

PERTURBATIVE QCD AT THE PRECISION FRONTIER*

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In this contribution, we give a brief overview of the status of perturbative quantum chromodynamics calculations and some recent advances in computational techniques. We also touch on one particular determination of the strong coupling constant and highlight the important role played by precise perturbative calculations in this measurement.

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1. Introduction

The successful operation of the Large Hadron Collider (LHC) at CERN has opened up a new era of exploration in particle physics, the outstanding highlight of which so far has been the discovery of the Higgs boson [1, 2]. However, as the direct detection of new phenomena not captured by the Standard Model of particle physics has eluded us so far, the search for subtle deviations of measured data from theoretical predictions is taking center stage. The increased sensitivity and precision of the experiments pose a formidable theoretical challenge though, as predictions must be computed at similarly high accuracies. In particular, the sophisticated modeling of the strong interaction in particle collisions is indispensable.

2. Perturbative QCD

Quantum chromodynamics (QCD) is the non-Abelian gauge theory of the strong interaction between quarks mediated by gluons [3]. It is asymptotically free, which means that the strength of the interaction diminishes as the energy scale is raised. This implies that high-energy particle interactions in QCD can be studied using *perturbation theory*. In this approach,

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quantities of interest such as cross sections are computed as expansions in some small parameter characterizing the strength of the interaction

$$\sigma = \alpha_S^p(\mu) [\sigma^{\text{LO}} + \alpha_S(\mu)\sigma^{\text{NLO}}(\mu) + \alpha_S^2(\mu)\sigma^{\text{NNLO}}(\mu) + \dots]. \quad (1)$$

In the equation above, $\alpha_S(\mu)$ denotes the *strong coupling* which plays the role of the expansion parameter, while σ^{LO} , $\sigma^{\text{NLO}}(\mu)$, and $\sigma^{\text{NNLO}}(\mu)$ refer to the *leading-order* (LO), *next-to-leading order* (NLO), and *next-to-next-to-leading order* (NNLO) contributions to the cross section. The numerical value of α_S at typical LHC energies is around 0.1, so a naive counting puts the size of the NLO and NNLO corrections at around 10% and 1%, respectively. However, in practice, this naive estimate can be off by as much as an order of magnitude. Furthermore, notice the quantity μ in Eq. (1). This denotes the renormalization scale whose value is chosen to be some typical energy scale in the particular process under study. As the equation implies, the full cross section on the left-hand side, σ , is in principle independent of μ . However, due to the unavoidable truncation of the perturbative series in practical calculations, perturbative QCD predictions retain some μ -dependence and hence come with an associated theoretical uncertainty. The magnitude of this uncertainty can be decreased by computing higher-order perturbative corrections. Thus, precise predictions require the evaluation of higher-order corrections not only from the point of view of the series expansion, but also from the point of view of controlling the theoretical uncertainty.

The straightforward application of QCD perturbation theory beyond leading order faces two conceptual challenges. First, one must compute the quantum mechanical transition amplitudes that describe the scattering process one is interested in and treat their ultraviolet divergences through renormalization. In the language of Feynman diagrams, higher-order corrections correspond to diagrams with virtual emissions (loops), and one has to evaluate the corresponding multi-loop Feynman integrals, which is a highly non-trivial task beyond the one-loop level. Second, these amplitudes must be used to compute measurable observables such as cross sections. Careful considerations show that this requires one to also include so-called real emission contributions, where the emitted extra radiation is not reabsorbed as in a loop diagram, but is rather “unresolved” (*e.g.*, soft, or collinear to another parton) in the final state. However, it turns out that even though predictions for physical observables are finite at each perturbative order (for properly defined so-called infrared and collinear-safe quantities), the various virtual and real contributions are separately infrared divergent. These divergences must then be regularized and properly treated before any numerical calculation can take place.

Both of the above issues are by now well-understood at NLO accuracy to the point where the automation of NLO QCD calculations for general processes has been realised in several program packages [4, 5] and these days, processes such as $e^+e^- \rightarrow 7j$ [6], $pp \rightarrow W + 5j$ [7], and $pp \rightarrow t\bar{t}b\bar{b} \rightarrow \mu^-\bar{\nu}_\mu e^+ \nu_e b\bar{b}b\bar{b}$ [8] (a $2 \rightarrow 8$ process) can be computed at NLO accuracy. Thus, current frontiers are the computations of 2-loop processes with 4 or more legs and several masses, as well as 3-loop massless processes on the one hand, but also the efficient treatment of infrared divergences at NNLO and beyond on the other.

In this contribution, we will focus on the issue of multi-loop integrals and present some of the recent progress in their evaluation. As this is a very large and very active field, the selection of topics to be discussed is necessarily incomplete and reflects the subjective choice of the author.

3. Multi-loop integrals

In order to get a basic idea about the mathematical difficulties associated with computing loop integrals, it is enough to examine a one-loop example. Hence, consider the one-loop diagram of Fig. 1, showing the production of a Higgs boson in gluon–gluon scattering through a top-quark loop. After

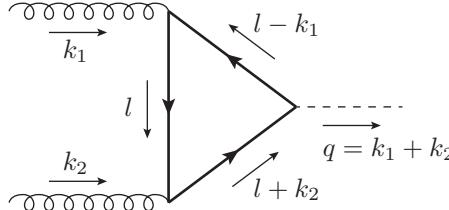


Fig. 1. One-loop diagram for $gg \rightarrow H$ mediated by a top-quark loop.

performing tensor reduction, this diagram leads to (among others) the following one-loop integral (we use dimensional regularization in $d = 4 - 2\epsilon$ spacetime dimensions):

$$\int \frac{d^d l}{(2\pi)^d} \frac{1}{(l^2 - m_t^2) \left[(l - k_1)^2 - m_t^2 \right] \left[(l + k_2)^2 - m_t^2 \right]}. \quad (2)$$

One can perform the integration over the loop momentum l symbolically and obtain a concrete integral representation of the result, *e.g.*, through Feynman parametrization (see *e.g.*, [9])

$$\frac{-i}{16\pi^2} \int_0^1 dx \int_0^1 dy \frac{y}{[m_t^2 - sxy(1-y)]} + \mathcal{O}(\epsilon), \quad (3)$$

where $s = q^2$. We have obtained a two-dimensional real integral representation. However, already for this simple case, the solution cannot be expressed in terms of elementary functions. In the multi-loop case, we generally encounter high-dimensional integrals that are very difficult to compute explicitly. Indeed, the concrete integrals one obtains in multi-loop computations become very cumbersome very quickly as the number of loops and/or the number of kinematic parameters (external momenta and particle masses) are increased and their direct evaluation is usually not possible.

One very fruitful approach to overcoming this issue is to focus on the *differential equations* (DE) satisfied by the function [10–12] in its kinematic parameters, rather than any specific integral representation. In principle, deriving the corresponding differential equations is algorithmic and proceeds through the solution of so-called *integration-by-parts* (IBP) identities [13, 14]. The basic idea is the following. Instead of concentrating on the integral in Eq. (2), let us consider the entire family of integrals

$$f(n_1, n_2, n_3) = \int \frac{d^d l}{(2\pi)^d} \frac{1}{(l^2 - m_t^2)^{n_1} [(l - k_1)^2 - m_t^2]^{n_2} [(l + k_2)^2 - m_t^2]^{n_3}}. \quad (4)$$

IBP identities now follow from the simple observation that, in dimensional regularization, the integral of a total derivative vanishes

$$0 = \int \frac{d^d l}{(2\pi)^d} \frac{\partial}{\partial l^\mu} \frac{v^\mu}{(l^2 - m_t^2)^{n_1} [(l - k_1)^2 - m_t^2]^{n_2} [(l + k_2)^2 - m_t^2]^{n_3}}, \quad (5)$$

where the four-vector v^μ can be chosen to be any external or loop momentum, $v^\mu = l^\mu, k_1^\mu, k_2^\mu$. It is not hard to see that explicitly performing the differentiation then leads to linear relations between f s with shifted arguments (IBP identities), implying that the set of $f(n_1, n_2, n_3)$ is not independent. In fact, it can be shown that the number of independent integrals is finite [15] and this (non-unique) set is called a set of *master integrals*. Evidently, any $f(n_1, n_2, n_3)$ can be written as a linear combination of master integrals. Although in principle this is straightforward [16], we stress that in practice, the efficient generation and solution of IBP identities is highly non-trivial and an active area of research.

It is now conceptually straightforward to derive a set of differential equations for the master integrals. Indeed, differentiating with respect to kinematic parameters (m_t and s in the example above) inside the integration,

it is clear that the derivative of any master integral (and any f in general) will be just a linear combination of f s with shifted arguments. But then this derivative can be written in terms of master integrals using the IBP identities. In this way, one can derive a system of first-order, homogeneous, linear differential equations for the master integrals of the form (here we use x_n to denote the set of kinematic parameters)

$$\partial_m \vec{f}(\epsilon, x_n) = A_m(\epsilon, x_n) \vec{f}(\epsilon, x_n), \quad (6)$$

where $\partial_m = \frac{\partial}{\partial x_m}$ and each A_m is an $N \times N$ matrix, where N is the number of master integrals. One may then attempt to solve this set of differential equations to obtain the master integrals which then allows one to compute any integral in the entire family.

The method of differential equations outlined above is in itself not new and has been used to evaluate multi-loop integrals for many important processes in the past. However, in recent years, several new developments have made the method even more powerful. In the following, we will briefly touch upon three broad directions of study:

1. Analytic approaches: recent advances include the understanding of a “good” choice of basis of master integrals and of the class of functions that arise as solutions when using such a basis.
2. Numerical methods: developments related to obtaining numerical solutions with “arbitrary” precision through generalized power series expansions.
3. Initial conditions: the auxiliary mass flow method provides a new, general solution for obtaining initial conditions.

Starting with developments in the analytic understanding of the DE method, a very important realization was that a proper choice of the basis of master integrals leads to an algorithmic solution of the DEs [17]. The idea is the following. In practical calculations, we are interested in the Laurent expansion of the solution in the parameter of dimensional regularization, ϵ . With this in mind, let us choose a new basis of master integrals, \vec{g} , related to our original basis as $\vec{f} = T \vec{g}$ for some invertible matrix $T(\epsilon, x_n)$. Substituting this into Eq. (6), we find

$$\partial_m \vec{g}(\epsilon, x_n) = B_m(\epsilon, x_n) \vec{g}(\epsilon, x_n), \quad (7)$$

where

$$B_m = T^{-1} A_m T - T^{-1} \partial_m T. \quad (8)$$

Now, if we are able to find a transformation T such that the ϵ dependence in B_m factorizes and appears only in the form

$$B_m(\epsilon, x_n) = \epsilon \tilde{B}_m(x_n), \quad (9)$$

then we can immediately construct the Laurent expansion (in ϵ) of the solution \vec{g} in terms of so-called *iterated integrals* [17]. In many cases, the iterated integrals which arise take the following form:

$$G(a_1, a_2, \dots, a_n; z) = \int_0^z \frac{dy_1}{y_1 - a_1} \int_0^{y_1} \frac{dy_2}{y_2 - a_2} \dots \int_0^{y_{n-1}} \frac{dy_n}{y_n - a_n}. \quad (10)$$

The functions $G(a_1, a_2, \dots, a_n; z)$ introduced above are called *multiple polylogarithms* (MPLs) [18] and due to the developments of the last decade [19–21], the properties of these functions are quite well understood. Indeed, many tools for the manipulation and numerical evaluation of MPLs have been implemented in publicly available packages [22–24] and analytic results obtained in terms of MPLs can readily be used in explicit computations of physical observables. Although a thorough understanding of MPLs has allowed very impressive progress in terms of obtaining analytic results, it is now well-established that not all loop integrals can be expressed in terms of them, and more complicated cases (typically at two or more loops and with massive particles) lead to iterated integrals beyond MPLs. Here we cannot enter into any of the rather elaborate technical details and note only that the study of the appropriate generalizations (such as elliptic MPLs) is currently a very active area of research.

Turning to the topic of numerical methods, we begin by noting that of course in practical calculations, what really matters is the ability to obtain the numerical value of the solution at any given point. Thus, the question arises as to whether it is possible to solve the set of DEs numerically. While the numerical solution of DEs is a very well-known problem of numerical analysis, the particularities of loop integrals demand some unique considerations. First, the structure of the solution for loop integrals is typically complicated and may contain poles, cuts, and logarithmic singularities. Hence, a naive numerical approach can easily be unstable or even deliver results that are outright wrong. Second, for phenomenological applications, it is of paramount importance to guarantee a high level of numerical accuracy, typically to at least 16 significant digits, the precision provided by standard double-precision floating-point arithmetic. These issues led in recent years to the development of the method of generalized power series for the numerical solution of DEs [25]. Without entering into technical details, the essential idea is that around any point s_0 , the solution to the DEs is locally represented by a generalized power series of the form

$$f(s) = \sum_{j=0}^{\infty} \sum_{k=0}^N c_{j,k} (s - s_0)^{r+j} \ln^k (s - s_0), \quad r \in \mathbb{Q}. \quad (11)$$

Here, s is a variable parametrizing a line segment in the neighbourhood of the point s_0 , where we assume an initial condition is known. After substituting a truncated form (in j) of this ansatz into the DEs, the $c_{j,k}$ coefficients can be determined algebraically. Numerical accuracy can be increased, in principle, arbitrarily by simply retaining more terms in the ansatz. As noted above, the form of the solution in Eq. (11) is valid only locally around the point s_0 . Hence, obtaining an evaluation at any given point generally requires that the solution be built up in several segments. Importantly, though, the construction of a suitable integration path can be performed algorithmically. This has allowed the construction of several packages implementing these ideas [26–28].

Last, we touch upon the issue of initial conditions. Obviously, in order to obtain explicit numbers from the solution of DEs, whether by evaluating an analytic formula or directly via numerical methods, initial conditions must be specified. Traditionally, initial conditions are computed by looking for a point or limit at which the integral simplifies and is amenable to direct calculation. Typical choices might be the vanishing of some mass parameter or kinematic invariant or the limit in which some mass or invariant goes to infinity, and the correct choice requires a case-by-case study of the problem. It is then important to understand if the computation of initial conditions can be made systematic. This question was answered in the affirmative in recent years and the so-called auxiliary mass flow (AMFlow) method [29] provides a general solution. The essential idea of the method is to introduce a non-physical mass-like parameter η into loop integrals (such that $\eta = 0$ corresponds to the original integral) and to study the behaviour of the solution with respect to this parameter. It is then found that in the $\eta \rightarrow \infty$ limit, the integrals always simplify, so this limit is a good choice for computing initial conditions. However, what makes the AMFlow method particularly powerful is that the basic construction can be iterated. Hence, if the $\eta \rightarrow \infty$ limit of the starting integral is still too difficult to compute, one can simply treat this as a new integral to be evaluated and apply the procedure once more, obtaining an initial condition for this new integral that is further simplified. It can be shown that in this way, any initial condition calculation can be reduced to a trivial one [30]. Finally, a differential equation for the η -dependence of any integral is constructed with the IBP method, and this DE is solved to evolve the initial condition at $\eta \rightarrow \infty$ to the physical point $\eta = 0$. The AMFlow method can naturally be merged with the method of generalized power series, which, in principle, allows the automation of the numerical calculation of loop integrals [31].

The advances for computing loop integrals described above (along with methods for dealing with IR singularities which we have not addressed) have led to a wealth of impressive results in recent years. Some selected highlights include the computation of: $H + j$ production at NLO with exact quark mass dependence [32, 33]; three-loop corrections to $gg \rightarrow H$ production with exact top-quark mass dependence [34, 35]; heavy-quark production in e^+e^- annihilation at N³LO [36]; 2-jet and 3-jet production at the LHC at NNLO [37, 38]; three-loop amplitudes for $2 \rightarrow 2$ parton scattering [39–41]; differential Higgs boson production at N³LO [42], and $pp \rightarrow WH/ZH$ production at N³LO [43].

4. The strong coupling from Z boson recoil: a recent precision highlight

Finally, to illustrate the impact of higher-order corrections in actual measurements, we consider the recent determination of the strong coupling from the recoil of Z bosons by the ATLAS experiment [44]. The leading-order process of Z -boson production and subsequent decay to a lepton pair proceeds via the electroweak interaction, and at this order, the transverse momentum p_T of the Z boson is zero. However, once QCD radiation from the initial-state quarks is taken into account, a non-trivial p_T spectrum is generated. Clearly, the hardness of this spectrum is a measure of the strength of the strong interaction and can be used to determine α_S . This measurement is particularly attractive not only due to the low backgrounds that allow one to collect very precise experimental data, but also due to the availability of highly accurate theoretical predictions.

In particular, perturbative predictions for fiducial cross sections for the basic $pp \rightarrow Z/\gamma^* \rightarrow l^+l^-$ process have been computed to N³LO accuracy in perturbative QCD [45] and even approximate N⁴LO results are now available [46]. Moreover, resummed predictions for small p_T have been computed at N⁴LL order [46]¹. Owing to the high perturbative order of the calculation, the theoretical predictions have very small uncertainty. Thus, the final extraction of the strong coupling yields the result

$$\alpha_S(M_Z) = 0.11828^{+0.00084}_{-0.00088}, \quad (12)$$

making this the most precise experimental measurement of $\alpha_S(M_Z)$. We stress that higher-order corrections play a crucial part in reducing theoretical uncertainty, which ultimately leads to the very impressive precision of the final result.

¹ It is beyond our scope to discuss resummation in any detail, but very roughly, it amounts to summing logarithmically enhanced (for small p_T) terms of the form $\alpha_S^n \ln^{2n-1}(p_T/Q)$ (“leading log”, LL), $\alpha_S^n \ln^{2n-2}(p_T/Q)$ (“next-to-leading log”, NLL), *etc.* to all orders in perturbation theory.

5. Conclusions

In this contribution, we gave a brief overview of some selected topics in perturbative QCD. In particular, we focused on modern developments in computational techniques used to evaluate loop integrals. In order to illustrate the impact of higher-order calculations in phenomenological studies, we briefly discussed a recent measurement of the strong coupling by the ATLAS Collaboration.

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