PROCEEDINGS OF SCIENCE

Towards QCD at Five Loops

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We report on recent progress on five-loop calculations in perturbative QCD. We discuss the computation of the perturbative quark condensate, decoupling in QCD, and the precision determination of charm and bottom quark masses. For the latter, we give some first results from a gauge-invariant subset of five-loop diagrams.

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1. Introduction

A cursory inspection of publications over the last two decades suggests that the first five-loop QCD calculation was completed as early as in 2005 [1], with more five-loop QCD results coming out over the following years [2–7], culminating in a flurry of activity in 2016 and 2017 [8–16], and further work afterwards [17, 18]. However, a second look reveals that almost all of these works use techniques like asymptotic expansion [19–22] or the R* operation [23–27] to reduce the number of loops to at most four. The only exception is a series of works [9, 11, 14] introducing an unphysical auxiliary mass [28–30], which means that the theory is arguably no longer QCD. It can therefore be argued that there are no genuine five-loop QCD results to date.

What could we hope to learn from a five-loop QCD calculation? The works cited above give us a first idea about the type of quantities that should be within reach soon. Order α_s^5 corrections to the Adler function and to total hadronic decay widths, e.g. of the τ or of the Z boson, are in principle desirable for determinations of the strong coupling. However, in general better data will be needed for a significant increase in precision. Next, the energy dependence of the strong coupling and the quark masses could be determined to formally six-loop order. This would include decoupling of heavy flavours at five loops. Another example is the calculation of five-loop moments of the total cross section for heavy hadroproduction at lepton colliders, which would greatly benefit charm- and bottom quark mass determinations.

Aside from the general interest in the precise knowledge of fundamental parameters, the masses of the charm and the bottom quark have to be known with high precision for applications in flavour physics and for future Higgs coupling measurements. Projections for the HL-LHC suggest that the strength of the Yukawa coupling to the bottom quark will be measured with statistical and systematic experimental uncertainties of about one per cent [31]. At a high-energy lepton collider, the overall uncertainty could be improved by at least a factor of two and per cent level precision is within reach for the charm Yukawa coupling [32]. In order to draw conclusions about the Higgs sector, this precision has to be matched by the Standard Model prediction. This means that the bottom-quark mass has to be known to within half a per cent and the charm quark mass to within one per cent.

Whether this level of precision has already been reached with present quark mass determinations depends on the way errors are assessed and propagated when evolving the quark masses from the scale at which they are determined up to the Higgs boson mass. Following the original four-loop determination [33, 34], the perturbative uncertainty amounts to 3 MeV for the bottom quark and 2 MeV for the charm quark and is therefore negligible. However, this viewpoint has been challenged in [35, 36], where the theory uncertainties are estimated at 10 MeV for the bottom quark and 21 MeV for the charm quark. A five-loop quark mass determination would resolve this disagreement and ensure that future Higgs coupling measurements are not limited by theory.

2. Massive QCD at Five Loops

The most promising candidates for the first genuine five-loop QCD calculations are quantities depending on a single scale, which can be factored out from all Feynman integrals. If this scale is an external momentum, one arrives at massless propagator-type Feynman diagrams. For this class of diagrams, a range of dedicated methods have been developed. For example, integration-by-parts

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reduction can be systematised for specific diagram topologies exploiting the triangle [37] and the diamond [38] rule. Diagrams can be simplified — sometimes even reduced to trivial base cases — with the help of graphical functions [39]. Thanks to the glue-and-cut method [40], all 281 master integrals are known [41]. Still, the fact that there are 64 diagram families with 15 propagators and 20 possible scalar products poses a considerable combinatorial challenge.

An alternative is to consider problems with a single non-zero internal quark mass and vanishing external momenta. If all external particles are massless, there are 34 families of massive five-loop vacuum diagrams, with 12 propagators and 15 possible scalar products. While there are only 156 master integrals, most of them remain unknown. In the following we will focus on this scenario.

2.1 General Setup

Our calculational setup is based on the standard steps of a multiloop calculation. Diagrams are generated with `QGRAF` [42]. Their families are identified using custom code [43] based on `nauty` and `Traces` [44]. We use `FORM` [45] for inserting the Feynman rules and simplifying the resulting expressions. The resulting scalar integrals are reduced to master integrals using integration-by-parts reduction [37] via Laporta's algorithm [46]. To this end, we use `crusher` [47] with `tinbox` [48] for reduction over finite fields [49–53].

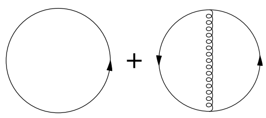
2.2 The Quark Condensate

The heavy quark condensate $\langle\bar\psi\psi\rangle$ appears in the leading non-analytic contribution of the Operator Product Expansion [54], or equivalently, in the asymptotic small-mass expansion. It has been suggested that its non-perturbative value can be obtained from a perturbative evaluation via renormalisation group optimised perturbation theory [55–59]. Its anomalous dimension is proportional to the vacuum anomalous dimension γ_0 [60], viz.

$$\mu^2 \frac{d}{d\mu^2} m\langle\bar\psi\psi\rangle = -4m^4\gamma_0, \tag{1}$$

which provides a powerful cross check of the five-loop result for γ_0 [16].

The first two orders of the perturbative expansion of the quark condensate correspond to the sum of only two vacuum diagrams:

$$\langle\bar\psi\psi\rangle =$$

$$+ \mathcal{O}(\alpha_s^2). \tag{2}$$

At five loops, 3451 diagrams contribute. After inserting the Feynman rules, we obtain approximately 400 000 scalar vacuum integrals with up to 4 dots (i.e. propagators raised by one power) and 4 powers of scalar products in the numerator. We consider different approaches for the numerical evaluation of the resulting 156 master integrals.

2.3 Numerical Evaluation of Master Integrals

Using `FIESTA` [61] for numerical sector decomposition [62], we obtain

$$\langle\bar{\psi}\psi\rangle\Big|_{(\frac{\alpha_s}{\pi})^4} = \frac{m^3}{16\pi^2}\Bigg[\frac{(-3.5 \pm 3.0)\times 10^{-8}}{\epsilon^{11}} + \frac{(-2.1 \pm 7.6)\times 10^{-6}}{\epsilon^{10}} + \frac{(0.2 \pm 2.1)\times 10^{-4}}{\epsilon^{9}} + \frac{(-0.5 \pm 7.5)\times 10^{-2}}{\epsilon^{8}} + O(\epsilon^{-7})\Bigg], \tag{3}$$

in $d = 4 - 2\epsilon$ dimensions, concluding that this approach alone is insufficient to obtain a meaningful result. We observe a loss of approximately two significant digits per order in the dimensional regulator ϵ, which suggests that master integrals have to be known with better than double precision. We have not found any significant improvement using quasi-Monte Carlo methods [63], a quasi-finite basis [64], tropical integration [65], or `pySecDec` [66].

To obtain high-precision results for the master integrals, we use two approaches. In the first approach, we raise one propagator power in the master integrals to a symbolic power x and obtain a coupled set of difference equations via integration-by-parts reduction. This system is solved numerically through a truncated factorial series ansatz inserting recursively determined boundary conditions for $x \to \infty$ [46, 67], where the integrals reduce to lower loops.

Alternatively, we evaluate the master integrals via numeric integration over a loop momentum, where the integrand is a propagator-type integral. It is then straightforward to evaluate the angular integral. The momentum routing can always be chosen such that the loop momentum flows through a massive line. Since all fermion lines are closed, this means that the propagator-type integrand has no massless cuts and is therefore infrared finite. Defining the loop integral measure as $[dq] \equiv \frac{d^dq}{i\pi^{d/2}}$, one arrives at the symbolic form

$$T = -\int_0^{-\infty} \frac{dq^2}{\Gamma(2-\epsilon)} \frac{(-q^2)^{1-\epsilon}}{(m^2-q^2)^a} P_0(q^2)\,, \tag{4}$$

where T denotes the original vacuum integral, a the power of the propagator with momentum q, and P_0 the remaining propagator-type integral after removing said propagator. The integrand can be made ultraviolet finite by either introducing a suitable subtraction term or by choosing a sufficiently large. In the latter case, the corresponding master integral (where typically $a = 1$) can be computed from T via integration-by-parts reduction.

To compute the integrand P_0 we derive a set of differential equations for the propagator-type master integrals P_i [68, 69], which we solve for $q^2 \to 0$ and $q^2 \to -\infty$ with generalised power series ansätze

$$P_i = \sum_{k=0}^{N-1} c_{ik} q^{2k} + O(q^{2N}), \tag{5}$$

$$P_i = \sum_{n=0}^{\#\text{loops}} \sum_{k=k_0}^{N-1} d_{ikn} \left(-\frac{1}{q^2}\right)^{k+n\epsilon} + O\left(\frac{1}{(-q^2)^N}\right). \tag{6}$$

The boundary conditions $b_{i,0}$ and $b_{i,k_0,n}$ correspond to products of known massive vacuum diagrams [70, 71] and massless propagators [40, 72] with at most four loops. After subtracting the

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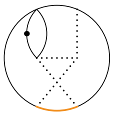
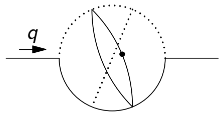
logarithmic high-energy contribution and performing a conformal mapping $q^2 \to \frac{4\omega}{(1+\omega)^2} m^2$ we construct a high-precision Padé approximation from the expansion coefficients [73–75]. A similar procedure was originally proposed in [76].

As an example, we consider the following vacuum diagram, routing the numerical integration momentum through the bottom-most line:



$$= -\int_0^{-\infty} \frac{dq^2}{\Gamma(2-\epsilon)} (-q^2)^{1-\epsilon} \quad \text{———} \quad \times \tag{7}$$



We derive the differential equations for the four-loop propagator in the integrand and insert the ansätze in equations (5), (6). For $N = 20$ we obtain the Padé approximations shown in figure 1.

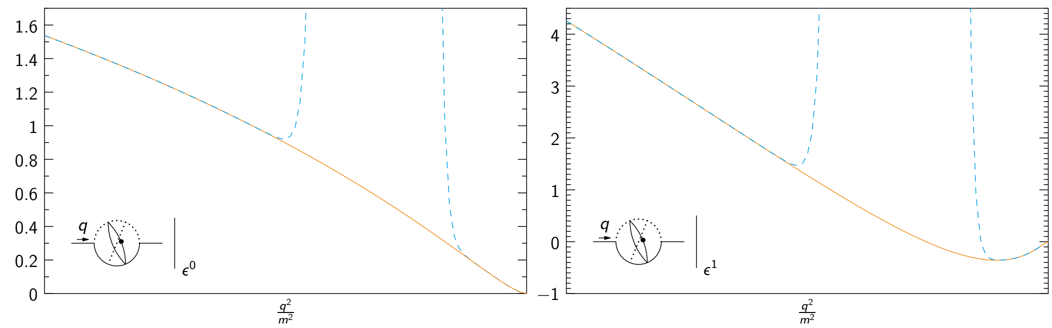
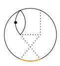


Figure 1: Padé approximations for the leading two coefficients in an expansion around $d = 4$ dimensions for a four-loop propagator-type diagram.

Numerical integration then yields



$$\times\, e^{5\gamma_E \epsilon} = 5.81253093584165969\,49 - 31.572349480122869826\epsilon + O(\epsilon^2). \tag{8}$$

Changing the integration contour in equation (4) to the line from 0 to $-i\infty$ changes the result by less than $10^{-19} + 2 \times 10^{-18}\epsilon$. Using $N = 25$ expansion terms reproduces the result within this uncertainty. We also find good agreement with a numerical evaluation using `FIESTA`, which yields $5.81409 - 31.58070(87)\epsilon$.

2.4 Decoupling

The presence of heavy quarks in virtual corrections is problematic in perturbative QCD in calculations where all other energy scales are much smaller than the heavy quark mass. On the purely practical level, diagrams with massive internal lines are notoriously hard to calculate. What is more, potentially large logarithms $\ln \frac{E}{m_Q}$, where m_Q is the heavy quark mass and E a typical energy for the process, can spoil the perturbative convergence in the $\overline{\text{MS}}$ scheme. The solution is to integrate out the heavy quark, i.e. to construct an effective n_l flavour theory, where $n_f = n_l + 1$ is the original number of quark flavours. The couplings can be related via

$$\alpha_s^{(n_l)} = \alpha_s^{(n_f)} \frac{\Delta_{cgg}}{\Pi_c^2 \Pi_g}, \tag{9}$$

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where Π_c and Π_g are the (scalar) ghost and gluon polarisation functions. Δ_{cgg} is the quantum correction to the truncated 1PI ghost-gluon vertex Γ_{cgg}, viz.

$$\Gamma_{cgg} = \Gamma^{(0)}_{cgg}(1 + \Delta_{cgg}), \tag{10}$$

where $\Gamma^{(0)}_{cgg}$ is the tree-level vertex. All Green functions are evaluated for vanishing external momentum and vanishing light quark masses. This decoupling relation is known to four-loop order [77].

At five-loop order, we obtain 131 860 803 scalar vacuum integrals with up to 7 dots and 6 scalar products. The reduction is currently ongoing, with 31 out of 34 integral families completed.

2.5 Heavy Quark Masses

The currently most precise determinations of heavy quark masses are based on sum rules. Let us define (inverse) moments $\mathcal{M}_n$ of the ratio $R_Q(s) = \frac{\sigma(e^+e^-\to Q\bar{Q})}{\sigma(e^+e^-\to\mu^+\mu^-)}$ as

$$\mathcal{M}_n = \int_{s_0}^{\infty} ds\, \frac{R_Q(s)}{s^{n+1}} = \frac{12\pi^2}{n!}\left[\left(\frac{d}{dq^2}\right)^n \Pi_Q(q^2)\right]_{q^2=0}, \tag{11}$$

where the proportionality to a derivative of the heavy-quark contribution Π_Q to the vacuum polarisation follows from a dispersion relation. These derivatives at vanishing external momentum can be evaluated perturbatively in terms of massive vacuum diagrams. The quark mass can then be extracted by comparing the calculated moments to moments obtained from the experimentally measured R_Q ratio or moments simulated on the lattice.

We have evaluated a gauge-independent subset of the five-loop contribution to the first moment. Concretely, for n_h degenerate massive quarks and n_l massless quarks, we have determined the contributions proportional to $n_h^4, n_h^3 n_l$, as well as the contribution from all diagrams with two or three massless quark loops. Using the setup outlined in section 2.1 we arrive at a result expressed in terms of the master integrals depicted in figure 2.

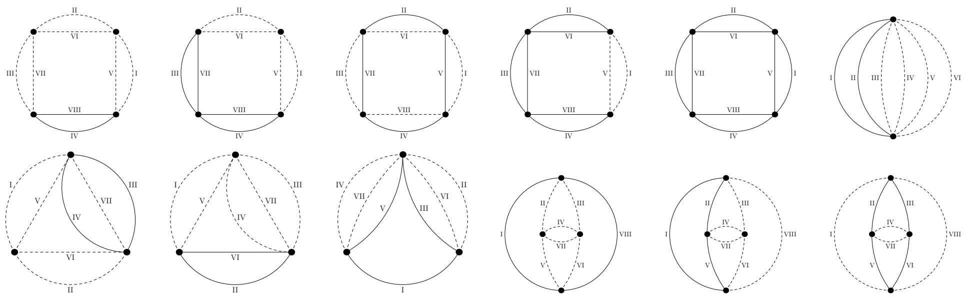

Figure 2: Master integrals originating from vacuum diagrams with at least two massless or at least three massive quark loops.

Evaluating the master integrals with sector decomposition yields

$$\begin{aligned}\mathcal{M}_1^{5\text{ loop}} = \frac{3\pi^2}{m_Q^2}\left(\frac{\alpha_s}{\pi}\right)^4 n_h C_F \Big[&0.6\, T_F^3 n_l^3 + 1.2\, T_F^3 n_l^2 n_h + 0.9\, T_F^3 n_l n_h^2 \\ &+ 0.2\, T_F^3 n_h^3 + (C_F - 5C_A) T_F^2 n_l^2 + \ldots\Big].\end{aligned} \tag{12}$$

3. Conclusions

While there is no complete genuine five-loop QCD result so far, a number of calculations are well underway. There is steady progress towards five-loop determinations of the heavy quark condensate, the decoupling coefficients, and the masses of charm and bottom quarks from sum rules.

The biggest remaining challenge seems to be a numerical high-precision evaluation of the master integrals corresponding to massive vacuum diagrams. Here, we use a combination of sector decomposition, recurrence equations, and direct integration over one loop momentum.

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