From Moments to Functions in Quantum Chromodynamics

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Single-scale quantities, like the QCD anomalous dimensions and Wilson coefficients, obey difference equations. Therefore their analytic form can be determined from a finite number of moments. We demonstrate this in an explicit calculation by establishing and solving large scale recursions by means of computer algebra for the anomalous dimensions and Wilson coefficients in unpolarized deeply inelastic scattering from their Mellin moments to 3-loop order.

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1. Introduction

Higher order calculations in Quantum Field Theories easily become tedious due to the larger number of terms emerging and the sophisticated form of the contributing Feynman parameter integrals. This applies already to *zero scale* and *single scale* quantities. Even more this is the case for problems containing more than one scale. While in the latter case the mathematical structure of the solution of the Feynman integrals is widely unknown, it is explored to a certain extent for zero- and single scale quantities. Zero scale quantities emerge as the expansion coefficients of the running couplings and masses, as fixed moments of splitting functions, etc. They can be expressed by rational numbers and certain special numbers as *multiple zeta-values (MZVs)* [1, 2] and related quantities.

Single scale quantities depend on a scale z which may be given as a ratio of Lorentz invariants s'/s in the respective physical problem. One may perform a *Mellin transform* over z

$$\int_0^1 dz\, z^{N-1} f(z) = M[f](N) \,.$$

All subsequent calculations are then carried out in Mellin space and one assumes $N \in \mathbf{N}$, $N > 0$. By this transformation the problem at hand becomes discrete. One may seek a description in terms of difference equations. Zero scale problems are obtained from single scale problems treating N as a fixed integer or considering the limit $N \to \infty$.

A main question concerning zero scale quantities is: Do the corresponding Feynman integrals always lead to MZVs? In the lower orders this is the case. However, starting at some order, even for single-mass problems, other special numbers will occur [3]. This makes it difficult to use methods like PSLQ [4] to determine the analytic structure of the corresponding terms even if one may calculate them numerically at high enough precision since one has to known the respective basis completely. [1]

Zero scale problems are much easier to calculate than single scale problems. In some analogy to the determination of the analytic structure in zero scale problems through integer relations over a known basis (PSLQ) one may think of an automated reconstruction of the all–N relation out of a *finite number* of Mellin moments given in analytic form. This is possible for recurrent quantities. At least up to 3-loop order, presumably even to higher orders, single scale quantities belong to this class. Here we report on a general algorithm for this purpose, which we applied to the problem being currently the most sophisticated one: the determination of the anomalous dimensions and Wilson coefficients to 3–loop order for unpolarized deeply-inelastic scattering [8]. Details of our calculation are given in Ref. [9].

2. Single Scale Feynman Integrals as Recurrent Quantities

For a large variety of massless problems single scale Feynman integrals can be represented as

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[1] In a recent analysis [2] the relations between all MZVs in the non-alternating and alternating case were determined up to weight $w = 12$ and up to $w = 24$ in the non-alternating case using shuffle-, stuffle- and generalized doubling relations. These relations lead to basis lengths according to the conjectures by Broadhurst [5] and Broadhurst-Kreimer-Zagier [6], which meets the upper bound set by Terasoma, Goncharov and Deligne [7]. In the non-alternating case we verified that the latter bound is valid at least to $w = 26$ and stopped the calculation afterwards due to the large complexity involved. All this does not exclude the existence of exotic relations reducing the basis further.

polynomials in the ring formed of the nested harmonic sums $S_{a_1,...,a_k}(N)$, [10, 11] and the MZVs $\zeta_{a_1,...,a_l}$ over the rational function field $\mathbf{Q}(N)$. Here,

$$S_{b,\vec{a}}(N) = \sum_{k=1}^{N} \frac{(\mathrm{sign}(b))^k}{k^{|b|}} S_{\vec{a}}(k), \qquad a_i, b \in \mathbf{Z}\backslash\{0\}, \tag{2.1}$$

$$\zeta_{b,\vec{a}} = \sum_{k=1}^{\infty} \frac{(\mathrm{sign}(b))^k}{k^{|b|}} S_{\vec{a}}(k), \qquad a_i, b \in \mathbf{Z}\backslash\{0\} .$$

If $b = 1$, the meaning of $\zeta_{b,\vec{a}}$ is symbolic, since it diverges. The degree of divergence is a positive power of $S_1(\infty)$. Rational functions in N and harmonic sums obey recurrence relations. Thus, due to closure properties [14] also any polynomial expression in such terms is a solution of a recurrence. Consider as an example the recursion

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

It is solved by $S_a(N)$. Corresponding difference equations hold for harmonic sums of deeper nestedness. Feynman integrals can often be decomposed into a combination containing terms of the form

$$\int_0^1 dz \frac{z^{N-1}-1}{1-z} H_{\vec{a}}(z), \quad \int_0^1 dz \frac{(-z)^{N-1}-1}{1+z} H_{\vec{a}}(z) ,$$

with $H_{\vec{a}}(z)$ being a harmonic polylogarithm, [12]. This structure also leads to recurrences, cf. [13]. It is very likely that single scale Feynman diagrams do always obey difference equations.

3. Establishing and Solving Recurrences

We assume that a sufficiently large set of moments at integer values N_i is given for a physical quantity, which obeys a recurrence relation. One seeks

$$\sum_{k=0}^{l} \left[\sum_{i=0}^{d} c_{i,k} N^i \right] F(N+k) = 0 . \tag{3.1}$$

The method for determining potential recurrences is available in standard packages [14]. The corresponding linear system is dense. Rational number arithmetics is not feasible for the large systems to be solved. Let us consider as an example the difference equation being associated to the contribution of the color factor C_F^3 for the 3-loop Wilson coefficient $C_{2,q}^{(3)}$ in unpolarized deeply inelastic scattering. 11 Tb of memory would be required to establish (3.1) in a naive way. Therefore refined methods have to be applied. We use arithmetic in finite fields together with Chinese remaindering [15], which reduces the storage requirements to a few Gb of memory. The linear system approximately minimizes for $l \approx d$. If one finds more than one recurrence the different recurrences are joined to reduce l to a minimal value. It seems to be a general phenomenon that the recurrence of minimal order is this with the smallest integer coefficients, cf. also [16]. For even larger problems than those dealt with in the present paper, a series of further technical improvements may be carried out, [17].

For the solution of the recurrence low orders are clearly preferred. It is solved in depth-optimal $\Pi\Sigma$ fields [18]; here we apply advanced symbolic summation methods as: efficient recurrence solvers and refined telescoping algorithms. They are available in the summation package `Sigma` [19] implemented in the computer algebra system Mathematica.

The solutions are found as linear combinations of rational terms in N combined with functions, which cannot be further reduced in the $\Pi\Sigma$ fields. In the present application they turn out all to be nested harmonic sums $S_{\vec{b}}(N)$, (2.1). Other or higher order applications may lead to sums of *different type* as well, which are uniquely found by the present algorithm.

4. Determination of the 3-Loop Anomalous Dimensions and Wilson Coefficients

We apply the method to determine the unpolarized anomalous dimensions and Wilson coefficients to 3-loop order. Here we use the above method to all the contributions to a single color/ζ_i-factor. These are 186 terms. As input to the calculation we use the respective Mellin moments, which were calculated by a `MAPLE`-code based on the harmonic sum representation [8]. We need very high moments and calculate the input recursively. As an example, let us illustrate the size of the moments for the C_F^3-contribution to the Wilson coefficient $C_{2,q}(N)$. The highest moment required is $N = 5114$. It cannot be calculated simply with `summer` [11] because of time and storage reasons. The highest moment is a rational number with a numerator of 13388 and a denominator 13381 digits. Below we give the moments for $N = 3$ and $N = 500$.

```
N=3:
#11 digits / #10 digits

-98268084191 / 1166400000

N=500:
#1262 digits / #1256 digits

16418407704241967809530206191763765062843035444812620830571976007465070084937939 94
42241103234415916303114822220582876889422095708591511216773075853139951009783631 79
25189528176220340371861328469746270216726780129136750995112038078119385930439108 03
50443459202186960525883320363553250899983613542268823673221490376310537617643487 72
54038108742649687295200756192272854718024194037272078224737659999002363837403152 99
20505336016334843482494547575553446642108141111400647539113679868916741006507667 49
35787094786833905739774100135208949944639092913274258157665663863972761583173877 48
59454713926460897008751574450750731923285428909654620048057119987481444143793860 93
99373617980290444257899537261336751997905237704272985005100634640619858400662960 71
33725430156489191559640696069945973638863011850678272919370653007547869470636728 48
93820819268710786003286281319367660574759704508965566676221633658958087734281197 21
53527921310890635770450696939622130611988940570336060686956071232719697269810600 56
01158460943602399862339178722607222773226904501323768362535491521301166456705650 45
96669459201645860239580602717466067988988613607723330880307417756055465187887933 27
22643682970712174056544743758442382508892385389745484212981704259092517425594947 28
72017877003947396562261659860366839154407853462338171648227013134266795320251847
/
30574446142472253728825705143673586972781307413482821222064929328203524408504719 02
74910469621053366455636548736756907967139065656888203656019072637108639548263860 81
32275800378793618699410038028075908603588941428910467764471628959087879864232546 78
57767782833372317021306124994298195597985010740206762827692891029556794218857958 67
19829329986013203449719273749058899340599872719397602128363686195011892382154423 66
38057737019295092681577479928593848374037511830194236928685691682067897100475574 52
51312173822720602676814804962989755224676147078486397731859098582787997866373038 34
10171666762768475257047554931662632970797204707198136239015458119538539864565335 43
99941820505518279599887601211684907454769692594684546134316241791988607515130764 81
03047342059267031385194185757313159443748738978736467069936208256972185233163755 59
40682220047659627159242085261060081097404023801262609475246405093612838027557221 32
48566900515257246859197926415060823075679569623285600734710867992871312875646684 41
62566980835042338974364847020024713143308034214677739255411512739249859461787711 89
23124371622134381377038960647349871570208014131535554353113267197391175990443419 13
59226935873738566095942459482374692931487025167140382970776938233225125536018104 7
49658623247509112659762997679737527882711111677459300352000000000000000000

N=5114:
#13388 digits / #13381 digits
```

The corresponding difference equations (3.1) are determined by a recurrence finder. Furthermore, the order of the difference equation is reduced to the smallest value possible. The difference equations are then solved order by order using the summation package `Sigma`.

For the C_F^3-term in $C_{2,q}(N)$ the recurrence was established after 20.7 days of CPU time. Here 4h were required for the modular prediction of the dimension of the system, 5.8 days were spent on solving modular linear systems, and 11 days for the modular operator GCDs. The Chinese remainder method and rational reconstruction took 3.8 days. 140 word size primes were needed. As output one obtains a recurrence of 31 Mb, which is of order 35 and degree 938, with a largest integer of 1227 digits. The recurrence was solved by `Sigma` after 5.9 days. We reached a compactification from 289 harmonic sums needed in [8] to 58 harmonic sums, where the representation in [8] (see a corresponding attachment) has already been compactified following an idea of one of the present authors. The determination of the 3-loop anomalous dimensions is a much smaller problem. Here the computation takes about 18 h only for the complete result.

For the three most complicated cases, establishing and solving of the difference equations took $3+1$ weeks each, requiring ≤ 10Gb on a 2 GHz processor. This led to an overall computation time of about sixteen weeks, with the possibility to parallelize four times. Here we did not yet consider parallelization w.r.t. the 140 primes chosen, which would significantly reduce the computational time of the C_F^3 term discussed above and for other comparably large contributions.

In the final representation, we account for algebraic reduction [20]; for this task we used the package `HarmonicSums` [21] which complements the functionalities of `Sigma`. One observes that different color factor contributions lead to the same, or nearly the same, amount of sums at a given quantity. This points to the fact that the amount of sums contributing, after the algebraic reduction has been carried out, is governed by topology rather than the field- and color structures being involved. The linear harmonic sum representations used in [8] require many more sums than in the representation reached by the present analysis. A further reduction can be obtained using the *structural relations*, which leads to maximally 35 different sums up to the level the 3-loop Wilson coefficients [13]. It is not unlikely that the present method can be applied to single scale problems in even higher order. As has been found before in [13, 22–24] representing a large number of 2- and 3-loop processes in terms of harmonic sums, the basis elements emerging are always the same. This applies to the anomalous dimensions and Wilson coefficients of the space- and time-like polarized and unpolarized case, the polarized and unpolarized Drell-Yan process and hadronic Higgs-Boson production in the heavy mass limit, deep-inelastic heavy flavor production in the limit $Q^2 \gg m_Q^2$, higher order QED corrections in e^+e^- annihilation, as well as to soft and virtual corrections to Bhabha scattering.

In practice no method does yet exist to calculate such a high number of moments ab initio as required for the determination of the all *N* formulae in the 3–loop case. On the other hand, a proof of existence has been delivered of a quite general and powerful automatic difference-equation solver, standing rather demanding tests, which is ready to help in the solution of present day problems in higher order Quantum Field Theory. It opens up good prospects for the development of even more powerful methods.

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. To solve 3-loop problems this way is not possible at present, since the number of required moments is too large for the methods available. We established and solved the recurrences for all color resp. ζ-projections at once, which forms a rather voluminous problem. Yet we showed that giant difference equations [order 35; degree ~ 1000] can be reliably and fast established and solved unconditionally for the most advanced problems in Quantum Field Theory.

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