n\left(\frac{64(4n+1)}{9(n+1)^4} - \frac{32S_1}{3(n+1)^3}\right) \\
&+ \quad \frac{1336}{27}S_2 + S_{-2}\left(\frac{16\left(16n^2+10n-3\right)}{9n^2(n+1)^2} - \frac{320}{9}S_1 + \frac{64}{3}S_2\right) - \frac{8\left(14n^2+14n+3\right)S_3}{3n(n+1)} + \frac{80}{3}S_4 \\
&+ \quad \frac{32\left(10n^2+10n-3\right)S_{-2,1}}{9n(n+1)} + S_1\Biggl(-\frac{4\left(209n^6+627n^5+627n^4+137n^3-108n^2-108n-54\right)}{27n^3(n+1)^3} \\
&+ \quad 16S_3 + \frac{64}{3}S_{-2,1}\Biggr) - \frac{32}{3}S_{2,-2} - \frac{64}{3}S_3,1 - \frac{128}{3}S_{-2,1,1}\Biggr] \\
&+ \quad C_AC_FN_F\zeta_3\left[\frac{8\left(3n^2+3n+2\right)}{n(n+1)} - 32S_1\right]
\end{aligned}
$$

$$
\begin{aligned}
P_{qq}^{2,-,dabc} &= \frac{d_{abc}d^{abc}}{N_c} N_F \Biggl[-\frac{P_8(n)}{3n^5(n+1)^5(n+2)^3} + \frac{4\left(n^2+n+2\right)S_{-3}}{n^2(n+1)^2} - \frac{P_9(n)S_1}{3n^4(n+1)^4(n+2)^3} \\
&+ S_{-2}\left(-\frac{8S_1\left(n^2+n+2\right)^2}{(n-1)n^2(n+1)^2(n+2)} - \frac{4\left(n^6+3n^5-8n^4-21n^3-23n^2-12n-4\right)}{(n-1)n^3(n+1)^3(n+2)} \right) \\
&+ (-1)^n \left(\frac{16\left(5n^6+29n^5+78n^4+118n^3+114n^2+72n+16\right)S_1}{3(n-1)n^2(n+1)^3(n+2)^3} \right. \\
&- \left. \frac{4\left(13n^8+74n^7+179n^6+314n^5+644n^4+1000n^3+816n^2+352n+64\right)}{3(n-1)n^3(n+1)^4(n+2)^3} \right) \\
&- \frac{2\left(n^2+n+2\right)S_3}{n^2(n+1)^2} - \frac{8\left(n^2+n+2\right)S_{-2,1}}{n^2(n+1)^2} \Biggr] \qquad (31)
\end{aligned}
$$

For brevity we abbreviated $S_{\vec{a}}(n) \equiv S_{\vec{a}}$. Here, $C_A = N_c, C_F = (N_c^2-1)/(2N_c)$ are $SU(N_c)$ color factors, N_F denotes the number of quark flavors and N_c is the number of colors, with $N_c = 3$ for Quantum Chromodynamics. We have accounted for the color factor $T_R = 1/2$ explicitly, which is the same for all groups $SU(N_c)$. d_{abc} denotes a $SU(N_c)$ structure constant and the Einstein convention is applied calculating $d_{abc}d^{abc}$.

The functions $P_i(n)$ which appear in Eqs. (26–31) are given by

$$
\begin{aligned}
P_1(n) &= 29n^{10}+145n^9+130n^8-146n^7-479n^6-11n^5-464n^4-1748n^3-1600n^2 \\
&\quad -752n-16 \qquad (32)\\
P_2(n) &= 1359n^{10}+6795n^9+15246n^8+15646n^7+3851n^6-35089n^5-34648n^4 \\
&\quad +12280n^3+32592n^2+17616n+3456 \qquad (33)\\
P_3(n) &= 4971n^{10}+24855n^9+11770n^8-86322n^7-150929n^6-135893n^5-85692n^4 \\
&+ -18992n^3+22824n^2+15840n+259 \qquad (34)\\
P_4(n) &= 29n^{10}+145n^9+226n^8+110n^7+353n^6+501n^5+976n^4+940n^3+576n^2 \\
&\quad +208n+32 \qquad (35)\\
P_5(n) &= 1359n^8+5436n^7+8274n^6+24524n^5+11103n^4+12528n^3+4120n^2 \\
&\quad -2560n-1584 \qquad (36)\\
P_6(n) &= 4971n^8+24855n^7+10762n^6-57138n^5-92033n^4-40901n^3+10692n^2 \\
&\quad +1216n-2904 \qquad (37)\\
P_7(n) &= 207n^8+828n^7+1491n^6+2291n^5+1338n^4+453n^3-8n^2-160n-72 \qquad (38)\\
P_8(n) &= 4\bigl(13n^{10}+97n^9+326n^8+720n^7+1399n^6+2416n^5+3017n^4+2412n^3 \\
&\quad +1184n^2+336n+48\bigr) \qquad (39)\\
P_9(n) &= 2\bigl(9n^9+41n^8-3n^7-505n^6-1719n^5-2951n^4-3092n^3-2032n^2 \\
&\quad -768n-144\bigr) \qquad (40)
\end{aligned}
$$

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