DESY 09-011
SFB-CPP-09/17

PROCEEDINGS OF SCIENCE

DESY 09-011
SFB-CPP-09/17

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.

XII Advanced Computing and Analysis Techniques in Physics Research
November 3–7 2008
Erice, Italy

[*] Speaker.

[†] This project was supported in part by German DFG SFB TR-9, Studienstiftung des Deutschen Volkes, projects P19462-N18, P20162-N18, and P20347-N18 of the Austrian FWF, and EC MRTN HEPTOOLS, contract MRTN-CT-2006-035505.

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arXiv:0902.4095v1 [hep-ph] 24 Feb 2009

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

[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 $S_{a_1,\ldots,a_k}(N)$, [10, 11] and the MZVs $\zeta_{a_1,\ldots,a_l}$ 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 ΠΣ 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 ΠΣ 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

164184077042419678095302061917637650628430354448126208305719760074650700849379399
422411032344159163031148222205828768894220957085915112167730758531399510097836317
925189528176220340371861328469746270216726780129136750995112038078119385930439108
504434592021869605258833203635532508999836135422688236732214903763105376176434877
540381087426496872952007561922728547180241940372720782247376599990023638374031529
920505336016334843482494547575553446642108141111400654753911367986891674100650767
357870947868339057397741001352089449446390929132742581576656638639727615831738774
859454713926460897008751574450750731923285428909654620048057119987481444143793860
993736179802904442578995372613367519979052377042729850051006346406198584006629607
337254301564891915596406960699459736388630118506782729193706530075478694706367284
938208192687107860032862813193676605747597045089655666762216336589580877342811972
153527921310890635770450696939622130611988940570336060686956071232719697269810600
011584609436023998623391787226072227732269045013237683625354915213011664567056504
966694592016458602395806027174660679889886136077233308803074177560554651878879332
722643682970712174056544743758442382508892385389745484212981704259095217425594947
287201787700394739656226165986036683915440785346233817164822701313426679532025184
730577446142472253728825705143673586972781307413482821222064929328203524408504719
749104696210533664556365487367569079671390656568882036560190726371086395482638608
132275800378793618699410038028075908603588941428910467764471628959087879864232546
577677828333723171021306124994298195597985010740206762827692891029556794218857958
198293299860132034497192737490588993405998727193976021283636861950118923821544236
638057737019295092681577479928593848374037511830194236928685691682067897100475574
513121738227206026768148049629897552246761470784863977318590985827879978663730383
410171666762768475257047554931662632970797204707198136239015458119538539864565335
999418205055182795998876012116849074547696925946845461343162417919886075151307648
103047342059267031385194185757313159443748738978736467069936208256972185233163755
594068222004765962715924208526106008109740402380126260947524640509361283802755722
485669005152572468591979264150608230756795696232856007347108679928713128756466844
162566980835042338974364847020024713143308034214677739255411512739249859461787711
892312437162213438137703896064734987157020801413153555435311326719739117599044341
913592269358737385660959424594823746929314870251671403829707763938233225125536018
104749658623247509112659762997679737527882711111677459300352000000000000000000
```

```
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 $\leq$ 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 $\sim$ 1000] can be reliably and fast established and solved unconditionally for the most advanced problems in Quantum Field Theory.

Acknowledgment. We would like to thank J. Vermaseren for discussions.

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