Loops and Legs

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DOI: http://dx.doi.org/10.3204/PUBDB-2018-00782/A9

We summarize the progress of the research performed in project A9 of the SFB 676 and highlight the most important results obtained.

1 Overview

Project A9 of the SFB 676 has produced 34 journal publications [1–34], three of which made it into *Physical Review Letters* [12, 28, 31]. Three papers are still under review [35–37]. Furthermore, nine proceedings contributions [38–44, 44, 45], two master theses [46, 47], and one PhD thesis [48] have emerged from SFB project A9. In the following, we review the scientific results achieved.

2 Loops and legs

The textbook approach (see e.g. Ref. [49]) to computing scattering amplitudes is through perturbation theory in appropriate coupling constants (which correlates with an expansion in Planck's constant) as applied to a path integral, schematically given as

$$\int d[\phi]\,(\ldots)\,e^{i\int d^D x \mathcal{L}(\phi)}\,. \tag{1}$$

The needed integrations are elegantly captured in the famous Feynman graph formalism. The fundamental difficulties faced by this method is illustrated in Table 1. At some point, the generated expressions will overwhelm even modern computing resources. As a rule of thumb, problems with fixed number of loops *plus* number of legs are in a universality class. Cutting edge phenomenological problems are currently roughly found at

$$\#\text{ loops} + \#\text{ legs} = 7\,. \tag{2}$$

Concrete results in this contribution include several which satisfy this rule of thumb.

The algebraic complexity of the final answer is determined to an extent by dimensional analysis. Scattering amplitudes have a fixed mass dimension, and the number of dimensionless ratios made out of all occurring scales (masses, momentum invariants) up to momentum conservation is the number of variables. Computational complexity, therefore, increases considerably and non-linearly with the number of legs. A roughly comparable increase in computational costs is associated to processes with increasing numbers of loops. These processes where particles split and join are inherently quantum effects and are, therefore, physically essential. For unobserved

# legs \ # loops	0	1	2	3	4	5	6
3	1	1	4	23	173	1587	17099
4	3	9	51	381	3477	37242	
5	15	87	675	6315	68745		
6	105	975	9930	113580			
7	945	12645	163170				
8	10395	187425					
9	135135						

Table 1: Feynman graph number statistics for a theory with only trivalent vertices (e.g. ϕ^3 theory), obtained using Ref. [50].

particles all quantum numbers must be summed over. By special relativity one particular, continuous quantum number is the Lorentz momentum, which must, therefore, be *integrated* over. Computing these so-called loop integrals are a major further obstacle to perform explicit computations.

The upshot of the mentioned complications is that, despite its age, the current frontier of calculations within the standard model (SM) of particle physics is given by Eq. (2). This holds even for the simpler case of massless particles only, which has less scales than the full SM. Truly general one-loop computations (the first quantum corrections!) have only become widely available over the last decade. The problem of computation has become even more pressing with the lack of smoking-gun evidence of beyond-the-SM (BSM) physics from LHC experiments. At the LHC, the main colliding particles are hadrons, which interact through all known nuclear forces. Since the strong force is much stronger than the electroweak force, this makes especially those effects captured by Quantum Chromodynamics (QCD) particularly important. Highly interesting physics including that of the Higgs boson, however, is contained in the electroweak sector of the theory. Hence the computation of QCD backgrounds alone is vital to the interpretation of almost any interesting BSM signal. Due to long lead times in next-generation collider building, precision is the most likely vector for discovery in the near- to medium-term future. This leads to a large motivation to develop tools and techniques to break the existing barriers already from a purely phenomenological point of view.

There are also more formal motivations to pursue such a development. The path integral of Eq. (1), for instance, requires a choice of field coordinates to define the integral. Any canonical transformation of these coordinates should leave physics invariant modulo potential anomalies. There is no known way, however, to utilize such symmetry much beyond linear transformations systematically. A general field transformation will, in fact, lead to a radically different looking Feynman graph series. This is one of the drivers of the huge complexity of Feynman-graph-based computations. Whenever a symmetry exists but is explicitly broken in the computation, an enormous intermediate expression swell occurs. An analogue of this in classical physics would be to compute the orbit of the earth around the sun in Cartesian coordinates centered around Pluto: the choice of coordinates leads to significantly larger intermediate expressions leaving the essential physics of the problem unchanged. Intriguingly, there are cases where the complicated Feynman graph computations yields simple answers for scattering amplitudes. This indeed suggests that physical symmetries have been missed, for instance in the example of the Parke–Taylor [51] amplitude in pure Yang–Mills theory (YM). Such examples motivate the search for computational techniques which bypass the intermediate complexity and intend to arrive straight at the answer.

The range of different motivations to study and develop the computation of observables has led to a healthy research effort throughout the history of quantum field theory, see e.g. https://en.wikipedia.org/wiki/Timeline_of_quantum_mechanics for historic aspects and Refs. [52, 53] for a general overview of recent developments.

The maximally supersymmetric $\mathcal{N} = 4$ Yang–Mills theory (SYM) has played a central role in pioneering new computational techniques. The addition of supersymmetry considerably simplifies many perturbative computations, while leaving in place some of the essential difficulties of especially high-loop computations. This makes $\mathcal{N} = 4$ SYM first of all an ideal toy model. Second, there are intriguing and not generically well-understood direct connections between QCD and $\mathcal{N} = 4$ SYM in perturbation theory at higher loop orders through certain number theory properties of the full results known as the maximal transcendentality principle (see below). Third, there is direct interest in studying the theory itself as it connects through AdS/CFT [54] directly to the strongly coupled version of this field theory in 't Hooft's planar limit [55]. In rare cases, this extra insight into the theory even enables the derivation of exact results. A prime example here is the Beisert–Eden–Staudacher (BES) [56] equation for the so-called cusp anomalous dimension in the planar limit. The first non-planar correction to the cusp anomalous dimension at four loops in $\mathcal{N} = 4$ SYM is in fact a central result of SFB project A9. This involves a single-scale problem at four loops with two on-shell and one off-shell legs. This problem satisfies Eq. (2).

On the other hand, the real world is certainly not manifestly supersymmetric and hence neither is the SM of particle physics. While using $\mathcal{N} = 4$ SYM as a toy model has undoubtedly fueled many developments, it has at times led to results which are hard to transpose to or toward the SM of particle physics. Within $\mathcal{N} = 4$ SYM, for instance, one naturally uses a chiral superspace formulated in terms of spinor helicity variables. These variables are hard-wired to four-dimensional physics, which does not mesh well with dimensional regularization in general. For supersymmetric theories, this is usually not a problem. For non-supersymmetric theories, work-arounds have been found at one loop or, on a case by case basis, at higher loops. The latter does not seem to generalize easily. A central product of Sec. 5 is a framework to compute scattering amplitudes without essential use of spinor helicity variables or supersymmetry, demonstrating its applicability, for instance, by computing for the first time analytic results for five gluons at two loops and four gluons at three loops. This involves a two-scale problem at three loops and a five-scale problem at two loops, both of which satisfy Eq. (2).

A particularly important motivational role in SFB project A9 was played by relations between the scattering of gravitons in general relativity (GR) and gluons in pure YM. Both parts can be traced back to this central idea which arose first in string theory. Early on in the development of this theory, Kawai, Lewellen and Tye (KLT) [57] noticed that the scattering of open-string states and that of closed-string states is intimately related at the string tree level. String scattering amplitudes of gravitons can be written as sums over products of string scattering amplitudes of gluons. In the point particle limit, this reduces to a relation between scattering gravitons in GR and gluons in YM. From the path integral point of view of field theory, this relation is rather mysterious but very welcome considering the complexity of Feynman graph perturbation theory in GR noted above. For quite some time, this relation was interpreted as a string theory artifact that was only valid at tree level. Even in this form, it is already useful to determine scattering amplitudes of gravitons through higher loop orders, as was pursued for instance in Ref. [58] for four-graviton scattering in maximal supergravity theory ($\mathcal{N} = 8$) to the three-loop level. The motivation here is the study of ultraviolet (UV) divergences: at the time, the consensus point of view was that these would set in first at three loops. Instead, using the flood of new insights into gluon scattering amplitudes at higher loop orders, it was initially found that the amplitude did not diverge as expected at this loop order. Instead, it behaved very much like four-gluon scattering amplitudes in $\mathcal{N} = 4$ SYM in the UV: they shared the same so-called critical dimension at the first four-loop orders. The natural conjecture that this persists to higher loop orders has since been pursued vigorously (e.g. in Refs. [59, 60]), and has very recently been disproved [61] at five loops. See Ref. [17] for a heuristic analysis.

3 Color-kinematic duality and amplitude relations at loop level

In systematizing high-loop graviton computations, a remarkable, double discovery was made by Bern, Carrasco and Johanson (BCJ) [62, 63]. First of all, these authors conjectured that gluon scattering amplitudes can always be written in a form where the kinematics-dependent parts obey a Jacobi identity, similar to that obeyed by the Lie algebra structure constants inherent in the formulation of YM. Secondly, these authors conjectured that replacing the color Lie algebra structures with a second copy of the kinematics-dependent parts will yield graviton scattering amplitudes. At tree level, both of these statements are known to hold through a variety of techniques, see e.g. Ref. [64] for an overview. At loop level, they have been verified mostly on a case-by-case basis for the integrands of scattering amplitudes. Together, the two conjectures are known as "color-kinematic duality." What is interesting in the context of this contribution is that, even in its current unproven form, color-kinematic duality functions as an ansatz generator. In short, one writes down an educated ansatz for the integrand of a certain scattering amplitude. Into this ansatz, flow beyond color-kinematic duality a number of expectations of the answer, such as expected manifest UV divergence and any graph symmetries. This ansatz will have a finite number of free parameters. Then Cutkosky-style unitarity cuts are used to match to the behavior of the physical amplitude, fixing terms in the ansatz. If the restricted ansatz matches on all D-dimensional unitarity cuts, one can be certain that it matches the full result as long as all propagators are strictly massless. Enforcing the Lie algebra structure conjectured by color-kinematic duality greatly simplifies a possible ansatz. Hence the conjecture offers a direct and concrete vector for explicit computation. A drawback is that a particular ansatz may not be general enough to capture the physical quantity, see e.g. Ref. [65] for a case where the ansatz needed to be unexpectedly complicated.

4 The full Sudakov form factor at four loops in $\mathcal{N} = 4$ super Yang–Mills theory

A full physical understanding or a derivation of color-kinematic duality has been lacking so far, especially on the gauge theory side. One idea would be to write a Lagrangian for YM whose vertices automatically generate a color-kinematic dual representation. This would immediately prove this part of the conjecture to all loop orders. Several attempts at a Lagrangian understanding of the duality exist [18, 66–68], with earlier, related work directed at the KLT relation [69]. Such a Lagrangian, if it existed, would have a further direct consequence: all observables in YM would have a color-kinematic-dual representation. The class of all observables is much larger than the set of all scattering amplitudes, containing for instance correlation functions of gauge-invariant operators. An even more general class of observables is formed by mixtures of gauge-invariant operators and on-shell states known as form factors.

The Sudakov form factor is an interesting observable that plays a central role in the analysis of infrared divergences, see e.g. Refs. [70–73]. Powerful theorems guarantee that the divergences of the Sudakov form factor in $\mathcal{N}=4$ SYM are governed by universal functions up to finite terms in the ϵ expansion of dimensional regularization, see Ref. [74]. These functions are the cusp and collinear anomalous dimensions. While the latter is regularization scheme dependent, the former is not. Both are truly universal functions for a given quantum field theory, appearing in a range of different situations. As noted above, the planar limit of the cusp anomalous dimension in the very special quantum field theory at hand is known to be given as the solution to a differential equation and has been computed up to many loops. The non-planar correction to this quantity first appears at four loops, which provides a major motivation to push to this order in perturbation theory. The motivation was further strengthened by a conjecture [75] that this particular correction vanishes in any quantum field theory. This conjecture was formulated by naive extrapolation of results through three loops to the four-loop order. Up to the three-loop order, the cusp anomalous dimension only depends on the quadratic Casimir invariant of the gauge group under study. The conjecture of Ref. [75], which became widely known as "Casimir scaling" (see e.g. Refs. [75–81]), was that this simply extrapolated to four-loop order for any quantum field theory, thereby implying the vanishing of the non-planar correction. Already prior to our work, there had been several indications that, beyond perturbation theory or in the Regge limit, the conjecture would not hold [82–84]. Eventually, the conjecture was settled conclusively in the negative for the first time in Ref. [31]. Here, the first non-planar correction to the cusp anomalous dimension was computed numerically in $\mathcal{N}=4$ SYM and shown not to vanish. The conclusion that Casimir scaling is violated at the four-loop order has since been supported by additional results in Ref. [85, 86], see also Ref. [34].

4.1 The general structure of cutting edge computations

Four-loop computations are, with few exceptions, a big challenge, even for current state-of-the-art computational tools. Hence, the results eventually presented in Ref. [31] were obtained in a number of smaller steps contained in several publications. These steps are, in fact, common to many modern computations of observables:

1. Generate an integrand for the quantity under study.
2. Project to scalar integrals.
3. Simplify the integrand by solving so-called integration-by-parts (IBP) identities. The result is then given in terms of a chosen basis of remaining so-called master integrals.
4. Compute the master integrals analytically or numerically, typically by expanding in terms of the dimensional-regularization parameter ϵ, and assemble the aimed-for physics result.

These steps will appear throughout this contribution.

Loop integrals arise necessarily in perturbative computations as explained above. Beyond the complexity highlighted above, there is a specific drawback of Feynman graphs in the context of maximally supersymmetric gauge theory: there is no known way of having this much supersymmetry manifest off-shell. Hence, cancellations induced by supersymmetry, such as the vanishing of UV divergences, are not directly manifest in Feynman graphs. This leads to considerably more complicated integrals being generated. In the context of the Sudakov form factor at four loops, this would be prohibitive. Another method to obtain the integrand is, as alluded to above, to write an ansatz large enough to contain the physical answer and to fix the coefficients in this ansatz by computing Cutkosky-style unitarity cuts. Crucially, these unitarity cuts contain only lower loop information. For many cuts, only tree-level information is needed. This type of unitarity-based approach is, in fact, the driving factor of the most recent round of advances at one loop in quite general quantum field theories, see, for instance, Refs. [87,88] and references thereto. In maximally supersymmetric theories, it is known that one can take the unitarity cuts not in $D = 4 - 2\epsilon$ dimensions, but instead in four dimensions. Here, the spinor helicity method allows manifest, linearized $\mathcal{N} = 4$ supersymmetry through Nair's [89] on-shell superspace formalism, which drastically simplifies many computations in this theory.

If the observable involves spinning particles, the integrand will typically involve polarization tensors, which keep track of the appropriate spin information. For gluons, for instance, polarization vectors would contract in general with all types of vectors in the problem at hand, including loop momenta. As a first step of simplifying the problem, one would like to reduce to integrals which only involve inner products of loop momenta and external momenta. This class of scalar integrals is referred to as "Feynman integrals." For maximally supersymmetric theories, such as the one under study here, the projection to scalar integrals is automatically performed using spinor helicity methods. This chiral-superspace formalism has also been extended to cover massive particles [2] and form factors [90]. In Sec. 5, an alternative reduction method to scalar integrals will be used and developed, which does not rely on supersymmetry.

Fixing the integrand and projecting to scalar integrals is certainly not enough for most physics goals. The integrals needed to achieve a given physics goal are in general very complicated. The integrand, however, is not nearly a unique object—the physical observables are, for instance, invariant under linear shifts of the loop integration variables. Infinitesimally, this invariance leads to IBP identities: full space-time derivatives with respect to the loop momenta of any integrand vanish after integration. It was realized early on [91, 92] that working out the derivatives gives a system of linear equations on the vector space spanned by a class of loop integrals. In Ref. [93], it was first realized that, if one introduces an ordering of the integrals in this class in terms of expected complexity, one can systematically solve complicated integrals in terms of simpler integrals by essentially a version of Gaussian elimination. This systematic method of solving IBP identities is known as Laporta's algorithm and has been implemented in several public codes such as `AIR` [94], `FIRE` [95–97], KIRA [98], and `Reduze` [99,100]. `LiteRed` [101,102] implements an approach somewhat distinct from IBP reduction. The output is a reduction in terms of a typically much smaller number of so-called master integrals, with the coefficient functions of the external-momentum invariants (generalizations of the traditional Mandelstam invariants) as well as the dimensional-regularization parameter. The master integrals are essentially a choice of basis. The number of master integrals tends to be fairly small and to be universal for classes of physical theories. Calculating master integrals becomes, therefore, a high-value target with benefits for several theories with different matter content at once.

Having expressed a physical result in terms of a basis of master integrals then leads to the postponed question of integrating these basis elements. Even though master integrals tend to be much simpler than the original integrals, the remaining challenge is, in many physically interesting cases, still a prohibitive obstacle. A variety of techniques have been developed over the years for this task aiming at typically either numerical or analytic integration. For the purposes of this contribution, two mostly numerical general techniques are especially relevant: integration using Mellin–Barnes (MB) integrals [103–105] or sector decomposition [106, 107]. Both of these are supported by a number of public codes, e.g. FIESTA [108–111] and SecDec [112–114] for sector decomposition and [105, 115–118] for MB representations. Both methods are under active development. Typically, the MB approach is numerically much faster and more reliable if efficient and valid MB representations can be found for the integrals at hand. This is known to be a generic problem for Feynman integrals with a non-planar topology [119], with partially automated resolution to the three-loop level [120]. Impressive analytic results have been obtained in those cases where a special form of a system of first-order differential equations with respect to kinematic invariants can be found [121]. Although work-around exists for lower loop orders [122, 123], these techniques do not directly apply to single-scale integrals, such as those that arise in the four-loop Sudakov form factor.

As an illustration of the general strategy for cutting-edge computation outlined here, consider the Sudakov form factor at three loops in massless QCD. Integrand generation and projection to scalar integrals are sub-leading problems here. Reduction to master integrals was reported in Ref. [124], with numeric integration reported first in Ref. [125], followed by several works culminating in the analytic expressions [126–128], see also Ref. [129]. The corresponding computation in $\mathcal{N} = 4$ SYM was performed after the QCD results in Ref. [130]. Below, a roughly similar series of steps will be shown to lead to the four-loop result, with the difference that $\mathcal{N} = 4$ SYM is the starting point.

4.2 The explicit computation

The first concrete step in the computation of the full Sudakov form factor at four loops in $\mathcal{N} = 4$ SYM was taken in Ref. [16]. This particular paper contains the first explicit exploration of color-kinematic duality for observables beyond scattering amplitudes (see also Ref. [131]). After outlining the general motivation and results, explicit examples are constructed for a range of examples in $\mathcal{N} = 4$ SYM, the most complicated one being the four-loop form factor for two on-shell multiplets and a member of the stress tensor multiplet: this is the Sudakov form factor. The approach for each is exactly as outlined above: an ansatz is created for which coefficients are fixed from unitarity cuts. The computation benefited greatly from previous developments for tree-level form factors in Ref. [90]. The result for the four-loop form factor obtained in Ref. [16] still contains a single free parameter, which could not be fixed from the cuts considered. The representation obtained through color-kinematic duality typically has good manifest UV properties in maximally supersymmetric theories, which translates into low numerator powers. This in turn corresponds to structurally simpler integrals. An interesting by-product of the methods developed in this paper is an analysis of the color structure of the Sudakov form factor through eight loops, using the computer algebra developed in Ref. [132]. In later work, a similar strategy yielded the integrand of the five-loop Sudakov form factor [133].

The next step according to the general scheme above for cutting-edge computation is the application of IBP identities to obtain an expression in terms of master integrals. The class of integrals involved, however, is highly complicated and presents a formidable challenge even to cutting-edge IBP reduction codes. The first reduction of integrals in this class was presented in Ref. [25]. The IBP reduction reported here was obtained by using the Reduze [99] code, modified to bypass a disk access problem. With this problem fixed, the code ran parallel on large computing resources for several months. To verify the obtained basis of integrals, a separate technique due to Ref. [134] for finding master integrals directly was explored. In essence, all steps performed by the MINT package were applied separately, and results were cross-compared. The free parameter left after comparing unitarity cuts turned out to drop out of the physical observable after applying IBP identities. To gauge the remaining difficulty of the master integrals, attempts were made to integrate the maximal propagator master integrals, which are the hardest cases numerically, with the FIESTA code. This was largely unsuccessful for the choice of master integrals used in Ref. [25], with an exception for one particular integral.

One particular problem of using IBP relations is that the result, in general, has complicated coefficients in a Laurent expansion around $\epsilon = 0$. This considerably complicates tracking the error budget at best and leads to large cancellation errors in the final result at worst. As an idea to combat this complexity, the use of 'rational' IBP relations was explored in Ref. [44]. Here, it was shown that a rational IBP reduction, i.e. one that does not depend on the dimensional regularization parameter ϵ, can be obtained as a sub-reduction of the IBP reduction obtained in Ref. [25]. This method does yield an expansion in terms of a choice of master integrals. It was also shown that different choices lead to vastly different expressions. By aiming at small rational expansion coefficients, a reasonably-looking expression was found for the non-planar part of the Sudakov form factor in $\mathcal{N} = 4$ SYM by hand. This again left the problem of integration.

What Ref. [44] clearly showed was the importance of picking a good basis of master integrals to expand the form factor in. Primarily, one would pick integrals for which the integrals are known as a basis. In the absence of advance knowledge of such integrals, such as in the case at hand, one can pick a basis that makes an expected property of the answer manifest. This is the starting point of Ref. [31], which uses a special property of $\mathcal{N} = 4$ SYM known as the "maximal transcendentality principle" [135, 136]. Many of the details of the computation reported here were presented in a longer paper [34].

Feynman integrals, in general, are known to have special number theory properties, especially for the transcendental constants generated by expanding Feynman integrals in the dimensional-regularization parameter. These constants can be assigned a so-called transcendental weight, which is typically a positive integer. Rational numbers are assigned weight zero. This weight is a number theory version of mass dimension and is, for instance, additive under multiplication. The maximal transcendental weight of the constants increases step-wise with the expansion in terms of ϵ, with the leading term being only rational. Most often, these constants fall into the class of multiple zeta values (MZVs), see e.g. Ref. [137] and references therein. For given transcendental weight, there is only a finite number of independent MZVs. It has been observed in many cases that, for $\mathcal{N} = 4$ SYM, a much stronger result holds: *only* MZV-valued terms of maximal weight appear, with potential sub-leading weight terms simply vanishing. Moreover, it has been conjectured [135, 136] that, for every result in QCD, one can match the leading transcendentality terms directly to the corresponding result in $\mathcal{N} = 4$ SYM. This is the aforementioned maximal transcendentality principle.

Given this principle, it is reasonable to expect that the Sudakov form factor at four loops in $\mathcal{N} = 4$ SYM will have a maximally transcendental expansion. Another way of expressing this follows by assigning the dimensional-regularization parameter ϵ transcendental weight -1 and stating that the form factor should have uniform transcendentality $2l$, where l is the loop order. The driver of Ref. [31] is the question if integrals can be found such that this expected property is manifest. This is guaranteed if a basis of master integrals exists which are uniformly transcendental (UT), and, for the Sudakov form factor at three loops, such a basis was found explicitly in Ref. [138]. For the single-scale integrals of the problem at hand, there is a conjecture that the integrands of UT integrals have constant leading singularities (only simple poles) [123, 139]. In the reported work, this property was used to systematically search for UT integrals within a large enough set of integrals. With additional work to find a reasonably looking representation of these integrals and taking into account the targeted four-loop form factor, this eventually led to a list of master integrals highly likely to be UT. For several integrals, a so-called "dLog" form was found proving the uniform transcendentality property. For others, very extensive checks were made. Using the rational IBP relations found in Ref. [44], it was possible to express the integrand found in Ref. [16] in terms of this basis. Extensive effort was made to find a representation in terms of a small number of UT integrals of a form that can be used easily in available integration programs.

Expressing the four-loop Sudakov form factor in $\mathcal{N} = 4$ SYM in terms of a basis of UT master integrals shows that the expansion of this quantity is indeed highly likely to be UT. This is already an interesting result, especially in the non-planar sector. It immediately implies that the cusp and collinear anomalous dimensions are, in this sector, also maximally transcendental. A second result first reported in Ref. [31] is that UT integrals turn out to be much easier to integrate numerically than generic integrals in the same class. Although this effect can be understood heuristically, both MB integrals as well as sector decomposition do not seem to be related directly to the number theory properties of the integrals. This effect is highly useful as is shown in Ref. [31], where it has resulted in a numerical result for the four-loop non-planar cusp anomalous dimension. This step involves extensive computing resources and careful management of results. Cross-checks between MB and sector decomposition results were obtained for cases where an efficient MB representation could be obtained.

The final result for the non-planar cusp anomalous dimension is statistically significantly non-zero, disproving the Casimir scaling conjecture. At the time it appeared, this result was the first for any four-loop non-planar cusp anomalous dimension in any quantum field theory. Several groups have confirmed the breakdown of Casimir scaling since [85,86,140]. Many of the details of the computation, including a full analysis of the errors in the computation and a first result for the non-planar collinear anomalous dimension, can be found in Ref. [34]. The errors can be analyzed by using the UT property to change the first five expansion coefficients into simple rational numbers times single, known MZVs using the PSLQ algorithm. Taking these to be the exact results then allows an estimate of the numerical error of the computation. Hence this procedure uses number theory properties to verify numerical integration results.

5 Scattering amplitudes and integrands from first principles

Where Sec. 4 has dealt with a specific observable at four loops and three legs, in this section tools and techniques for observables with more legs but mostly less loops are developed, including cases satisfying Eq. (2). This includes several observations for tree-level amplitudes. A prime motivation for many of the developments reported in this section is exactly the drive to bypass path integrals and Feynman graphs as crutches used for explicit computations highlighted above. One of the outputs of this section is a complete calculational engine directly based on physical first principles for scattering amplitudes. Another is a thorough physical understanding of perturbative gauge-gravity double-copy-type relations. A third output is a number of techniques and observations that hint at remarkable additional structure in cutting-edge computations, as will be demonstrated by exploring, for instance, the planar three-loop, four-point and two-loop, five-point gluon amplitudes, solving the remaining bottlenecks to complete analytic computation of the scattering amplitudes.

The input for Sec. 5 was, as was already highlighted above, the quest for the physical origin of color-kinematic duality. Even in its current state, this is already a powerful calculational tool, as was illustrated in Sec. 4 for a specific observable. The duality idea offers, however, no intrinsic, physical understanding where the extra structure comes from, neither in gauge theory itself nor in the relation to perturbative gravity. At tree level, much more is known about scattering amplitudes in general, as they are functionally rational functions of polarizations and momenta. Here, color-kinematic duality has two direct physical consequences: the KLT relations between YM and GR amplitudes and the BCJ relations for YM amplitudes. A first question, therefore, would be to find a physical understanding of these relations. For the BCJ relations, a first paper in this direction was Ref. [141], where the physical origin of the BCJ relations was traced to on-shell gauge invariance, coupled with what amounts to a power counting criterion. On-shell gauge invariance is a fundamental constraint on scattering amplitudes of massless matter [142]. This then begs the question if this can be extended to the KLT relations. This question was answered to the affirmative in Ref. [28]. This work first streamlined and generalized the work of Ref. [141], re-phrasing first-principle constraints on scattering amplitudes into systems of linear equations. Scattering amplitudes become generically vectors in a vector space. Using computer algebra, the dimensions of these vector spaces were mapped for classes of gluon and graviton scattering amplitudes. For gluon scattering through eight points, this shows directly the existence of BCJ relations for scattering amplitudes in pure YM. Up to five gravitons, it was then shown also to lead directly to the KLT relations, taking into account a power counting criterion. In addition, explicit scattering amplitudes were computed by requiring only physical poles to appear, a point emphasized in even greater detail from a different point of view in the later works of Refs. [143,144]. A point of fundamental interest is the observation that scattering amplitudes of gravitons exist which cannot be traced to sum over products of gluon amplitudes. The relation to color-kinematic duality should follow at tree level for all multiplicities by an extension of the techniques of Ref. [17]. Basically, this maps the solutions of two different linear problems to one another.

Having obtained first results mostly at tree level, a natural question is whether these techniques apply at the loop level, where knowledge for scattering amplitudes in general and for color-kinematic duality in particular is rather limited. Both of these are especially true for theories without supersymmetry. To use the first-principle approach effectively at the loop level requires a further idea, the origin of which is described in Ref. [49]. A classic computation described in this textbook is that of the gyromagnetic ratio (colloquially known as "$g-2$") in quantum electrodynamics. This quantity can be isolated from the computation of a form factor with two on-shell legs, basically expanding this quantity in solutions to the first principles used in the work described previously. A particular expansion coefficient then defines the gyromagnetic ratio. This gyromagnetic-ratio computation has recently reached the four-loop level analytically [145]. For scattering amplitudes, one can explore a similar strategy by expanding them into solutions to the on-shell constraints, see for instance Ref. [146] for an example. Central are a number of algebraic manipulations in linear algebra for a choice of basis for all scattering amplitudes for fixed external-particle content. This is a core part of Ref. [33]. This paper showcases a complete strategy for scattering amplitudes beyond path integrals with many example computations. Three-point amplitudes are covered thoroughly as illustrations of the general approach. For four-particle scattering, a complete basis for four-gluon and four-graviton scattering amplitudes is constructed (see also Ref. [147]). Both are shown to admit a factorization which is closely related to Bose symmetry. This factorization simplifies the analysis. Reference [33] contains additional formal results beyond perturbative gauge-gravity relations. A particularly appealing one is the result that self-interacting theories of massless spin-one bosons with a single dimensionless coupling constant in four dimensions necessarily involve Lie-algebra-valued coupling constants. Special results for scattering in three space-time dimensions are derived, including Hodge duality for gluons and the triviality of graviton scattering. A further formal and interesting result is the four-graviton amplitude at the one-loop order. This result is not new in itself, but is obtained here in such a straightforward computation that it holds the promise of pushing one loop order further, where only the four-helicity-equal amplitude has been obtained recently [148].

Phenomenologically, the results on the integrand of planar four-gluon scattering through two loops are especially promising in Ref. [33]. The one-loop computation could even be performed for basically any theory of gluons, including full effective field theories. This also forms the basis of a technique to iterate the computation of certain cuts to all loop orders, through a version of the so-called rung rule of maximally supersymmetric Yang–Mills theories. This technique tends to introduce highly non-local apparent poles into the computations rendering it less directly useful for explicit computation. The two-loop computation shows clearly how to merge computations of unitarity cuts with the solution of IBP relations obtained using computer algebra. The relation to the spinor helicity method was worked out explicitly. Different renormalization schemes were highlighted, differing in their treatment of the dimensionality of the particles in the loops and on the outside. Instrumental here was the approach to derive rational IBP relations as pioneered in Ref. [44]. It was also shown how color quantum numbers can be studied effectively using projectors. The same computer algebra techniques to compute color factors for form factors deployed in Ref. [16] were used here. Comparisons were made to results in the literature where available, finding full agreement.

The true litmus test for any new calculational technology in high-energy physics is the question if it can tackle cutting-edge computations. While the planar four-gluon, two-loop amplitude has been known for some time, the five-point version of this has been the subject of major recent efforts. Interestingly, the integration of a set of planar master integrals was obtained here first in two contemporaneous publications [149,150], with recent advances for the non-planar integrals [151,152]. The first steps in the general calculational scheme outlined above are, therefore, a bottleneck. Obtaining the integrand with Feynman graphs is, in the case at hand, impractical, requiring some application of unitarity methods. The traditional method to reduce the integrand to scalar integrals is the use of spinor helicity variables for the gluons. IBP reduction is furthermore a major problem previously considered undoable by public codes. Two papers presenting semi-numerical methods to obtain this particular scattering amplitude were presented very recently in Refs. [153, 154], presenting the amplitudes evaluated in a particular phase space point and finding agreement. There have been several works for the special helicity-equal amplitude at two loops through seven external gluons in Refs. [155–157]. The two-loop scattering amplitude for five planar gluons was a prime motivation for Ref. [37]. There are two main obstacles for scaling the techniques of Ref. [33] to say the two-loop planar five-gluon amplitude and beyond: algebraic complexity of the basis manipulations and solving the IBP reduction. In Ref. [37], the first obstacle is removed for most phenomenological applications featuring external bosons. The driver is a clever choice of basis. The basis choice can be motivated by extending the double-copy idea of perturbative gauge-gravity relations. After all, if graviton amplitudes are a double copy of gluons, can the gluons be written as copies of simpler building blocks as well? The conjecture in Ref. [37], verified up to six external gluons and four external gravitons, is that very simple one- and two-gluon building blocks suffice to span the space of all scattering amplitudes of a given class as tensor products. The tensor product structure greatly facilitates explicit analytic computations of needed matrix inverses, allowing even computation of leading-singularity cuts beyond the demarcation line set by Eq. (2).

The second obstacle to explicit analytic computation of the planar two-loop, five-gluon amplitude is the solution of the systems of IBP relations. In this context, it was observed that a good choice of coordinates for planar integrals can be formed out of coordinates of one-loop progenitors. For the case at hand, these are two one-loop pentagon topologies, glued along a common line. This choice of coordinates is good, as it clearly shows that one particular topology for the chosen parameterization is slightly simpler as an expression than the others—this is critical for being able to solve the required IBP relations using the FIRE code on fairly large computing resources. Intuitively, the good choice of coordinates likely translates into algebraically simpler IBP relations that are, therefore, computationally easier to solve. This then yields a form of the planar five-gluon, two-loop integrand in terms of a chosen basis of master integrals. A similar approach was also explored for the planar four-gluon, three-loop integrand.

The approach through a basis for scattering amplitudes makes clear that the integrand of a scattering amplitude in a basis of master integrals will generically contain manifest nonphysical poles in addition to the expected poles from infrared physics. For planar amplitudes, these are tree-level poles in physically forbidden channels. This is the multi-loop and multi-leg extension of a phenomenon observed in Ref. [33] as well (see also Ref. [158]). The real question is if these poles have non-vanishing residues. In Ref. [33], the explicit integration of the box function was needed to show that these residues vanish. In Ref. [37], it is pointed out that the expansion around these poles can be systematically constructed from differential equations with respect to kinematic invariants. Differential equations have been studied in depth recently following Ref. [121], where a special basis was proposed. Beyond consistency, it is highly interesting that expansions around nonphysical poles involve relations between a-priori independent master integral coefficients. To demonstrate the potential, the contribution of massive particles to four-gluon scattering at one loop is studied. It is well known in the field, see e.g. Ref. [159] for a discussion, that massive particles in loops lead to master integrals that evade all unitarity cuts. At one loop, these are the massive tadpole integrals. Hence, for massive particles flowing in loops, one typically has to resort to various laborious techniques to fix the coefficients of these integrals. Absence of nonphysical singularities, analyzed through differential equations as advocated in Ref. [37], turns out to suffice to fix this coefficient up to an additive renormalization factor. Massive particles are, of course, experimentally highly relevant.

6 Special functions

A powerful illustration of the wide applications the development of basic technology can have may be found within SFB project A9. Special attention was focused on hypergeometric functions, which play a central role in applications of quantum field theory to high-energy physics. In fact, Feynman diagrams may be reduced via MB representations to hypergeometric functions. The differential-reduction algorithm then allows one to systematically relate hypergeometric functions whose parameters differ by integers [13]. In this way, Feynman diagrams may be efficiently reduced to minimal bases of hypergeometric functions [13]. This provides a powerful alternative to the well-established IBP technique and is even superior than the latter because it can actually lead to a lesser number of master integrals, i.e. the counting of master integrals and their classification are achieved more efficiently and economically. This is bound to lead to dramatic simplifications in calculations of Feynman diagrams and scattering amplitudes because solving the master integrals is frequently the bottleneck to analytic expressions. In fact, in the case of the two-loop sunset diagram with different masses and space-like on-shell kinematics, it could be shown that one of the three master integrals produced by the standard IBP technique is redundant [4], a result which can be recovered by the IBP procedure only after applying the trick of eliminating a one-loop subdiagram in favor of an effective mass to be integrated over, as shown in Ref. [11]. A number of irreducible master integrals for L-loop sunrise-type and bubble Feynman diagrams with generic values of masses and external momenta were explicitly evaluated via the MB representation [30]. The differential-reduction algorithm also allows one to efficiently extract in analytic form the coefficients of the Laurent expansions of Feynman integrals in the parameter $\epsilon = 2 - D/2$ of dimensional regularization [160]. We released a Mathematica-based program package for the differential reduction of hypergeometric functions, called `HYPERDIRE`, which is available from the program library of *Computer Physics Communication*, where a detailed description and a useful manual may be found. Its current version can handle the generalized hypergeometric function ${}_{p+1}F_p$ with one argument, the Appell functions F_p $(p = 1, \ldots, 4)$ with two arguments [3], the residual Horn-type hypergeometric functions of two variables [21], the F_D and F_S Horn-type hypergeometric functions of three variables [22], as well as the Lauricella function F_C of three variables [27], which frequently appear in multi-loop calculations relevant for high-energy physics. This may be applied to Feynman diagrams with arbitrary powers of propagators and arbitrary masses. Another highly efficient method of finding relationships between hypergeometric functions is by comparing the results for Feynman integrals evaluated using different techniques [5].

In Ref. [20], the expansion method for ${}_3F_2$ hypergeometric functions developed by members of SFB project A9 [160] was applied to the field theory expansion of five-point superstring amplitudes on a flat background. Here, the role of the dimensional-regularization parameter ϵ is basically played by the string scale α'. The developed code turns out to be quite a bit faster than two methods proposed almost simultaneously [161, 162].

We also considered the derivatives of Horn hypergeometric functions of any number variables with respect to their parameters [36]. We demonstrated that the derivative of the function in n variables is expressed as a Horn hypergeometric series of $n + 1$ infinite summations depending on the same variables and with the same region of convergence as for original Horn function. The derivatives of Appell functions, generalized hypergeometric functions, confluent and non-confluent Lauricella series and generalized Lauricella series were explicitly presented. Applications to the calculation of Feynman diagrams were discussed, especially the series expansion in ϵ within dimensional regularization. Connections with other classes of special functions were discussed as well.

In Ref. [32], we evaluated the three-loop massive vacuum bubble diagrams in terms of polylogarithms up to weight six. We also constructed the basis of irrational constants being harmonic polylgarithms of arguments $\exp(ki\pi/3)$.

In Ref. [14], we showed that multi-fold MB transforms of Usyukina–Davydychev (UD) functions, which appear in connection with triangle ladder-like scalar diagrams in $D = 4$ dimensions, may be reduced to two-fold MB transforms, which come as as polynomials of logarithms of ratios of Mandelstam variables with certain coefficients. We also showed that these coefficients have a combinatoric origin. In Ref. [19], we presented an explicit formula for these coefficients. The procedure of recovering the coefficients is based on taking the double-uniform limit in certain series of smooth functions of two variables, which is constructed according to a pre-determined iterative way. This finite double-uniform limit was represented in terms of a differential operator with respect to an auxiliary parameter which acts on the integrand of a certain two-fold MB integral. We demonstrated that our result is compatible with original representations of UD functions. In Ref. [14], a chain of recurrence relations for analytically regularized UD functions was obtained implicitly by comparing the left- and right-hand sides of relations between diagrams of different loop orders. In Ref. [29], we reproduced these recurrence relations by calculating explicitly, via Barnes lemmas, the contour integrals produced by the left-hand sides of the diagrammatic relations. In this way, we explicitly calculated a family of multi-fold contour integrals of certain ratios of Euler gamma functions. We conjectured that similar results for the contour integrals are valid for a wider family of smooth functions which includes the MB transforms of UD functions.

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