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RunDec: a Mathematica package for running and decoupling of the strong coupling and quark masses

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Abstract

In this paper the formulae are collected which are needed for the computation of the strong coupling constant and quark masses at different energy scales and for different number of active flavours. All equations contain the state-of-the-art QCD corrections up to three- and sometimes even four-loop order. For the practical implementation `Mathematica` is used and a package containing useful procedures is provided.

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Program Summary

Title of program: `RunDec`

Available from:
`http://www-ttp.physik.uni-karlsruhe.de/Progdata/ttp00/ttp00-05/`

Computer for which the program is designed and others on which it is operable: Any work-station or PC where `Mathematica` is running.

Operating system or monitor under which the program has been tested: UNIX, Mathematica 4.0

No. of bytes in distributed program including test data etc.: 65000

Distribution format: ASCII

Keywords: Quantum Chromodynamics, running coupling constant, running quark mass, on-shell mass, $\overline{\rm MS}$ mass, decoupling of heavy particles

Nature of physical problem: The values for the coupling constant of Quantum Chromodynamics, $\alpha_s^{(n_f)}(\mu)$, actually depends on the considered energy scale, μ, and the number of active quark flavours, n_f. The same applies to light quark masses, $m_q^{(n_f)}(\mu)$, if they are, e.g., evaluated in the $\overline{\rm MS}$ scheme. In the program `RunDec` all relevant formulae are collected and various procedures are provided which allow for a convenient evaluation of $\alpha_s^{(n_f)}(\mu)$ and $m_q^{(n_f)}(\mu)$ using the state-of-the-art correction terms.

Method of solution: `RunDec` uses `Mathematica` functions to perform the different mathematical operations.

Restrictions on the complexity of the problem: It could be that for an unphysical choice of the input parameters the results are nonsensical.

Typical running time: For all operations the running time does not exceed a few seconds.

1 Introduction

Quantum Chromodynamics (QCD) is nowadays well established as the theory of strong interaction within the Standard Model of elementary particle physics. In recent years there has been a wealth of theoretical results (for a review see [1]). At the same time perturbative QCD has been extremely successful in describing the experimental data with high precision.

The fundamental quantity of QCD is the so-called beta function which connects the value of the strong coupling constant, $\alpha_s(\mu)$, at different energy scales μ. It is thus particularly important to know the beta function as precise as possible. In [2] the four-loop corrections were evaluated allowing for a consistent running at order α_s^4. In the majority of all computations performed in QCD the $\overline{\rm MS}$ renormalization scheme [3] is adopted. In this scheme the Appelquist-Carazzone decoupling theorem [4] is not directly applicable. When crossing flavour thresholds, it is thus important to perform the decoupling "by hand". In order to be consistent, four-loop running must go along with the three-loop decoupling relation which was evaluated in [5].

Similar considerations are also valid for quark masses. Also here the renormalization group function is available up to the four-loop level [6] and the corresponding decoupling relation up to order α_s^3 [7] (see also [8]).

In this paper all relevant formulae are collected which are necessary for the running and decoupling of α_s and for quark masses. Their proper use is discussed and easy-to-use `Mathematica` [9] procedures collected in the package `RunDec` are provided. Their handling is described and examples are given.

The outline of the paper is as follows. In the next Section the formulae are presented which are needed for the running of the strong coupling constant up to the four-loop level. The corresponding equations for the quark masses are presented in Section 3. In addition the conversion formulae between the $\overline{\rm MS}$ and on-shell scheme are discussed in some detail. Section 4 is concerned with the decoupling of the strong coupling and quark masses. Finally, in Section 5, the most important procedures of the package `RunDec` are described in an easy-to-use way. For most practical applications they should be sufficient. In the Appendix the complete collection of procedures is given.

2 Running strong coupling constant

The beta function governing the running of the coupling constant of QCD is defined through

$$\mu^2\frac{\mathrm{d}}{\mathrm{d}\mu^2}\frac{\alpha_s^{(n_f)}(\mu)}{\pi} \;=\; \beta^{(n_f)}\left(\alpha_s^{(n_f)}\right) \;=\; -\sum_{i\ge0}\beta_i^{(n_f)}\left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^{i+2}\,, \tag{1}$$

where n_f is the number of active flavours. The coefficients are given by [10, 11, 12, 2]

$$\begin{aligned}
\beta_0^{(n_f)} &= \frac{1}{4}\left[11-\frac{2}{3}n_f\right]\,,\\
\beta_1^{(n_f)} &= \frac{1}{16}\left[102-\frac{38}{3}n_f\right]\,,\\
\beta_2^{(n_f)} &= \frac{1}{64}\left[\frac{2857}{2}-\frac{5033}{18}n_f+\frac{325}{54}n_f^2\right]\,,\\
\beta_3^{(n_f)} &= \frac{1}{256}\left[\frac{149753}{6}+3564\zeta_3+\left(-\frac{1078361}{162}-\frac{6508}{27}\zeta_3\right)n_f\right.\\
&\quad\left.+\left(\frac{50065}{162}+\frac{6472}{81}\zeta_3\right)n_f^2+\frac{1093}{729}n_f^3\right]\,.
\end{aligned} \tag{2}$$

ζ is Riemann's zeta function, with values $\zeta_2 = \pi^2/6$ and $\zeta_3 \approx 1.202\,057$. It is convenient to introduce the following notation:

$$
\begin{aligned}
b_i^{(n_f)} &= \frac{\beta_i^{(n_f)}}{\beta_0^{(n_f)}}\,, \\
a^{(n_f)}(\mu) &= \frac{\alpha^{(n_f)}(\mu)}{\pi}\,.
\end{aligned}
\tag{3}
$$

In the following the labels μ and n_f are omitted if confusion is impossible.

Integrating Eq. (1) leads to

$$
\begin{aligned}
\ln\frac{\mu^2}{\Lambda^2} &= \int \frac{da}{\beta(a)} \\
&= \frac{1}{\beta_0}\left[\frac{1}{a} + b_1 \ln a + (b_2 - b_1^2)a + \left(\frac{b_3}{2} - b_1 b_2 + \frac{b_1^3}{2}\right)a^2\right] + C,
\end{aligned}
\tag{4}
$$

where an expansion in a has been performed. The integration constant is conveniently split into Λ, the so-called asymptotic scale parameter, and C. The conventional $\overline{\mathrm{MS}}$ definition of Λ, which we shall adopt in the following, corresponds to choosing $C = (b_1/\beta_0)\ln\beta_0$ [3, 13].

Iteratively solving Eq. (4) yields [5]

$$
\begin{aligned}
a &= \frac{1}{\beta_0 L} - \frac{b_1 \ln L}{(\beta_0 L)^2} + \frac{1}{(\beta_0 L)^3}\left[b_1^2(\ln^2 L - \ln L - 1) + b_2\right] \\
&\quad + \frac{1}{(\beta_0 L)^4}\left[b_1^3\left(-\ln^3 L + \frac{5}{2}\ln^2 L + 2\ln L - \frac{1}{2}\right) - 3 b_1 b_2 \ln L + \frac{b_3}{2}\right],
\end{aligned}
\tag{5}
$$

where $L = \ln(\mu^2/\Lambda^2)$ and terms of $\mathcal{O}(1/L^5)$ have been neglected. Λ is defined in such a way that Eq. (5) does not contain a term proportional to (const.$/L^2$) [3].

The canonical way to compute $a(\mu_2)$ when $a(\mu_1)$ is given for a fixed number of flavours is as follows:

1. Determine Λ. There are several possibilities to do this. One could, e.g., use the explicit solution given in Eq. (4). Another possibility is the use of (5) and solve the equation iteratively for Λ. Furthermore the first line of (4) could be used and the integral could be solved numerically without performing any expansion in α_s. We will see in the examples below that the numerical differences are small.

2. $a(\mu_2)$ is computed with the help of Eq. (5) where the value of Λ is inserted and μ is set to μ_2.

It is also possible to avoid the introduction of Λ in intermediate steps and to solve the differential equation (1) numerically using $a(\mu)|_{\mu=\mu_1} = a(\mu_1)$ as initial condition. This convention requires the knowledge of both α_s and the scale μ in order to determine α_s at the new scale. Frequently, $\mu = M_Z$ is used as reference scale.

On the other hand Λ plays the role of an universal parameter which at the same time sets the characteristic scale of QCD.

At this point it is instructive to consider an example. Let us assume that α_s is given at the Z-boson scale: $\alpha_s^{(5)}(M_Z) = 0.118$. Let us further assume that it is determined from the experiment with three-loop accuracy, which means that in the β function (2) only the coefficients up to β_2 are considered and β_3 is neglected. Let us now evaluate the strong coupling at the scale $\mu = M_b$ and compare the results obtained with the different strategies outlined above. In the following a possible `Mathematica` session is shown. `NumDef` is a set of `Mathematica` rules which assigns typical values to the physical parameters used in our procedures. The numbers used in this paper can be found in Eq. (36) and the procedures are described in the Appendix.

```
In[1]:= <<RunDec.m;
```

Comment: evaluation of Λ from $\alpha_s^{(5)}(M_Z)$ based on the explicit solution, Eq. (4), and subsequent evaluation of $\alpha_s^{(5)}(M_b)$ from Λ based on Eq. (5).

```
In[2]:= lamex = LamExpl[asMz/.NumDef,Mz/.NumDef,5,3]

Out[2]= 0.208905

In[3]:= AlphasLam[lamex,Mb/.NumDef,5,3]

Out[3]= 0.216610
```

Comment: evaluation of Λ from $\alpha_s^{(5)}(M_Z)$ based on Eq. (5), and subsequent evaluation of $\alpha_s^{(5)}(M_b)$ from Λ based on Eq. (5).

```
In[4]:= lamim = LamImpl[asMz/.NumDef,Mz/.NumDef,5,3]

Out[4]= 0.208348

In[5]:= AlphasLam[lamim,Mb/.NumDef,5,3]

Out[5]= 0.216444
```

Comment: evaluation of $\alpha_s^{(5)}(M_b)$ from $\alpha_s^{(5)}(M_Z)$ based on Eq. (1).

```
In[6]:= AlphasExact[asMz/.NumDef,Mz/.NumDef,Mb/.NumDef,5,3]

Out[6]= 0.216712
```

Rounding to three significant digits leads to a difference of ± 1 in the last digit. Considering the direct integration of (1) as the most precise one we can conclude $\alpha_s^{(5)}(M_b) = 0.217$ assuming three-loop accuracy.

number of loops	highest coefficient in β function	$\alpha_s^{(5)}(M_b)$ (a)	(b)	(c)	$\alpha_s^{(5)}(1\text{ GeV})$ (c)
1	β_0	0.2059	0.2059	0.2059	0.3369
2	β_1	0.2123	0.2173	0.2161	0.3965
3	β_2	0.2166	0.2164	0.2167	0.4029
4	β_3	0.2174	0.2173	0.2169	0.4065

Table 1: $\alpha_s^{(5)}(M_b)$ and $\alpha_s^{(5)}(1\text{ GeV})$ computed from $\alpha_s^{(5)}(M_Z)$ using different number of loops for the running. For the computation `LamExpl[]` (a), `LamImpl[]` (b) (both in combination with `AlphasLam[]`) and `AlphasExact[] (c)` is used.

In Tab. 1 the influence of the number of loops is studied in the evaluation of $\alpha_s^{(5)}$ at the scale M_b and the (hypothetical) scale 1 GeV using $\alpha_s^{(5)}(M_Z)$ as input. (For the latter only the function `AlphasExact[]` is used for the computation.) It can be seen that the inclusion of β_1 leads to a significant jump in $\alpha_s^{(5)}(M_b)$ whereas the effect of the three- and four-loop coefficients, i.e. β_2 and β_3, is only marginal. Their influence is more pronounced for $\mu = 1$ GeV.

3 Quark masses in the $\overline{\rm MS}$ and on-shell scheme

In the $\overline{\rm MS}$ scheme the running of the quark masses is governed by the function $\gamma_m(\alpha_s)$

$$\mu^2 \frac{d}{d\mu^2} m^{(n_f)}(\mu) = m^{(n_f)}(\mu)\,\gamma_m^{(n_f)}\left(\alpha_s^{(n_f)}\right) = -m^{(n_f)}(\mu)\sum_{i\geq 0}\gamma_{m,i}^{(n_f)}\left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^{i+1}, \quad (6)$$

where the coefficients $\gamma_{m,i}$ are known up to the four-loop order [14, 15, 16, 6]

$$\begin{aligned}
\gamma_{m,0}^{(n_f)} &= 1\,,\\
\gamma_{m,1}^{(n_f)} &= \frac{1}{16}\left[\frac{202}{3} - \frac{20}{9}n_f\right],\\
\gamma_{m,2}^{(n_f)} &= \frac{1}{64}\left[1249 + \left(-\frac{2216}{27} - \frac{160}{3}\zeta_3\right)n_f - \frac{140}{81}n_f^2\right],\\
\gamma_{m,3}^{(n_f)} &= \frac{1}{256}\left[\frac{4603055}{162} + \frac{135680}{27}\zeta_3 - 8800\zeta_5 + \left(-\frac{91723}{27} - \frac{34192}{9}\zeta_3 + 880\zeta_4\right.\right.\\
&\quad \left. + \frac{18400}{9}\zeta_5\right)n_f + \left(\frac{5242}{243} + \frac{800}{9}\zeta_3 - \frac{160}{3}\zeta_4\right)n_f^2\\
&\quad \left. + \left(-\frac{332}{243} + \frac{64}{27}\zeta_3\right)n_f^3\right],
\end{aligned} \quad (7)$$

with $\zeta_3 \approx 1.202\,057$, $\zeta_4 = \pi^4/90$ and $\zeta_5 \approx 1.036\,928$. In analogy to (3) we define

$$c_i^{(n_f)} = \frac{\gamma_{m,i}^{(n_f)}}{\beta_0^{(n_f)}}. \tag{8}$$

Combining Eqs. (1) and (6) leads to a differential equation for $m(\mu)$ as a function of $\alpha_s(\mu)$. It has the solution [17]

$$\frac{m(\mu)}{m(\mu_0)} = \frac{c(\alpha_s(\mu)/\pi)}{c(\alpha_s(\mu_0)/\pi)}, \tag{9}$$

with [6]

$$\begin{aligned} c(x) &= x^{c_0}\Big\{1 + (c_1 - b_1 c_0)x + \frac{1}{2}\Big[(c_1 - b_1 c_0)^2 + c_2 - b_1 c_1 + b_1^2 c_0 - b_2 c_0\Big]x^2 \\ &+ \Big[\frac{1}{6}(c_1 - b_1 c_0)^3 + \frac{1}{2}(c_1 - b_1 c_0)\Big(c_2 - b_1 c_1 + b_1^2 c_0 - b_2 c_0\Big) \\ &+ \frac{1}{3}\Big(c_3 - b_1 c_2 + b_1^2 c_1 - b_2 c_1 - b_1^3 c_0 + 2 b_1 b_2 c_0 - b_3 c_0\Big)\Big]x^3\Big\}, \end{aligned} \tag{10}$$

where terms of $\mathcal{O}(x^4)$ have been neglected. For a given mass, m, at scale μ_0 and $\alpha_s(\mu_0)$ the scale invariant mass $\mu_m = m(\mu_m)$ can be obtained from Eq. (9) by iteration. Note the appearance of $\alpha_s(\mu)$ on the r.h.s. of (9). Thus for the computation of μ_m it is convenient to use in a first step $\alpha_s(\mu_0)$ in combination with Eq. (5) to determine Λ. Afterwards Eq. (5) is used again for the calculation of $\alpha_s(\mu)$ which is inserted in (9) before the iteration.

From Eq. (9) it appears natural to define the mass [18]

$$\hat{m} \equiv \frac{m(\mu)}{c(\alpha_s(\mu)/\pi)}, \tag{11}$$

which is often used in the context of lattice calculations. By construction the mass $\hat{m}$ is scale independent. It is furthermore scheme independent (as far as mass-independent schemes are concerned). This can be seen by considering the r.h.s. of (11) in the limit $\mu \to \infty$

$$\hat{m} = \lim_{\mu\to\infty} m(\mu)\left(\frac{\alpha_s(\mu)}{\pi}\right)^{-\frac{\gamma_{m,0}}{\beta_0}}, \tag{12}$$

and by recalling the fact that the coefficients β_0 and $\gamma_{m,0}$ are scheme independent. In the following we will refer to $\hat{m}$ as renormalization group invariant mass.

In the following we want to provide the relations between the $\overline{\rm MS}$ and the on-shell mass. Whereas the coefficient of order α_s^2 has been available since quite some time [17, 19] only recently the three-loop result could be obtained [20, 21]. In [20] an asymptotic expansion in combination with conformal mapping and Padé approximation has been used in order to obtain a numerical result for the $\overline{\rm MS}$–on-shell conversion formula. The numerical results of [20] are in perfect agreement with the subsequent analytical calculation of [21] (cf. Tab. 2). For a given on-shell mass the $\overline{\rm MS}$ quantity can be computed with the help of

$$
\begin{aligned}
\frac{m(\mu)}{M} &= 1+\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\left[-\frac{4}{3}-l_{\mu M}\right]+\left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^2\Bigg[-\frac{3019}{288}-2\zeta_2-\frac{2}{3}\zeta_2\ln 2+\frac{1}{6}\zeta_3 \\
&\quad -\frac{445}{72}l_{\mu M}-\frac{19}{24}l_{\mu M}^2+\left(\frac{71}{144}+\frac{1}{3}\zeta_2+\frac{13}{36}l_{\mu M}+\frac{1}{12}l_{\mu M}^2\right)n_l-\frac{4}{3}\sum_{1\le i\le n_l}\Delta\left(\frac{M_i}{M}\right)\Bigg] \\
&\quad +\left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^3\Bigg[z_m^{(3)}(M)+\left(-\frac{165635}{2592}-\frac{25}{3}\zeta_2-\frac{25}{9}\zeta_2\ln 2+\frac{55}{36}\zeta_3\right)l_{\mu M} \\
&\quad -\frac{11779}{864}l_{\mu M}^2-\frac{475}{432}l_{\mu M}^3+n_l\left(\left(\frac{10051}{1296}+\frac{37}{18}\zeta_2+\frac{2}{9}\zeta_2\ln 2+\frac{7}{9}\zeta_3\right)l_{\mu M}+\frac{911}{432}l_{\mu M}^2\right. \\
&\quad \left.+\frac{11}{54}l_{\mu M}^3\right)+n_l^2\left(\left(-\frac{89}{648}-\frac{1}{9}\zeta_2\right)l_{\mu M}^2-\frac{13}{216}l_{\mu M}^2-\frac{1}{108}l_{\mu M}^3\right)\Bigg]\,, \qquad (13)
\end{aligned}
$$

where $\zeta_2=\pi^2/6$ and $l_{\mu M}=\ln\mu^2/M^2$. n_l is the number of light quarks. The function $\Delta(x)$ arises from the two-loop diagram with a second fermion-loop [17]. For $0\le x\le 1$ it is approximated within an accuracy of 1% by

$$
\Delta(x) \;=\; \frac{\pi^2}{8}\,x-0.597\,x^2+0.230\,x^3\,. \qquad (14)
$$

The corresponding mass effects at order α_s^3 are not yet known. In the argument of $\Delta(x)$ the ratio of the on-shell mass of the light quarks, M_i, and the heavy one, M, appears.

The coefficients $z_m^{(3)}(M)$ can be found in Tab. 2 for different values of n_l where both the results of [20] and [21] are listed. For completeness also the corresponding two-loop coefficients (without the contribution from $\Delta(x)$) are given. The analytical result for $z_m^{(3)}(M)$ reads [21]

$$
\begin{aligned}
z_m^{(3)}(M) &= -\frac{9478333}{93312}+\frac{55}{162}\ln^4 2+\left(-\frac{644201}{6480}+\frac{587}{27}\ln 2+\frac{44}{27}\ln^2 2\right)\zeta_2-\frac{61}{27}\zeta_3 \\
&\quad +\frac{3475}{432}\zeta_4+\frac{1439}{72}\zeta_2\zeta_3-\frac{1975}{216}\zeta_5+\frac{220}{27}a_4+n_l\Bigg[\frac{246643}{23328}-\frac{1}{81}\ln^4 2 \\
&\quad +\left(\frac{967}{108}+\frac{22}{27}\ln 2-\frac{4}{27}\ln^2 2\right)\zeta_2+\frac{241}{72}\zeta_3-\frac{305}{108}\zeta_4-\frac{8}{27}a_4\Bigg] \\
&\quad +n_l^2\left[-\frac{2353}{23328}-\frac{13}{54}\zeta_2-\frac{7}{54}\zeta_3\right]\,, \qquad (15)
\end{aligned}
$$

where $a_4=\mathrm{Li}_4(1/2)\approx 0.517\,479$.

Iterating (13) leads to a relation between the scale-invariant mass, $\mu_m=m(\mu_m)$, and the on-shell mass

$$
\frac{\mu_m}{M} \;=\; 1+\frac{\alpha_s^{(n_f)}(M)}{\pi}\left[-\frac{4}{3}\right]+\left(\frac{\alpha_s^{(n_f)}(M)}{\pi}\right)^2\Bigg[-\frac{2251}{288}-2\zeta_2-\frac{2}{3}\zeta_2\ln 2+\frac{1}{6}\zeta_3
$$

	$z_m(M) = m(M)/M$			$z_m^{SI}(M) = \mu_m/M$			$z_m^{inv}(m) = M/\mu_m$		
n_l	$\mathcal{O}(\alpha_s^2)$	$\mathcal{O}(\alpha_s^3)$ [20]	$\mathcal{O}(\alpha_s^3)$ [21]	$\mathcal{O}(\alpha_s^2)$	$\mathcal{O}(\alpha_s^3)$ [20]	$\mathcal{O}(\alpha_s^3)$ [21]	$\mathcal{O}(\alpha_s^2)$	$\mathcal{O}(\alpha_s^3)$ [20]	$\mathcal{O}(\alpha_s^3)$ [21]
0	−14.33	−202(5)	−198.7	−11.67	−170(5)	−166.3	13.44	194(5)	190.6
1	−13.29	−176(4)	−172.4	−10.62	−146(4)	−142.5	12.40	168(4)	164.6
2	−12.25	−150(3)	−147.5	−9.58	−123(3)	−120.0	11.36	143(3)	139.9
3	−11.21	−126(3)	−123.8	−8.54	−101(3)	−98.76	10.32	119(3)	116.5
4	−10.17	−103(2)	−101.5	−7.50	−81(2)	−78.86	9.28	96(2)	94.42
5	−9.13	−82(2)	−80.40	−6.46	−62(2)	−60.27	8.24	75(2)	73.64

Table 2: Two- and three-loop coefficients of the relation between on-shell and $\overline{\rm MS}$ mass. The choice $\mu^2 = M^2$, respectively, $\mu^2 = m^2$ has been adopted.

$$+ n_l\left(\frac{71}{144} + \frac{1}{3}\zeta_2\right) - \frac{4}{3}\sum_{1\le i\le n_l}\Delta\left(\frac{M_i}{M}\right)\Bigg] + \left(\frac{\alpha_s^{(n_f)}(M)}{\pi}\right)^3 z_m^{SI,(3)}(M)\,. \qquad (16)$$

Inverting Eq. (13) leads to

$$\begin{aligned}\frac{M}{\mu_m} &= 1 + \frac{\alpha_s^{(n_f)}(\mu_m)}{\pi}\frac{4}{3} + \left(\frac{\alpha_s^{(n_f)}(\mu_m)}{\pi}\right)^2\left[\frac{307}{32} + 2\zeta_2 + \frac{2}{3}\zeta_2\ln 2 - \frac{1}{6}\zeta_3\right.\\ &\left. + n_l\left(-\frac{71}{144} - \frac{1}{3}\zeta_2\right) + \frac{4}{3}\sum_{1\le i\le n_l}\Delta\left(\frac{m_i}{\mu_m}\right)\right] + \left(\frac{\alpha_s^{(n_f)}(\mu_m)}{\pi}\right)^3 z_m^{inv,(3)}(\mu_m)\,,\end{aligned} \qquad (17)$$

where for convenience $\mu^2 = m^2$ has been chosen. The numerical values of the coefficients z_m^{SI} and z_m^{inv} can also be found in Tab. 2. Their analytic expressions are easily obtained from Eqs. (13) and (15).

Eq. (17) can be used to compute the on-shell quark mass if the corresponding mass in the $\overline{\rm MS}$ scheme is provided. In order to avoid large logarithms it is suggestive to use in a first step the renormalization group equation (9) and evaluate μ_m. In a second step Eq. (17) is used for $\mu = \mu_m$. Also in the case when the on-shell mass is given it is advantageous to use Eq. (17) for the computation of the $\overline{\rm MS}$ mass. The reason is that Eq. (13) contains contributions from the ill-defined pole mass of the light quarks like, e.g., the strange quark. In the case of the top quark it is safe to use (13) as in general the contributions for the charm and strange quark masses can be neglected.

Concerning the determination of the quark masses a crucial role is played by lattice calculations. There it is not possible to use directly the $\overline{\rm MS}$ scheme as it is tightly connected to dimensional regularization. Rather one has to use a prescription which is based on the so-called momentum subtraction scheme. In general these schemes have the disadvantages that they are not mass independent. Recently, however, a mass definition based on momentum subtraction — the regularization invariant (RI) mass — has been proposed which enjoys this feature [22]. In [25] the relation to the $\overline{\rm MS}$ mass has been evaluated to three-loop accuracy. It reads:

$$\frac{m^{(n_f)}(\mu)}{m^{RI}(\mu)} = 1 + \frac{\alpha_s^{(n_f)}(\mu)}{\pi}\left[-\frac{4}{3}\right] + \left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^2\left[-\frac{995}{72} + \frac{19}{6}\zeta_3 + \frac{89}{144}n_f\right]$$

number of loops	$m_b^{(5)}(M_Z)$ (GeV)	M_b (GeV)	$m_b^{RI}(M_Z)$ (GeV)
1	2.903	4.332	3.048
2	2.715	4.545	2.885
3	2.696	4.692	2.872
4	2.693	—	—

Table 3: Computation of $m_b^{(5)}(M_Z)$, M_b and $m^{RI}(M_Z)$ from $\mu_b = m_b^{(5)}(\mu_b) = 3.97$ GeV for different number of loops.

$$+\left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^3\left[-\frac{6663911}{41472}+\frac{408007}{6912}\zeta_3-\frac{185}{36}\zeta_5+\left(\frac{118325}{7776}+\frac{5}{12}\zeta_4\right.\right.$$
$$\left.\left.-\frac{617}{216}\zeta_3\right)n_f+\left(-\frac{4459}{23328}-\frac{1}{54}\zeta_3\right)n_f^2\right]. \tag{18}$$

Let us at this point consider an explicit example. For a given mass $\mu_b = m_b^{(5)}(\mu_b) = 3.97$ GeV five-flavour running (cf. Eqs. (9) and (10)) is used in order to obtain $m_b^{(5)}(M_Z)$ and the on-shell mass is computed with the help of Eq. (17). Furthermore the value for $m^{RI}(M_Z)$ is evaluated. In Tab. 3 the results are listed for different number of loops.

At the end of this section we want to summarize the different mass definitions introduced in this section in the following table:

M	on-shell mass
$m(\mu)$	$\overline{\text{MS}}$ mass
μ_m	scale invariant mass
$\hat{m}$	renormalization group invariant mass
m^{RI}	regularization invariant mass

4 Decoupling at flavour thresholds

In MS-like renormalization schemes, the Appelquist-Carazzone decoupling theorem [4] does not in general apply to quantities that do not represent physical observables, such as beta functions or coupling constants, i.e., quarks with masses much larger than the considered energy scale do not automatically decouple. The standard procedure to circumvent this problem is to render decoupling explicit by using the language of effective field theory. The formulae presented below are valid for QCD with $n_l = n_f - 1$ massless quark flavours and one heavy flavour h, with mass m_h which is supposed to be much larger than the energy scale. Then, one constructs an effective n_l-flavour theory by requiring consistency with the full n_f-flavour theory at an energy scale comparable to m_h, the heavy-quark threshold $\mu^{(n_f)} = \mathcal{O}(m_h)$. This leads to a nontrivial matching condition between the couplings and light masses, m_q, of the two theories. Although, $\alpha_s^{(n_l)}(m_h) = \alpha_s^{(n_f)}(m_h)$ and $m_q^{(n_l)}(m_h) = m_q^{(n_f)}(m_h)$ at leading and next-to-leading order, this relation does not generally hold at higher orders in the $\overline{\rm MS}$ scheme. At $\mathcal{O}(\alpha_s^2)$ the corresponding correction terms have been computed in [26, 27, 28].

The connection between the strong coupling constant in the effective and the full theory is given by

$$\alpha_s^{(nf-1)}(\mu) \;=\; \zeta_g^2 \alpha_s^{(n_f)}(\mu)\,, \tag{19}$$

where ζ_g is known up to the three-loop order [5, 7]:

$$\begin{aligned}
\left(\zeta_g^{MS}\right)^2 \;=\;& 1+\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\left(-\frac{1}{6}\ln\frac{\mu^2}{m_h^2}\right)+\left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^2\left(\frac{11}{72}-\frac{11}{24}\ln\frac{\mu^2}{m_h^2}+\frac{1}{36}\ln^2\frac{\mu^2}{m_h^2}\right)\\
&+\left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^3\left[\frac{564731}{124416}-\frac{82043}{27648}\zeta_3-\frac{955}{576}\ln\frac{\mu^2}{m_h^2}+\frac{53}{576}\ln^2\frac{\mu^2}{m_h^2}\right.\\
&\left.-\frac{1}{216}\ln^3\frac{\mu^2}{m_h^2}+n_l\left(-\frac{2633}{31104}+\frac{67}{576}\ln\frac{\mu^2}{m_h^2}-\frac{1}{36}\ln^2\frac{\mu^2}{m_h^2}\right)\right]\,.
\end{aligned}\tag{20}$$

In this equation the $\overline{\rm MS}$ mass $m_h(\mu)$ — indicated by the superscript MS — is chosen for the parameterization of the heavy quark mass and μ represents the renormalization scale. Often it is convenient to express ζ_g through the scale invariant mass, denoted by $\mu_h = m_h(\mu_h)$:

$$\begin{aligned}
\left(\zeta_g^{SI}\right)^2 \;=\;& 1+\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\left(-\frac{1}{6}\ln\frac{\mu^2}{\mu_h^2}\right)+\left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^2\left(\frac{1}{36}\ln^2\frac{\mu^2}{\mu_h^2}-\frac{19}{24}\ln\frac{\mu^2}{\mu_h^2}+\frac{11}{72}\right)\\
&+\left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^3\left[-\frac{1}{216}\ln^3\frac{\mu^2}{\mu_h^2}-\frac{131}{576}\ln^2\frac{\mu^2}{\mu_h^2}+\frac{1}{1728}\ln\frac{\mu^2}{\mu_h^2}(-6793+281\,n_l)\right.\\
&\left.-\frac{82043}{27648}\zeta_3+\frac{564731}{124416}-\frac{2633}{31104}n_l\right]\,.
\end{aligned}\tag{21}$$

Transforming the heavy quark mass into the on-shell scheme leads to

$$\begin{aligned}
\left(\zeta_g^{OS}\right)^2 \;=\;& 1+\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\left(-\frac{1}{6}\ln\frac{\mu^2}{M_h^2}\right)+\left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^2\left(-\frac{7}{24}-\frac{19}{24}\ln\frac{\mu^2}{M_h^2}+\frac{1}{36}\ln^2\frac{\mu^2}{M_h^2}\right)\\
&+\left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^3\left[-\frac{58933}{124416}-\frac{2}{3}\zeta_2\left(1+\frac{1}{3}\ln 2\right)-\frac{80507}{27648}\zeta_3-\frac{8521}{1728}\ln\frac{\mu^2}{M_h^2}\right.\\
&\left.-\frac{131}{576}\ln^2\frac{\mu^2}{M_h^2}-\frac{1}{216}\ln^3\frac{\mu^2}{M_h^2}+n_l\left(\frac{2479}{31104}+\frac{\zeta_2}{9}+\frac{409}{1728}\ln\frac{\mu^2}{M_h^2}\right)\right]\,.
\end{aligned}\tag{22}$$

In practical applications also the inverted formulae are needed which read for Eqs. (20), (21) and (22):

$$
\begin{aligned}
\frac{1}{\left(\zeta_g^{MS}\right)^2} &= 1+\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\left(\frac{1}{6}\ln\frac{\mu^2}{m_h^2}\right)+\left(\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\right)^2\left(-\frac{11}{72}+\frac{11}{24}\ln\frac{\mu^2}{m_h^2}+\frac{1}{36}\ln^2\frac{\mu^2}{m_h^2}\right)\\
&\quad+\left(\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\right)^3\left[-\frac{564731}{124416}+\frac{82043}{27648}\zeta_3+\frac{2645}{1728}\ln\frac{\mu^2}{m_h^2}+\frac{167}{576}\ln^2\frac{\mu^2}{m_h^2}\right.\\
&\quad\left.+\frac{1}{216}\ln^3\frac{\mu^2}{m_h^2}+n_l\left(\frac{2633}{31104}-\frac{67}{576}\ln\frac{\mu^2}{m_h^2}+\frac{1}{36}\ln^2\frac{\mu^2}{m_h^2}\right)\right], \qquad (23)\\
\frac{1}{\left(\zeta_g^{SI}\right)^2} &= 1+\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\left(\frac{1}{6}\ln\frac{\mu^2}{\mu_h^2}\right)+\left(\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\right)^2\left(-\frac{11}{72}+\frac{19}{24}\ln\frac{\mu^2}{\mu_h^2}+\frac{1}{36}\ln^2\frac{\mu^2}{\mu_h^2}\right)\\
&\quad+\left(\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\right)^3\left[-\frac{564731}{124416}+\frac{82043}{27648}\zeta_3+\frac{2191}{576}\ln\frac{\mu^2}{\mu_h^2}+\frac{511}{576}\ln^2\frac{\mu^2}{\mu_h^2}\right.\\
&\quad\left.+\frac{1}{216}\ln^3\frac{\mu^2}{\mu_h^2}+n_l\left(\frac{2633}{31104}-\frac{281}{1728}\ln\frac{\mu^2}{\mu_h^2}\right)\right], \qquad (24)\\
\frac{1}{\left(\zeta_g^{OS}\right)^2} &= 1+\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\left(\frac{1}{6}\ln\frac{\mu^2}{M_h^2}\right)+\left(\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\right)^2\left(\frac{7}{24}+\frac{19}{24}\ln\frac{\mu^2}{M_h^2}+\frac{1}{36}\ln^2\frac{\mu^2}{M_h^2}\right)\\
&\quad+\left(\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\right)^3\left[\frac{58933}{124416}+\frac{2}{3}\zeta_2\left(1+\frac{1}{3}\ln 2\right)+\frac{80507}{27648}\zeta_3+\frac{8941}{1728}\ln\frac{\mu^2}{M_h^2}\right.\\
&\quad\left.+\frac{511}{576}\ln^2\frac{\mu^2}{M_h^2}+\frac{1}{216}\ln^3\frac{\mu^2}{M_h^2}+n_l\left(-\frac{2479}{31104}-\frac{\zeta_2}{9}-\frac{409}{1728}\ln\frac{\mu^2}{M_h^2}\right)\right]. \qquad (25)
\end{aligned}
$$

The decoupling relations (20)–(25) have to be applied whenever a flavour threshold is to be crossed.

At this point we briefly want to comment on the order of α_s which has to be used for the running, respectively, the decoupling if the analysis should be consistent. If the μ evolution of $\alpha_s^{(n_f)}(\mu)$ is to be performed at $N+1$ loops, i.e., with the highest coefficient in Eq. (1) being $\beta_N^{(n_f)}$, then consistency requires the matching conditions to be implemented in terms of N-loop formulae. Then, the residual μ dependence of physical observables will be of order $N+2$.

As an example let us compute $\alpha_s^{(4)}(M_c)$ from $\alpha_s^{(5)}(M_Z)=0.118$. Let us furthermore consider the on-shell definition of the heavy quark, M_b, i.e. we use Eq. (22) for the analysis. For the scale μ in (19) where the matching is performed we choose $\mu_{th}=M_b$. Assuming four-loop accuracy for the beta function and (as a consequence) three-loop accuracy for the matching computation one would proceed as follows (see Appendix for a description of the procedures):

```
In[2]:= (alsmuth = AlphasExact[asMz/.NumDef,Mz/.NumDef,Mb/.NumDef,5,4])
```

number of loops (running)	$\alpha_s^{(4)}(M_c)$		
	$(\mu_{th} = M_Z)$	$(\mu_{th} = M_b)$	$(\mu_{th} = 1$ GeV$)$
1	0.3213	0.2918	0.2784
2	0.3387	0.3318	0.3222
3	0.3396	0.3364	0.3319
4	0.3399	0.3378	0.3350

Table 4: Computation of $\alpha_s^{(4)}(M_c)$ from $\alpha_s^{(5)}(M_Z) = 0.118$ for different number of loops. For the matching scale M_Z, M_b and 1 GeV has been chosen.

```
Out[2]= 0.2169467

In[3]:= (alsmuthp = DecAsDownOS[alsmuth,Mb/.NumDef,Mb/.NumDef,4,4])

Out[3]= 0.2163396

In[4]:= (alsMc = AlphasExact[alsmuthp,Mb/.NumDef,Mc/.NumDef,4,4])

Out[4]= 0.337848
```

Finally one arrives at $\alpha_s^{(4)}(M_c) = 0.338$. These steps are summarized in the function `AsRunDec[]` where the corresponding call would read

```
In[5]:= AsRunDec[asMz/.NumDef,Mz/.NumDef,Mc/.NumDef,4]

Out[5]= 0.337848
```

Note that the loop-argument of the function `DecAsDownOS[]` (last argument) refers to the order used for the running, i.e. in the considered case the "4" means that the three-loop relation is used for the decoupling. In this example the effect of the decoupling is quite small. It is actually comparable to the uncertainty from using different methods for the running (cf. Tab. 1). However, one has to remember that for the matching scale the heavy quark mass itself has been used, whence all logarithms in Eq. (22) vanish. A different choice would lead to a different result for $\alpha_s^{(4)}(M_c)$. On the other hand, on general grounds, the decoupling procedure should not depend on the choice of that scale, respectively, the dependence should become weaker when going to higher orders. In Tab. 4 the dependence of $\alpha_s^{(4)}(M_c)$ on the number of loops is shown. For the matching scale M_Z, M_b and 1 GeV has been chosen. It can be clearly seen that the four-loop analysis provides the most stable values — even in the case when the matching is performed at the a high scale like the Z boson mass. This is expected on general grounds as physical results should not depend on the matching scale.

We should mention that in case the $\overline{\rm MS}$ definition for the heavy quark is used in a first step $m_h(\mu_{th})$ has to be evaluated. The corresponding formulae can be found in Section 3. They are also implemented as `Mathematica` procedures and described in the Appendix.

In Fig. 1 it is demonstrated that the inclusion of the four-loop coefficient β_3 accompanied by the three-loop matching leads to an independence of $\mu_{th} = \mu^{(5)}$ over a very broad range [7]. The plot shows the dependence of $\alpha_s^{(5)}(M_Z)$ on the matching scale (denoted by $\mu^{(5)}$) where $\alpha_s^{(4)}(M_\tau)$ is used as starting point. Our procedure to get the different curves is as follows. We first calculate $\alpha_s^{(4)}(\mu^{(5)})$ by exactly integrating Eq. (1) with the initial condition $\alpha_s^{(4)}(M_\tau) = 0.36$, then obtain $\alpha_s^{(5)}(\mu^{(5)})$ from Eqs. (25) with $M_b = 4.7$ GeV, and finally compute $\alpha_s^{(5)}(M_Z)$ with Eq. (1). For consistency, N-loop evolution must be accompanied by $(N-1)$-loop matching, i.e. if we omit terms of $\mathcal{O}(\alpha_s^{N+2})$ on the right-hand side of Eq. (1), we need to discard those of $\mathcal{O}(\alpha_s^N)$ in Eq. (25) at the same time. In Fig. 1, the variation of $\alpha_s^{(5)}(M_Z)$ with $\mu^{(5)}/M_b$ is displayed for the various levels of accuracy, ranging from one-loop to four-loop evolution. For illustration, $\mu^{(5)}$ is varied by almost two orders of magnitude. While the leading-order result exhibits a strong logarithmic behaviour, it stabilizes as we go to higher orders. The four-loop curve is almost flat for $\mu^{(5)} \gtrsim 1$ GeV. Besides the $\mu^{(5)}$ dependence of $\alpha_s^{(5)}(M_Z)$, also its absolute normalization is significantly affected by the higher orders. At the central matching scale $\mu^{(5)} = M_b$, we encounter a rapid, monotonic convergence behaviour.

Fig. 1 can immediately be reproduced with the help of the procedure `AlL2AlH[]` described in the Appendix.

Up to now only the decoupling of the coupling constant has been considered. However, also the (relatively) lighter quark masses undergo a decoupling procedure when crossing a flavour threshold. If we define the connection between the quark mass in the effective and full theory through

$$m_q^{(n_f-1)} = \zeta_m m_q^{(n_f)}\,, \tag{26}$$

the decoupling constant ζ_m is given by [7]

$$\begin{aligned}
\zeta_m^{MS} &= 1 + \left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^2 \left(\frac{89}{432} - \frac{5}{36}\ln\frac{\mu^2}{m_h^2} + \frac{1}{12}\ln^2\frac{\mu^2}{m_h^2}\right) + \left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^3 \left[\frac{2951}{2916}\right. \\
&\quad - \frac{407}{864}\zeta_3 + \frac{5}{4}\zeta_4 - \frac{1}{36}B_4 + \left(-\frac{311}{2592} - \frac{5}{6}\zeta_3\right)\ln\frac{\mu^2}{m_h^2} + \frac{175}{432}\ln^2\frac{\mu^2}{m_h^2} \\
&\quad \left. + \frac{29}{216}\ln^3\frac{\mu^2}{m_h^2} + n_l\left(\frac{1327}{11664} - \frac{2}{27}\zeta_3 - \frac{53}{432}\ln\frac{\mu^2}{m_h^2} - \frac{1}{108}\ln^3\frac{\mu^2}{m_h^2}\right)\right]\,,
\end{aligned} \tag{27}$$

where [29]

$$\begin{aligned}
B_4 &= 16\,\mathrm{Li}_4\left(\frac{1}{2}\right) - \frac{13}{2}\zeta_4 - 4\zeta_2\ln^2 2 + \frac{2}{3}\ln^4 2 \\
&\approx -1.762\,800\,.
\end{aligned} \tag{28}$$

Note that all three quantities in Eq. (26) depend on the renormalization scale μ.

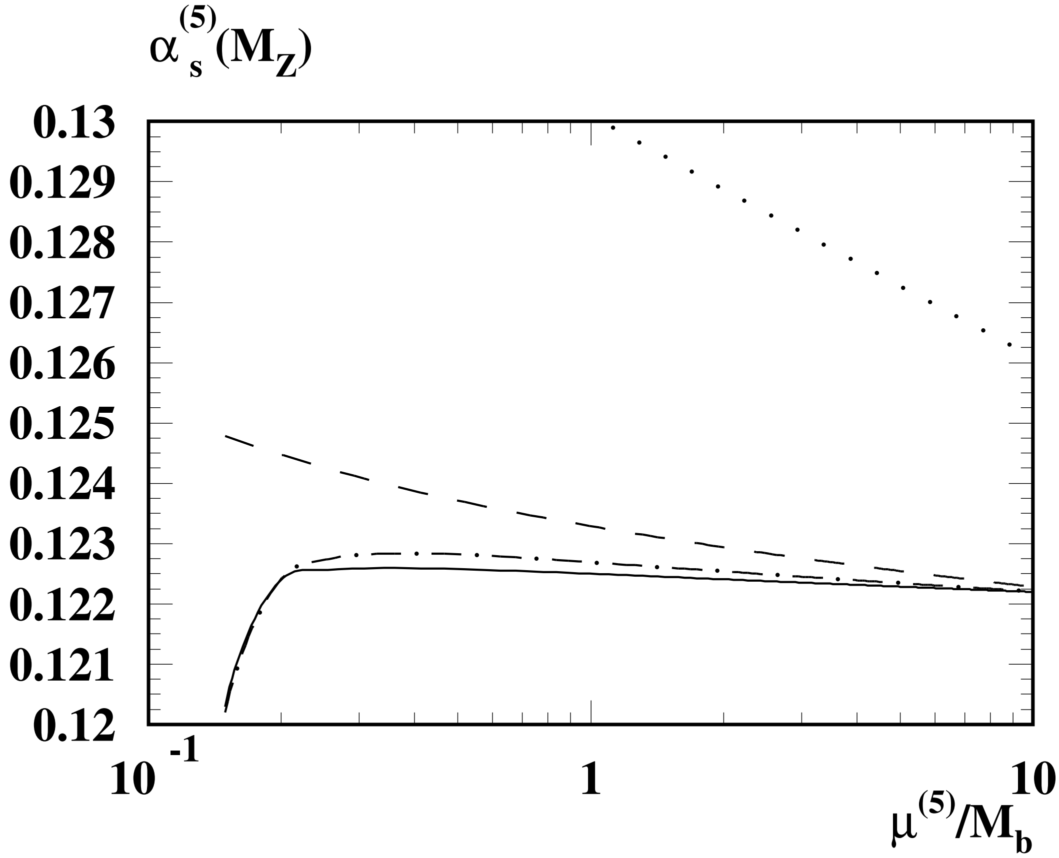

Figure 1: $\mu^{(5)}$ dependence of $\alpha_s^{(5)}(M_Z)$ calculated from $\alpha_s^{(4)}(M_\tau) = 0.36$ and $M_b = 4.7$ GeV using Eq. (1) at one (dotted), two (dashed), three (dot-dashed), and four (solid) loops in connection with Eq. (25) at the respective orders.

Again it turns out to be useful to consider in addition to (27) the quantities where the scale invariant and the on-shell mass, respectively, has been used for the parameterization of the heavy quark:

$$
\begin{aligned}
\zeta_m^{SI} &= 1 + \left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^2 \left(\frac{89}{432} - \frac{5}{36}\ln\frac{\mu^2}{\mu_h^2} + \frac{1}{12}\ln^2\frac{\mu^2}{\mu_h^2}\right) + \left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^3 \left[\frac{2951}{2916}\right. \\
&\quad - \frac{407}{864}\zeta_3 + \frac{5}{4}\zeta_4 - \frac{1}{36}B_4 + \left(-\frac{1031}{2592} - \frac{5}{6}\zeta_3\right)\ln\frac{\mu^2}{\mu_h^2} + \frac{319}{432}\ln^2\frac{\mu^2}{\mu_h^2} \\
&\quad \left. + \frac{29}{216}\ln^3\frac{\mu^2}{\mu_h^2} + n_l\left(\frac{1327}{11664} - \frac{2}{27}\zeta_3 - \frac{53}{432}\ln\frac{\mu^2}{\mu_h^2} - \frac{1}{108}\ln^3\frac{\mu^2}{\mu_h^2}\right)\right], \qquad (29) \\
\zeta_m^{OS} &= 1 + \left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^2 \left(\frac{89}{432} - \frac{5}{36}\ln\frac{\mu^2}{M_h^2} + \frac{1}{12}\ln^2\frac{\mu^2}{M_h^2}\right) + \left(\frac{\alpha_s^{(n_f)}(\mu)}{\pi}\right)^3 \left[\frac{1871}{2916}\right.
\end{aligned}
$$

$$
-\frac{407}{864}\zeta_3+\frac{5}{4}\zeta_4-\frac{1}{36}B_4+\left(\frac{121}{2592}-\frac{5}{6}\zeta_3\right)\ln\frac{\mu^2}{M_h^2}+\frac{319}{432}\ln^2\frac{\mu^2}{M_h^2}
$$
$$
+\frac{29}{216}\ln^3\frac{\mu^2}{M_h^2}+n_l\left(\frac{1327}{11664}-\frac{2}{27}\zeta_3-\frac{53}{432}\ln\frac{\mu^2}{M_h^2}-\frac{1}{108}\ln^3\frac{\mu^2}{M_h^2}\right)\Bigg]\,. \qquad (30)
$$

The corresponding inverted relations read

$$
\begin{aligned}
\frac{1}{\zeta_m^{MS}} &= 1+\left(\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\right)^2\left(-\frac{89}{432}+\frac{5}{36}\ln\frac{\mu^2}{m_h^2}-\frac{1}{12}\ln^2\frac{\mu^2}{m_h^2}\right)+\left(\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\right)^3\Bigg[-\frac{2951}{2916}\\
&\quad+\frac{407}{864}\zeta_3-\frac{5}{4}\zeta_4+\frac{1}{36}B_4+\left(\frac{133}{2592}+\frac{5}{6}\zeta_3\right)\ln\frac{\mu^2}{m_h^2}-\frac{155}{432}\ln^2\frac{\mu^2}{m_h^2}\\
&\quad-\frac{35}{216}\ln^3\frac{\mu^2}{m_h^2}+n_l\left(-\frac{1327}{11664}+\frac{2}{27}\zeta_3+\frac{53}{432}\ln\frac{\mu^2}{m_h^2}+\frac{1}{108}\ln^3\frac{\mu^2}{m_h^2}\right)\Bigg]\,, \qquad (31)\\
\frac{1}{\zeta_m^{SI}} &= 1+\left(\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\right)^2\left(-\frac{89}{432}+\frac{5}{36}\ln\frac{\mu^2}{\mu_h^2}-\frac{1}{12}\ln^2\frac{\mu^2}{\mu_h^2}\right)+\left(\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\right)^3\Bigg[-\frac{2951}{2916}\\
&\quad+\frac{407}{864}\zeta_3-\frac{5}{4}\zeta_4+\frac{1}{36}B_4+\left(\frac{853}{2592}+\frac{5}{6}\zeta_3\right)\ln\frac{\mu^2}{\mu_h^2}-\frac{299}{432}\ln^2\frac{\mu^2}{\mu_h^2}\\
&\quad-\frac{35}{216}\ln^3\frac{\mu^2}{\mu_h^2}+n_l\left(-\frac{1327}{11664}+\frac{2}{27}\zeta_3+\frac{53}{432}\ln\frac{\mu^2}{\mu_h^2}+\frac{1}{108}\ln^3\frac{\mu^2}{\mu_h^2}\right)\Bigg]\,, \qquad (32)\\
\frac{1}{\zeta_m^{OS}} &= 1+\left(\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\right)^2\left(-\frac{89}{432}+\frac{5}{36}\ln\frac{\mu^2}{M_h^2}-\frac{1}{12}\ln^2\frac{\mu^2}{M_h^2}\right)+\left(\frac{\alpha_s^{(n_l)}(\mu)}{\pi}\right)^3\Bigg[-\frac{1871}{2916}\\
&\quad+\frac{407}{864}\zeta_3-\frac{5}{4}\zeta_4+\frac{1}{36}B_4+\left(-\frac{299}{2592}+\frac{5}{6}\zeta_3\right)\ln\frac{\mu^2}{M_h^2}-\frac{299}{432}\ln^2\frac{\mu^2}{M_h^2}\\
&\quad-\frac{35}{216}\ln^3\frac{\mu^2}{M_h^2}+n_l\left(-\frac{1327}{11664}+\frac{2}{27}\zeta_3+\frac{53}{432}\ln\frac{\mu^2}{M_h^2}+\frac{1}{108}\ln^3\frac{\mu^2}{M_h^2}\right)\Bigg]\,. \qquad (33)
\end{aligned}
$$

As an example we compute $m_c^{(5)}(M_Z)$ for different number of loops and different matching points μ_{th}. The results can be found in Tab. 5 where $\mu_{th} = M_Z,\ M_b$, and 1 GeV has been chosen. It can clearly be seen that the four-loop result provides the most stable values for $m_c^{(5)}(M_Z)$.

A similar analysis as in Fig. 1 may be performed for the light-quark masses as well. For illustration, let us investigate how the $\mu^{(5)}$ dependence of the relation between $\mu_c = m_c^{(4)}(\mu_c)$ and $m_c^{(5)}(M_Z)$ changes under the inclusion of higher orders in evolution and matching. As typical input parameters, we choose $\mu_c = 1.2$ GeV, $M_b = 4.7$ GeV, and $\alpha_s^{(5)}(M_Z) = 0.118$. We first evolve $m_c^{(4)}(\mu)$ from $\mu = \mu_c$ to $\mu = \mu_{th} = \mu^{(5)}$ via Eq. (10), then obtain $m_c^{(5)}(\mu^{(5)})$ from Eqs. (33), and finally evolve $m_c^{(5)}(\mu)$ from $\mu = \mu^{(5)}$ to $\mu = M_Z$ via Eq. (10). In all steps, $\alpha_s^{(n_f)}(\mu)$ is evaluated with the same values of n_f and μ as $m_c^{(n_f)}(\mu)$. In Fig. 2, we show the resulting values of $m_c^{(5)}(M_Z)$ corresponding to N-loop evolution with $(N-1)$-loop matching for $N = 1, \ldots, 4$. Similarly to Fig. 1, we observe a rapid, monotonic convergence behaviour at the central matching scale $\mu^{(5)} = M_b$. Again,

number of loops (running)	$m_c^{(5)}(M_Z)$		
	$(\mu_{th} = M_Z)$	$(\mu_{th} = M_b)$	$(\mu_{th} = 1$ GeV$)$
1	0.6968	0.7174	0.7207
2	0.6025	0.6051	0.6236
3	0.5846	0.5852	0.5984
4	0.5798	0.5801	0.5783

Table 5: Computation of $m_c^{(5)}(M_Z)$ from $\mu_c = m_c(\mu_c) = 1.2$ GeV for different number of loops. For the matching scale M_Z, M_b and 1 GeV has been chosen.

the prediction for $N = 4$ is remarkably stable under the variation of $\mu^{(5)}$ as long as $\mu^{(5)} \gtrsim 1$ GeV. Fig. 2 can easily be reproduced with the help of the procedure `mL2mH[]` (see Appendix).

If one chooses to perform the running of $\alpha_s(\mu)$ with the help of Λ it is useful to have an equation at hand which relates this parameter in the full and effective theory. Combining Eqs. (4), (5) and (21) one obtains [5]

$$\begin{aligned}
\beta_0' \ln \frac{\Lambda'^2}{\Lambda^2} &= (\beta_0' - \beta_0) l_h + (b_1' - b_1) \ln l_h - b_1' \ln \frac{\beta_0'}{\beta_0} \\
&+ \frac{1}{\beta_0 l_h} \left[b_1 (b_1' - b_1) \ln l_h + b_1'^2 - b_1^2 - b_2' + b_2 + \frac{11}{72} \right] \\
&+ \frac{1}{(\beta_0 l_h)^2} \left\{ -\frac{b_1^2}{2} (b_1' - b_1) \ln^2 l_h + b_1 [-b_1' (b_1' - b_1) \right. \\
&+ b_2' - b_2 - \frac{11}{72}] \ln l_h + \frac{1}{2} (-b_1'^3 - b_1^3 - b_3' + b_3) \\
&\left. + b_1' (b_1^2 + b_2' - b_2 - \frac{11}{72}) + \frac{564731}{124416} - \frac{82043}{27648} \zeta_3 - \frac{2633}{31104} n_l \right\} , \qquad (34)
\end{aligned}$$

where $l_h = \ln(\mu_h^2/\Lambda^2)$ and the primed quantities refer to the $(n_f - 1)$-flavour effective theory. In this equation μ_h has been chosen for the matching scale which is particularly convenient, since it eliminates the renormalization group logarithms in (21). This choice is furthermore justified with the help of Figs. 1 and 2 where it can be seen that, in higher orders, the actual value of the matching scale does not matter as long as it is comparable to the heavy-quark mass. In Eq. (34) the four different powers in l_h correspond to the different loop orders. Whereas at one-loop accuracy only the linear term in l_h has to be taken into account at four-loop order also the $1/l_h^2$ contribution has to be considered. Eq. (34) is implemented in the procedure `DecLambdaDown[]`.

For completeness we also display the inverted relation of Eq. (34):

$$\beta_0 \ln \frac{\Lambda^2}{\Lambda'^2} = (\beta_0 - \beta_0') l_h' + (b_1 - b_1') \ln l_h' - b_1 \ln \frac{\beta_0}{\beta_0'}$$

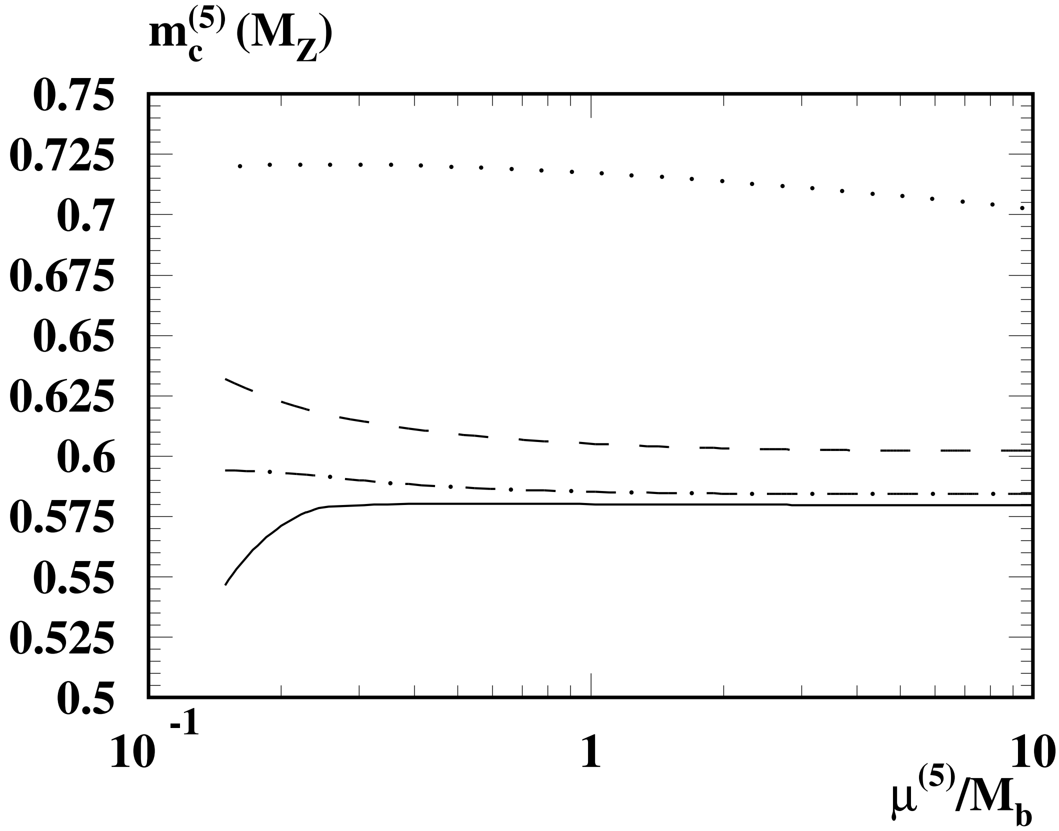

Figure 2: $\mu^{(5)}$ dependence of $m_c^{(5)}(M_Z)$ calculated from $\mu_c = m_c^{(4)}(\mu_c) = 1.2$ GeV, $M_b = 4.7$ GeV and $\alpha_s^{(5)}(M_Z)$ using Eq. (6) at one (dotted), two (dashed), three (dot-dashed), and four (solid) loops in connection with Eq. (33) at the respective orders.

$$
\begin{aligned}
&+ \frac{1}{\beta_0' l_h'}\left[b_1'(b_1 - b_1')\ln l_h' + b_1^2 - b_1'^2 - b_2 + b_2' - \frac{11}{72}\right] \\
&+ \frac{1}{(\beta_0' l_h')^2}\left\{-\frac{b_1'^2}{2}(b_1 - b_1')\ln^2 l_h' + b_1'[-b_1(b_1 - b_1') \right. \\
&+ b_2 - b_2' + \frac{11}{72}]\ln l_h' + \frac{1}{2}(-b_1^3 - b_1'^3 - b_3 + b_3') \\
&\left. + b_1(b_1'^2 + b_2 - b_2' + \frac{11}{72}) - \frac{564731}{124416} + \frac{82043}{27648}\zeta_3 + \frac{2633}{31104}n_l\right\}, \qquad (35)
\end{aligned}
$$

with $l_h' = \ln(\mu_h^2/(\Lambda')^2)$. It is realized in the procedure `DecLambdaUp[]`.

At this point we would like to mention that next to the coupling constant and quark masses also the gauge parameter and the quark and gluon fields obey decoupling relations. The corresponding equations and results can be found in [7].

5 Description of the main procedures

In this section we describe the procedures which are most important for the practical applications, namely the combined running and decoupling of the strong coupling and the conversion of the on-shell mass to the $\overline{\rm MS}$ one and vice versa.

In `RunDec.m` some masses and couplings are set to default values which are used if they are not specified explicitly. They are collected in the set `NumDef` and read (also the corresponding symbol used in `RunDec` is given):

$$
\begin{array}{llllll}
\texttt{Mtau}: & M_\tau = 1.777\text{ GeV}\,, & \texttt{Mc}: & M_c = 1.6\text{ GeV}\,, & \texttt{Mb}: & M_b = 4.7\text{ GeV}\,, \\
\texttt{Mt}: & M_t = 175\text{ GeV}\,, & \texttt{muc}: & \mu_c = 1.2\text{ GeV}\,, & \texttt{mub}: & \mu_b = 3.97\text{ GeV}\,, \\
\texttt{Mz}: & M_Z = 91.18\text{ GeV}\,, & \texttt{asMz}: & \alpha_s^{(5)}(M_Z) = 0.118\,. & &
\end{array}
\qquad (36)
$$

The following procedure computes $\alpha_s^{(m)}(\mu)$ where $\alpha_s^{(n)}(\mu_0)$ is used as input parameter. As input only $\alpha_s(\mu_0)$, μ_0, μ and the number of loops have to be specified. Both n and m are determined according to the values of the quark masses given in `NumDef`. In case $n \neq m$ the heavy quarks are consistently decoupled at the heavy quark scale itself where for the mass definition the on-shell scheme is used.

- `AsRunDec`:
  - *input:* $\alpha_s^{(n)}(\mu_0)$, μ_0, μ, number of loops
  - *output:* $\alpha_s^{(m)}(\mu)$
  - *uses:* `AlphasExact[]`, `AlL2AlH[]` and `AlH2AlL[]`
  - *comments:* The decoupling is performed automatically at the pole mass of the heavy quark where the values defined in `Numdef` are taken. If μ is lower than M_c, $m = 3$ is chosen, i.e. the strange quark is not decoupled.
  - *example:* In order to compute $\alpha_s^{(6)}(500\text{ GeV}) = 0.952$ with four-loop accuracy if $\alpha_s^{(5)}(M_Z) = 0.118$ is given one has to use the command `AsRunDec[asMz/.NumDef,Mz/.NumDef,500,4]`.

The conversion of the on-shell mass M to the $\overline{\rm MS}$ mass, m, can be computed with the help of the procedure `mOS2mMS[]`:

- `mOS2mMS`:
  - *input:* M, n_f, number of loops
  - *output:* $m^{(n_f)}(M)$
  - *uses:* `AsRunDec[]` and `mOS2mMS[]` (from the appendix)
  - *comments:* The relation is implemented up to order α_s^3 (three loops). n_f is the number of active flavours. $\alpha_s^{(n_f)}(M)$ is evaluated at the scale M where $\alpha_s^{(5)}(M_Z)$, as defined in `Numdef`, serves as a starting point. For the running and decoupling the procedure `AsRunDec` is used.

  - *example:* In the case of the top quark the $\overline{\rm MS}$ mass $m_t(M_t) = 164.6$ GeV is obtained via `mOS2mMS[175,6,3]` where $M_t = 175$ GeV has been chosen.

The inverted relation is implemented in

- `mMS2mOS`:
  - *input:* $\mu_m = m^{(n_f)}(\mu_m)$, n_f, number of loops
  - *output:* M
  - *uses:* `AsRunDec[]` and `mMS2mOS[]` (from the appendix)
  - *comments:* The relation is implemented up to order α_s^3 (three loops). n_f is the number of active flavours. $\alpha_s^{(n_f)}(\mu_m)$ is evaluated at the scale μ_m where $\alpha_s^{(5)}(M_Z)$, as defined in `Numdef`, serves as a starting point. For the running and decoupling the procedure `AsRunDec` is used.
  - *example:* In the case of the top quark the on-shell mass $M_t = 174.7$ GeV is obtained via `mMS2mOS[165,6,3]` where $m_t(M_t) = 165$ GeV has been chosen.

In the above procedures all quarks lighter than the one under consideration are assumed to be massless. More specialized procedures providing more freedom in the choice of parameters and the running presentations can be found in the Appendix.

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Appendix: Detailed presentation of the `Mathematica` modules contained in `RunDec`

In the following we list the procedures contained in the program package `RunDec` and provide a brief description. The order of the parameters specified in the field *input* corresponds to the order required in the `Mathematica` procedures. The precision used for most of the numerical evaluations is controlled with the variable `$NumPrec`. For the procedures involving, e.g., numerical solutions of differential equations or recursive solutions of equations the default precision of `Mathematica` is kept which is for all practical purposes more than enough. Note that often the precision requested for with `$NumPrec` can not be reached when the input data are only known to a few digits.

`AsRunDec[]` is not listed as it can already be found in Section 5.

Procedures related to the strong coupling constant

- `LamExpl`:
  - *input:* $\alpha_s^{(n_f)}(\mu)$, μ, n_f, number of loops
  - *output:* $\Lambda^{(n_f)}$
  - *uses:* Eq. (4)
  - *comments:* —
  - *example:* From the knowledge of $\alpha_s^{(5)}(M_Z) = 0.118$ the computation of $\Lambda^{(5)} = 0.2089$ to three-loop accuracy proceeds as follows: `LamExpl[asMz/.NumDef,Mz/.NumDef,5,3]`.

- `LamImpl`:
  - *input:* $\alpha_s^{(n_f)}(\mu)$, μ, n_f, number of loops
  - *output:* $\Lambda^{(n_f)}$
  - *uses:* Eq. (5)
  - *comments:* Solves Eq. (5) numerically for $\Lambda^{(n_f)}$.
  - *example:* If $\alpha_s^{(5)}(M_Z) = 0.118$ is given the computation of $\Lambda^{(5)} = 0.2083$ to three-loop accuracy proceeds as follows: `LamImpl[asMz/.NumDef,Mz/.NumDef,5,3]`.

- `AlphasLam`:
  - *input:* $\Lambda^{(n_f)}$, μ, n_f, number of loops
  - *output:* $\alpha_s^{(n_f)}(\mu)$
  - *uses:* Eq. (5)
  - *comments:* An explicit warning is printed on the screen if the ratio $\mu/\Lambda^{(n_f)}$ is too small.
  - *example:* For $\Lambda^{(5)} = 0.208$ and $M_b = 4.7$ GeV the value of $\alpha_s^{(5)}(M_b) = 0.2163$ is obtained to three-loop accuracy with `AlphasLam[0.208,4.7,5,3]`.

- `AlphasExact`:
  - *input:* $\alpha_s^{(n_f)}(\mu_0)$, μ_0, μ, n_f, number of loops
  - *output:* $\alpha_s^{(n_f)}(\mu)$
  - *uses:* Eq. (1)
  - *comments:* Solves the differential equation numerically using $\alpha_s(\mu_0)$ as initial condition. An explicit warning is printed on the screen if the ratio $\mu/\Lambda^{(n_f)}$ is too small where $\Lambda^{(n_f)}$ is obtained with the help of `LamExpl[]`.

– *example:* $\alpha_s^{(5)}(M_b) = 0.2167$ is computed from $\alpha_s^{(5)}(M_Z)$ through `AlphasExact[asMz/.NumDef,Mz/.NumDef,Mb/.NumDef,5,3]` where the three-loop formulae are used.

Procedures relating different mass definitions

- `mOS2mMS`:
  - *input:* M, $\{M_q\}$, $\alpha_s^{(n_f)}(\mu)$, μ, n_f, number of loops
  - *output:* $m^{(n_f)}(\mu)$
  - *uses:* Eq. (13) and Tab. 2
  - *comments:* The relation is implemented up to order α_s^3 (three loops). $\{M_q\}$. is a set of light quark masses which can also be empty. For consistency reasons their values must correspond to the on-shell mass.

    Note that the name of the procedure is the same as the one introduced in Section 5. The distinction is only in the number of the arguments.
  - *example:* The $\overline{\rm MS}$ mass corresponding to the on-shell top quark mass of 175 GeV is computed via `mOS2mMS[175,{},0.107,175,6,3]` where $\alpha_s^{(6)}(175\text{ GeV}) = 0.107$ has been chosen. The result reads $m_t(175\text{ GeV}) = 164.64$ GeV. Terms up to order α_s^3 have been used and light quark mass effects have been neglected.

- `mMS2mOS`:
  - *input:* $m^{(n_f)}(\mu)$, $\{m_q\}$, $\alpha_s^{(n_f)}(\mu)$, μ, n_f, number of loops
  - *output:* M
  - *uses:* Eq. (17) for general μ and Tab. 2
  - *comments:* The relation is implemented up to order α_s^3 (three loops). In this case the light quark masses are defined in the $\overline{\rm MS}$ scheme $\{m_q\}$.

    Note that the name of the procedure is the same as the one introduced in Section 5. The distinction is only in the number of the arguments.
  - *example:* The on-shell mass corresponding to the $\overline{\rm MS}$ top quark mass $m_t(175\text{ GeV}) = 165$ GeV is computed via `mMS2mOS[165,{},0.107,175,6,3]` where $\alpha_s^{(6)}(175\text{ GeV}) = 0.107$ has been chosen. The result reads $M_t = 175.35$ GeV. Terms up to order α_s^3 have been used and light quark mass effects have been neglected.

- `mOS2mMSrun`:
  - *input:* M, $\{M_q\}$, $\alpha_s^{(n_f)}(\mu)$, μ, n_f, number of loops
  - *output:* $m^{(n_f)}(\mu)$

- *uses:* `AlphasExact[]`, `mOS2mSI[]` and `mMS2mMS[]`
- *comments:* In a first step μ_m is computed and afterwards $m^{(n_f)}(\mu)$ is evaluated. The usage is identical to `mOS2mMS[]`.
- *example:* (analog to `mOS2mMS[]`)

• `mMS2mOSrun`:

- *input:* $m^{(n_f)}(\mu)$, $\{m_q\}$, $\alpha_s^{(n_f)}(\mu)$, μ, n_f, number of loops
- *output:* M
- *uses:* `AlphasLam[]`, `LamImpl[]`, `mMS2mMS[]` and `mMS2mOS[]`
- *comments:* In a first step μ_m is computed. Then Eq. (17) only has to be used for $\mu = \mu_m$. The usage is identical to `mMS2mOS[]`.
- *example:* (analog to `mMS2mOS[]`)

• `mOS2mMSit`:

- *input:* M, $\{m_q\}$, $\alpha_s^{(n_f)}(\mu)$, μ, n_f, number of loops
- *output:* $m^{(n_f)}(\mu)$
- *uses:* Eq. (17) for general μ and Tab. 2
- *comments:* For the computation Eq. (17) is used in order to avoid the on-shell masses of the light quark masses $\{m_q\}$. The usage is identical to `mOS2mMS[]`.
- *example:* (analog to `mOS2mMS[]`).

• `mOS2mSI`:

- *input:* M, $\{M_q\}$, $\alpha_s^{(n_f)}(M)$, n_f, number of loops
- *output:* $\mu_m = m^{(n_f)}(\mu_m)$
- *uses:* Eq. (16) and Tab. 2
- *comments:* The scale invariant mass is computed from the on-shell mass.
- *example:* In the case of the bottom quark, the mass $\mu_b = 3.97$ GeV is evaluated via `mOS2mSI[Mb/.NumDef,{1.6},0.217,5,3]` where $\alpha_s^{(5)}(M_b) = 0.217$ has been chosen. In the mass relation terms up to order α_s^3 have been used and quark mass effects arising from M_c/M_b with $M_c = 1.6$ GeV have been taken into account.

• `mMS2mMS`:

- *input:* $m^{(n_f)}(\mu_0)$, $\alpha_s^{(n_f)}(\mu_0)$, $\alpha_s^{(n_f)}(\mu)$, n_f, number of loops
- *output:* $m^{(n_f)}(\mu)$
- *uses:* Eqs. (9) and (10)

- *comments:* —
- *example:* From $m_b(M_b) = 3.85$ GeV one finds $m_b(M_Z) = 2.69$ GeV with the help of `mMS2mMS[3.85,0.217,asMz/.NumDef,5,4])` where $\alpha_s^{(5)}(M_b) = 0.217$ and $\alpha_s^{(5)}(M_Z) = 0.217$ has been used. For the running the four-loop expressions have been used.

• `mMS2mSI`:

- *input:* $m^{(n_f)}(\mu)$, $\alpha_s^{(n_f)}(\mu)$, μ, n_f, number of loops
- *output:* $\mu_m = m(\mu_m)$
- *uses:* Eqs. (9) and (10)
- *comments:* The scale invariant mass is computed from the $\overline{\mathrm{MS}}$ mass.
- *example:* $\mu_b = 3.97$ GeV is computed from the input $m_b(M_b) = 3.85$ GeV, $M_b = 4.7$ GeV and $\alpha_s^{(5)}(M_b) = 0.217$ via the command `mMS2mSI[3.85,0.217,4.7,5,4]`. For the running the four-loop expressions have been used.

• `mMS2mRI`:

- *input:* $m^{(n_f)}(\mu)$, $\alpha_s^{(n_f)}(\mu)$, n_f, number of loops
- *output:* m^{RI}
- *uses:* inverted equation of (18)
- *comments:* The relation is implemented up to order α_s^3 (three loops).
- *example:* The regularization invariant mass, $m_b^{RI}(M_Z)$, corresponding to the $\overline{\mathrm{MS}}$ bottom quark mass $m_b(M_Z) = 2.695$ GeV is computed via `mMS2mRI[2.695,asMz/.NumDef,5,3]` where $\alpha_s^{(5)}(M_Z) = 0.118$ has been chosen. The result reads $m_b^{RI}(M_Z) = 2.872$ GeV where terms up to order α_s^3 have been used.

• `mRI2mMS`:

- *input:* $m^{RI}(\mu)$, $\alpha_s^{(n_f)}(\mu)$, n_f, number of loops
- *output:* $m^{(n_f)}(\mu)$
- *uses:* Eq. (18)
- *comments:* The relation is implemented up to order α_s^3 (three loops).
- *example:* The $\overline{\mathrm{MS}}$ mass corresponding to the regularization invariant top quark mass of $m_t^{RI} = 175$ GeV is computed via `mRI2mMS[175,0.107,175,6,3]` where $\alpha_s^{(6)}(175 \text{ GeV}) = 0.107$ has been chosen. The result reads $m_t(175 \text{ GeV}) = 165.6$ GeV where terms up to order α_s^3 have been used.

- `mMS2mRGI`:
  - *input:* $m^{(n_f)}(\mu)$, $\alpha_s^{(n_f)}(\mu)$, n_f, number of loops
  - *output:* $\hat{m}$
  - *uses:* Eq (11)
  - *comments:* —
  - *example:* The renormalization group invariant bottom quark mass corresponding to the $\overline{\rm MS}$ mass $m_b^{(5)}(M_Z) = 2.69$ GeV is computed via `mMS2mRGI[2.69,asMz/.NumDef,5,4]` where $\alpha_s^{(5)}(M_Z) = 0.118$ has been chosen. The result reads $m_b^{RGI} = 14.25$ GeV assuming four-loop accuracy.

- `mRGI2mMS`:
  - *input:* $\hat{m}$, $\alpha_s^{(n_f)}(\mu)$, n_f, number of loops
  - *output:* $m^{(n_f)}(\mu)$
  - *uses:* Eq (11)
  - *comments:* —
  - *example:* The $\overline{\rm MS}$ mass corresponding to the renormalization group invariant bottom quark mass of 14.25 GeV is computed via `mRGI2mMS[14.25,asMz/.NumDef,5,4]` where $\alpha_s^{(5)}(M_Z) = 0.118$ has been chosen. The result reads $m_b(M_Z) = 2.69$ GeV assuming four-loop accuracy.

Decoupling of the strong coupling and the masses

At this point we once again want to stress, that the argument specifying the number of loops refers to the accompanied running, i.e. if "2" is chosen the decoupling relation is used to one-loop order. Furthermore, for the argument ruling the number of active flavours the number of light quarks, $n_l = n_f - 1$, is chosen.

- `DecAsUpOS`:
  - *input:* $\alpha_s^{(n_l)}(\mu_{th})$, M_{th}, μ_{th}, n_l, number of loops
  - *output:* $\alpha_s^{(n_l+1)}(\mu_{th})$
  - *uses:* Eq. (25)
  - *comments:* For the heavy mass the on-shell definition is used.
  - *example:* The computation of $\alpha_s^{(6)}(M_Z) = 0.1169$ from the knowledge of $\alpha_s^{(5)}(M_Z) = 0.118$ proceeds via `DecAsUpOS[asMz/.NumDef,175,Mz/.NumDef,5,4]` where $M_t = 175$ GeV has been chosen and terms of order α_s^3 (indicated by the "4" in the last argument) have been included.

- `DecAsDownOS`:
  - *input:* $\alpha_s^{(n_l+1)}(\mu_{th})$, M_{th}, μ_{th}, n_l, number of loops
  - *output:* $\alpha_s^{(n_l)}(\mu_{th})$
  - *uses:* Eq. (22)
  - *comments:* For the heavy mass the on-shell definition is used.
  - *example:* The computation of $\alpha_s^{(5)}(200\text{ GeV}) = 0.1047$ from the knowledge of $\alpha_s^{(6)}(200\text{ GeV}) = 0.105$ proceeds via `DecAsDownOS[0.105,175,200,6,4]` where $M_t = 175$ GeV has been chosen and terms of order α_s^3 (indicated by the "4" in the last argument) have been included.

- `DecAsUpMS`:
  - *input:* $\alpha_s^{(n_l)}(\mu_{th})$, $m_{th}(\mu_{th})$, μ_{th}, n_l, number of loops
  - *output:* $\alpha_s^{(n_l+1)}(\mu_{th})$
  - *uses:* Eq. (23)
  - *comments:* The heavy mass is evaluated in the $\overline{\text{MS}}$ scheme at the scale μ_{th}.
  - *example:* The computation of $\alpha_s^{(6)}(M_Z) = 0.1170$ from the knowledge of $\alpha_s^{(5)}(M_Z) = 0.118$ proceeds via `DecAsUpMS[asMz/.NumDef,165,Mz/.NumDef,5,4]` where $m_t(M_Z) = 165$ GeV has been chosen and terms of order α_s^3 (indicated by the "4" in the last argument) have been included.

- `DecAsDownMS`:
  - *input:* $\alpha_s^{(n_l+1)}(\mu_{th})$, $m_{th}(\mu_{th})$, μ_{th}, n_l, number of loops
  - *output:* $\alpha_s^{(n_l)}(\mu_{th})$
  - *uses:* Eq. (20)
  - *comments:* The heavy mass is evaluated in the $\overline{\text{MS}}$ scheme at the scale μ_{th}.
  - *example:* The computation of $\alpha_s^{(5)}(200\text{ GeV}) = 0.1048$ from the knowledge of $\alpha_s^{(6)}(200\text{ GeV}) = 0.105$ proceeds via `DecAsDownMS[0.105,165,200,6,4]` where $m_t(M_Z) = 165$ GeV has been chosen and terms of order α_s^3 (indicated by the "4" in the last argument) have been included.

- `DecAsUpSI`:
  - *input:* $\alpha_s^{(n_l)}(\mu_{th})$, $\mu_{m_{th}}$, μ_{th}, n_l, number of loops
  - *output:* $\alpha_s^{(n_l+1)}(\mu_{th})$
  - *uses:* Eq. (24)
  - *comments:* Here the scale invariant mass $\mu_{m_{th}}$ is chosen for heavy mass.

- *example:* (analog to `DecAsUpMS[]`)

- `DecAsDownSI`:
  - *input:* $\alpha_s^{(n_l+1)}(\mu_{th})$, $\mu_{m_{th}}$, μ_{th}, n_l, number of loops
  - *output:* $\alpha_s^{(n_l)}(\mu_{th})$
  - *uses:* Eq. (21)
  - *comments:* Here the scale invariant mass $\mu_{m_{th}}$ is chosen for heavy mass.
  - *example:* (analog to `DecAsDownMS[]`)

- `DecMqUpOS`:
  - *input:* $m_q^{(n_l)}(\mu_{th})$, $\alpha_s^{(n_l)}(\mu_{th})$, M_{th}, μ_{th}, n_l, number of loops
  - *output:* $m_q^{(n_l+1)}(\mu_{th})$
  - *uses:* Eq. (33)
  - *comments:* For the heavy mass the on-shell definition is used.
  - *example:* The computation of $m_b^{(6)}(M_Z) = 2.697$ GeV from $m_b^{(5)}(M_Z) = 2.7$ GeV with order α_s^3 accuracy is performed via `DecMqUpOS[2.7,asMz/.NumDef,175,Mz/.NumDef,5,4]`. Here, $\alpha_s^{(5)}(M_Z) = 0.118$ and $M_t = 175$ GeV have been used.

- `DecMqDownOS`:
  - *input:* $m_q^{(n_l+1)}(\mu_{th})$, $\alpha_s^{(n_l+1)}(\mu_{th})$, M_{th}, μ_{th}, n_l, number of loops
  - *output:* $m_q^{(n_l)}(\mu_{th})$
  - *uses:* Eq. (30)
  - *comments:* For the heavy mass the on-shell definition is used.
  - *example:* The computation of $m_c^{(4)}(M_Z) = 0.583$ GeV from $m_c^{(5)}(M_Z) = 0.58$ GeV with order α_s^3 accuracy is performed via `DecMqDownOS[0.58,asMz/.NumDef,4.7,Mz/.NumDef,5,4]`. Here, $\alpha_s^{(5)}(M_Z) = 0.118$ and $M_b = 4.7$ GeV have been used.

- `DecMqUpMS`:
  - *input:* $m_q^{(n_l)}(\mu_{th})$, $\alpha_s^{(n_l)}(\mu_{th})$, $m_{th}(\mu_{th})$, μ_{th}, n_l, number of loops
  - *output:* $m_q^{(n_l+1)}(\mu_{th})$
  - *uses:* Eq. (31)
  - *comments:* The heavy mass is evaluated in the $\overline{\mathrm{MS}}$ scheme at the scale μ_{th}.
  - *example:* (analog to `DecMqUpOS[]`)

- `DecMqDownMS`:
  - *input:* $m_q^{(n_l+1)}(\mu_{th})$, $\alpha_s^{(n_l+1)}(\mu_{th})$, $m_{th}(\mu_{th})$, μ_{th}, n_l, number of loops
  - *output:* $m_q^{(n_l)}(\mu_{th})$
  - *uses:* Eq. (27)
  - *comments:* The heavy mass is evaluated in the $\overline{\mathrm{MS}}$ scheme at the scale μ_{th}.
  - *example:* (analog to `DecMqDownOS[]`)
- `DecMqUpSI`:
  - *input:* $m_q^{(n_l)}(\mu_{th})$, $\alpha_s^{(n_l)}(\mu_{th})$, $\mu_{m_{th}}$, μ_{th}, n_l, number of loops
  - *output:* $m_q^{(n_l+1)}(\mu_{th})$
  - *uses:* Eq. (32)
  - *comments:* Here the scale invariant mass $\mu_{m_{th}}$ is chosen for heavy mass.
  - *example:* (analog to `DecMqUpOS[]`)
- `DecMqDownSI`:
  - *input:* $m_q^{(n_l+1)}(\mu_{th})$, $\alpha_s^{(n_l+1)}(\mu_{th})$, $\mu_{m_{th}}$, μ_{th}, n_l, number of loops
  - *output:* $m_q^{(n_l)}(\mu_{th})$
  - *uses:* Eq. (29)
  - *comments:* Here the scale invariant mass $\mu_{m_{th}}$ is chosen for heavy mass.
  - *example:* (analog to `DecMqUpMS[]`)
- `DecLambdaUp`:
  - *input:* $\Lambda^{(n_l)}$, $\mu_{m_{th}}$, n_l, number of loops
  - *output:* $\Lambda^{(n_l+1)}$
  - *uses:* Eq. (34)
  - *comments:* For the heavy mass the scale invariant mass $\mu_{m_{th}}$ is used.
  - *example:* From $\Lambda^{(4)} = 0.2876$ one can compute $\Lambda^{(5)} = 0.208$ with the help of `DecLambdaUp[0.287,3.97,4,4]` where $\mu_b = 3.97$ and four-loop accuracy has been chosen.
- `DecLambdaDown`:
  - *input:* $\Lambda^{(n_l+1)}$, $\mu_{m_{th}}$, n_l, number of loops
  - *output:* $\Lambda^{(n_l)}$
  - *uses:* Eq. (35)

- *comments:* For the heavy mass the scale invariant mass $\mu_{m_{th}}$ is used.
- *example:* From $\Lambda^{(5)} = 0.208$ one can compute $\Lambda^{(4)} = 0.208$ with the help of `DecLambdaDown[0.208,3.97,4,4]` where $\mu_b = 3.97$ and four-loop accuracy has been chosen.

Miscellaneous procedures

The following modules provide some simple examples which mostly combine the modules described above. "L" stands for low and "H" for high. The condition $l < h$ is assumed in all four procedures.

- `AlL2AlH`:
  - *input:* $\alpha_s^{(l)}(\mu_1)$, μ_1, $\{\{n_{f_1}, M_{th_1}, \mu_{th_1}\}, \{n_{f_2}, M_{th_2}, \mu_{th_2}\}, \ldots\}$, μ_2, number of loops
  - *output:* $\alpha_s^{(h)}(\mu_2)$
  - *uses:* `AlphasExact[]` and `DecAsUpOS[]`
  - *comments:* The set in the third argument may contain several triples indicating the number of flavours, the heavy (on-shell) quark mass and the scale at which the decoupling is performed.
  - *examples:* 1. For the computation of $\alpha_s^{(6)}(500 \text{ GeV}) = 0.0952$ from $\alpha_s^{(4)}(M_c = 1.6 \text{ GeV}) = 0.338$ to $\mathcal{O}(\alpha_s^3)$ accuracy the input would look as follows: `AlL2AlH[0.338,1.6,{{5,4.7,5},{6,175,200}},500,4]` Here, the matching is performed at 5 GeV and 200 GeV, respectively.

    2. Fig. 1 can be reproduced with the help of the following input `AlL2AlH[0.36,1.777,{{5,4.7,mu5}},91.187,l]` where $l = 1, 2, 3, 4$ corresponds to the number of loops and `mu5/4.7` is the scale on the abscissa.
- `AlH2AlL`:
  - *input:* $\alpha_s^{(h)}(\mu_1)$, μ_1, $\{\{n_{f_1}, M_{th_1}, \mu_{th_1}\}, \{n_{f_2}, M_{th_2}, \mu_{th_2}\}, \ldots\}$, μ_2, number of loops
  - *output:* $\alpha_s^{(l)}(\mu_2)$
  - *uses:* `AlphasExact[]` and `DecAsDownOS[]`
  - *comments:* The set in the third argument may contain several triples indicating the number of flavours, the heavy (on-shell) quark mass and the scale at which the decoupling is performed.
  - *example:* Consider the inverse order of the first example of the previous procedure. The input `AlH2AlL[0.0952,500,{{6,175,200},{5,4.7,5}},1.6,4]`, indeed leads to $\alpha_s^{(4)}(1.6 \text{ GeV}) = 0.338$.

- `mL2mH`:
  - *input:* $m_q^{(l)}(\mu_1)$, $\alpha_s^{(l)}(\mu_1)$, μ_1, $\{\{n_{f_1}, M_{th_1}, \mu_{th_1}\}, \{n_{f_2}, M_{th_2}, \mu_{th_2}\}, \ldots\}$, μ_2, number of loops
  - *output:* $m_q^{(h)}(\mu_2)$
  - *uses:* `AlphasExact[]`, `mMS2mMS[]` `DecMqUpOS[]` and `DecAsUpOS[]`
  - *comments:* The set in the fourth argument may contain several triples indicating the number of flavours, the heavy (on-shell) quark mass and the scale at which the decoupling is performed.
  - *example:* Using $\alpha_s^{(4)}(1.2 \text{ GeV}) = 0.403$ and $m_c^{(4)}(1.2 \text{ GeV}) = 1.2$ GeV one finds $m_c^{(5)}(M_Z) = 0.580$ GeV with the help of `mL2mH[1.2,0.403,1.2,{{5,4.7,5.0}},Mz/.NumDef,4]`. The decoupling of $M_b = 4.7$ GeV is performed at 5.0 GeV. In this way the results of Fig. 2 can be reproduced.
- `mH2mL`:
  - *input:* $m_q^{(h)}(\mu_1)$, $\alpha_s^{(h)}(\mu_1)$, μ_1, $\{\{n_{f_1}, M_{th_1}, \mu_{th_1}\}, \{n_{f_2}, M_{th_2}, \mu_{th_2}\}, \ldots\}$, μ_2, number of loops
  - *output:* $m_q^{(l)}(\mu_2)$
  - *uses:* `AlphasExact[]`, `mMS2mMS[]` `DecMqDownOS[]` and `DecAsDownOS[]`
  - *comments:* The set in the fourth argument may contain several triples indicating the number of flavours, the heavy (on-shell) quark mass and the scale at which the decoupling is performed.
  - *example:* Using $\alpha_s^{(5)}(M_Z) = 0.118$ and $m_c^{(5)}(M_Z) = 0.580$ GeV one finds $m_c^{(4)}(1.2 \text{ GeV}) = 1.20$ GeV with the help of `mH2mL[0.580,asMz/.NumDef,Mz/.NumDef,{{5,4.7,5.0}},1.2,4]`. The decoupling of $M_b = 4.7$ GeV is performed at 5.0 GeV.

References

[1] K.G. Chetyrkin, J.H. Kühn, and A. Kwiatkowski, *Phys. Reports* **277** (1996) 189.

[2] T. van Ritbergen, J.A.M. Vermaseren, and S.A. Larin *Phys. Lett.* **B 400** (1997) 379.

[3] G. 't Hooft, *Nucl. Phys.* **B 61** (1973) 455;
W.A. Bardeen, A.J. Buras, D.W. Duke, and T. Muta, *Phys. Rev.* **D 18** (1978) 3998.

[4] T. Appelquist and J. Carazzone, *Phys. Rev.* **D 11** (1975) 2856.

[5] K.G. Chetyrkin, B.A. Kniehl, and M. Steinhauser, *Phys. Rev. Lett.* **79** (1997) 2184.

[6] K.G. Chetyrkin, *Phys. Lett.* **B 404** (1997) 161;
S.A. Larin, T. van Ritbergen, and J.A.M. Vermaseren, *Phys. Lett.* **B 405** (1997) 327.

[7] K.G. Chetyrkin, B.A. Kniehl, and M. Steinhauser, *Nucl. Phys.* **B 510** (1998) 61.

[8] G. Rodrigo and A. Santamaria, *Phys. Lett.* **B 313** (1993) 441;
G. Rodrigo, A. Pich, and A. Santamaria, *Phys. Lett.* **B 424** (1998) 367.

[9] S. Wolfram, *Mathematica — a system for doing mathematics by computer* (Addison-Wesley, New York, 1988).

[10] D.J. Gross and F. Wilczek, *Phys. Rev. Lett.* **30** (1973) 1343; *Phys. Rev.* **D 8** (1973) 3633;
H.D. Politzer, *Phys. Rev. Lett.* **30** (1973) 1346.

[11] D.R.T. Jones, *Nucl. Phys.* **B 75** (1974) 531;
W.E. Caswell, *Phys. Rev. Lett.* **33** (1974) 244;
É.Sh. Egoryan and O.V. Tarasov, *Teor. Mat. Fiz.* **41** (1979) 26; *Theor. Math. Phys.* **41** (1979) 863.

[12] O.V. Tarasov, A.A. Vladimirov, and A.Yu. Zharkov, *Phys. Lett.* **B 93** (1980) 429;
S.A. Larin and J.A.M. Vermaseren, *Phys. Lett.* **B 303** (1993) 334.

[13] W. Furmanski and R. Petronzio, *Z. Phys.* **C 11** (1982) 293.

[14] R. Tarrach, *Nucl. Phys.* **B 183** (1981) 384.

[15] O.V. Tarasov, Report No.: preprint JINR P2-82-900 (1982).

[16] S.A. Larin, Report Nos.: Preprint NIKHEF-H/92-18 (1992), hep-ph/9302240; In Proc. of the Int. Baksan School "Particles and Cosmology" (April 22-27, 1993, Kabardino-Balkaria, Russia), eds. E.N. Alexeev, V.A. Matveev, Kh.S. Nirov, V.A. Rubakov (World Scientific, Singapore, 1994).

[17] N. Gray, D.J. Broadhurst, W. Grafe, and K. Schilcher, *Z. Phys.* **C 48** (1990) 673.

[18] E.G. Floratos, S. Narison and E. de Rafael, *Nucl. Phys.* **B 155** (1979) 115.

[19] J. Fleischer, F. Jegerlehner, O.V. Tarasov, and O.L. Veretin, *Nucl. Phys.* **B 539** (1999) 671, hep-ph/9803493 (v5).

[20] K.G. Chetyrkin and M. Steinhauser, *Phys. Rev. Lett.* **83** (1999) 4001;
K.G. Chetyrkin and M. Steinhauser, Report Nos.: DESY 99–174, TTP99–47, hep-ph/9911434 (Hamburg, Karlsruhe, 1999) (*Nucl. Phys.* **B** in press).

[21] K. Melnikov and T. van Ritbergen, Report Nos.: SLAC-PUB-8321, TTP99–51 and hep-ph/9912391.

[22] G. Martinelli et al., *Nucl. Phys.* **B 445** (1995) 81;
see also [23, 24].

[23] S. Weinberg, *Phys. Rev.* **D 8** (1973) 3497.

[24] E. Franco and V. Lubicz, *Nucl. Phys.* **B 531** (1998) 641.

[25] K.G. Chetyrkin and A. Rétey, Report Nos.: TTP99–43 (Karlsruhe 1999) and hep-ph/9910332.

[26] S. Weinberg, *Phys. Lett.* **B 91** (1980) 51;
B.A. Ovrut and H.J. Schnitzer, *Phys. Lett.* **B 100** (1981) 403.

[27] W. Wetzel, *Nucl. Phys.* **B 196** (1982) 259;
W. Bernreuther and W. Wetzel, *Nucl. Phys.* **B 197** (1982) 228;
W. Bernreuther, *Ann. Phys.* **151**1983127; *Z. Phys.* **C 20** (1983) 331.

[28] S.A. Larin, T. van Ritbergen and J.A.M. Vermaseren, *Nucl. Phys.* **B 438** (1995) 278.

[29] D.J. Broadhurst, *Z. Phys.* **C 54** (1992) 599.