

Heavy Quarks in a Can and the QCD Coupling

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The Lambda parameter of three flavor QCD is obtained by computing the running of a renormalized finite volume coupling from hadronic to very high energies where connection with perturbation theory can safely be made. The theory of decoupling allows us to perform the bulk of the computation in pure gauge theory. The missing piece is then an accurate matching of a massive three flavor coupling with the pure gauge one, in the continuum limit of both theories. A big challenge is to control the simultaneous continuum and decoupling limits, especially when chiral symmetry is broken by the discretization.

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1. Strong Coupling

The quark masses and the coupling of QCD are free parameters, that have to be determined experimentally before any predictions can be made. For a long time the most precise determinations of the coupling were based on perturbative calculations of high energy processes. When confronted with experiment, the coupling can be treated as a fit parameter, and one is thus able to extract its value at a scale close to the typical energy scale of the process. The scale dependence of a renormalized coupling \bar{g}_s in scheme “ s ” (or $\alpha_s(\mu) \equiv \bar{g}_s^2(\mu)/(4\pi)$) is governed by its β -function $\beta_s = \mu \frac{d\bar{g}_s}{d\mu} \stackrel{\bar{g}_s \rightarrow 0}{\sim} -\bar{g}_s^3(b_0 + b_1 \bar{g}_s^2 + b_{s,2} \bar{g}_s^4 + \dots)$. The first two coefficients in the perturbative expansion are scheme independent (for mass independent schemes). The renormalization group invariant (RGI) Λ parameter can be obtained from the coupling at any scale by the relation

$$\Lambda_s = \mu \varphi_s(\bar{g}_s(\mu)), \quad (1)$$

$$\varphi_s(\bar{g}_s) = (b_0 \bar{g}_s^2)^{-b_1/(2b_0^2)} e^{-1/(2b_0 \bar{g}_s^2)} \times \exp \left\{ - \int_0^{\bar{g}_s} dx \left[\frac{1}{\beta_s(x)} + \frac{1}{b_0 x^3} - \frac{b_1}{b_0^2 x} \right] \right\}.$$

This holds beyond perturbation theory but requires the full non-perturbative β -function. To compare different determinations, one can either extract the Λ -parameter (the scheme dependence of Λ is usually known exactly), or one can agree on a scheme and a scale at which the comparison is made. The PDG for instance uses $\alpha_{\overline{\text{MS}}}(M_Z)$ as a reference point. Similarly, a renormalized mass $\bar{m}_s(\mu)$ can be traded for an RGI mass M that is independent of scheme and scale.

More recently [1] the most precise determinations of the strong coupling are based on low energy experimental quantities, for which perturbation theory is not applicable. For instance on the values of light hadron masses or the pion/kaon decay constant. This is only possible when combined with lattice QCD calculations. The experimental inputs are used to “set the scale”, i.e. to establish a relation between the bare coupling g_0 of the discretized QCD and the lattice spacing a in physical units. This involves expensive large volume simulations with (close-to) physical quark masses. From there on one can broadly distinguish between two types of coupling determinations. The first type is somewhat similar to the high energy determinations: a suitable high energy quantity for which high order perturbation theory is available is determined on the lattice, using essentially the same ensembles as for scale setting. The nonperturbative lattice QCD result is then fitted to a function in which the renormalized coupling is one of many fit parameters. Such a quantity can for instance be the static quark potential at short distance [2], a current two point function [3–5] or a small Wilson loop [6]. The statistical precision of such determinations is usually very high, and the final error is dominated by systematic effects. These can be large, because of the multi-scale nature of the problem. The typical energy μ of the quantity must be high in order to control perturbative truncation errors. Lattice spacings should be small $a \ll \mu^{-1}$ in order to justify continuum extrapolations based on the expected asymptotic behavior. At the same time the box length L has to be large enough to be safe from finite size effects $L \gg m_\pi^{-1}$. Reducing perturbative truncation errors is exponentially hard, because at fixed L and $a\mu$, $\bar{g}^{-2} \sim \ln(L/a)$. A maximal feasible lattice size of around $L/a \approx 100$ means that compromises have to be made. The second type of coupling determinations circumvents the multi-scale problem by finite size scaling techniques [7]. A renormalized finite volume coupling $\bar{g}_s(L^{-1})$ is introduced, i.e. the energy scale

of the coupling is identified with the inverse box size¹. In these schemes only $L \gg a$ is necessary, which is easily achieved, but to change the scale μ a new simulation is necessary. When such a coupling is computed at the same bare couplings g_0 which were also used in the large-volume scale-setting simulations, the lattice spacing and hence the scale L^{-1} are known. To extract the Λ parameter however, the non-perturbative β -function is required. This is typically obtained from fits to the step-scaling function $\sigma(u) = \bar{g}^2(2L)|_{\bar{g}^2(L)=u}$. More precisely, the renormalized coupling is computed at a value of L/a and $2L/a$, while all bare parameters are kept the same. This yields one point of the lattice step-scaling function $\Sigma(u, a/L)$, which needs to be computed over a wide range of u and a/L values, in order to be able to continuum-extrapolate to $\sigma(u)$ and hence to obtain the β -function. This procedure is computationally quite expensive, because it requires many simulations with massless fermions on lattices which often reach $2L/a = 48$. This calculation of the β function is responsible for the main part of the final error in the determinations of Λ by finite size scaling techniques. It has been carried out many times in the past, with various definitions of a finite size coupling and for many theories, e.g. with the Schrödinger-Functional (SF) coupling [8] for QCD with $N_f = 0$ [9, 10], $N_f = 2$ [11], $N_f = 3$ [12], $N_f = 4$ [13, 14] and more recently with the Gradient-Flow (GF) coupling [15, 16] for QCD with $N_f = 0$ [17, 18] and $N_f = 3$ [19]. See [20] for a recent review.

The method presented during this conference allows to compute the $N_f = 3$ Λ -parameter using the very precise β -function of the $N_f = 0$ theory. The two theories are connected in the limit where the three quarks are very heavy. The method was first presented in [21] and a detailed study was published shortly after the conference [22]. The latter publication goes into more detail and contains many tables and figures that were omitted from this shorter proceeding.

2. Decoupling of Heavy Quarks

Decoupling of heavy quarks means that their leading effect on low energy observables can be absorbed in a redefinition of the parameters of the same theory but without the heavy fields [23]. It is best understood in terms of effective theories [24]. In our case the fundamental theory shall be QCD with three degenerate heavy quarks.

$$\mathcal{L} = -\frac{1}{2g^2} \text{tr}\{F_{\mu\nu}F_{\mu\nu}\} + \sum_{f=1}^3 \bar{\psi}_f [\not{D} + m]\psi_f, \quad (2)$$

with two parameters (coupling and mass). The low energy physics of this model can be described by an effective theory

$$\mathcal{L}^{\text{eff}} = \sum_{i=0}^n \frac{1}{M^i} \mathcal{L}_i, \quad (3)$$

and the Lagrangians of increasingly high dimension \mathcal{L}_i are linear combinations of local operators built from the light fields such that all symmetries of the fundamental theory are respected. In our case, where all quarks decouple, operators are built just from the gauge field. The effective Lagrangian is usually truncated leading to residual power corrections $1/M^{n+1}$. The first two orders

¹Often $\bar{g}(L)$ is written instead of $\bar{g}(L^{-1})$

for our setup (ignoring boundary effects) are

$$\mathcal{L}_0 = -\frac{1}{2g^2} \text{tr}\{F_{\mu\nu}F_{\mu\nu}\}, \quad (4)$$

$$\mathcal{L}_2 = \omega_1 \text{tr}\{D_\mu F_{\nu\rho}D_\mu F_{\nu\rho}\} + \omega_2 \text{tr}\{D_\mu F_{\mu\rho}D_\nu F_{\nu\rho}\}. \quad (5)$$

Note that no dimension 5 operators exist. In the case when the leading effective theory is used, $\mathcal{L}^{\text{eff}} = \mathcal{L}_0$, it only has one parameter, the coupling or equivalently the $\Lambda^{(0)}$ parameter. The theory is matched to the fundamental theory by demanding that one physical low energy quantity is the same in both theories. This fixes the $\Lambda^{(0)}$ parameter, and its value inherits a dependence on the mass M of the fundamental theory. All other physical low energy quantities computed in the matched effective theory will then be the same as in the fundamental theory, up to corrections $O(1/M^2)$. In a similar manner the matching can be performed in perturbation theory. In the $\overline{\text{MS}}$ -scheme one finds

$$\Lambda_{\overline{\text{MS}}}^{(0)}(M) = \Lambda_{\overline{\text{MS}}}^{(3)} \times P\left(M/\Lambda_{\overline{\text{MS}}}^{(3)}\right), \quad (6)$$

where P is a perturbative expression constructed from the 5-loop β -function [25, 26], the 4-loop anomalous mass dimension [27] and the 4-loop decoupling relation [28]. The expansions are in powers of $\bar{g}_{\overline{\text{MS}}}^2(m_\star)$, where the renormalization scale is given by the mass of the heavy quark $\bar{m}_{\overline{\text{MS}}}(m_\star) = m_\star$. It is known to be a very well behaved series already at scales as low as the charm quark mass [29], but will be used here at much higher scales. Figure 1 shows this perturbative function in the range of masses relevant for this project. Eq. (6) holds up to perturbative truncation errors, i.e. a high power in $\bar{g}_{\overline{\text{MS}}}(m_\star)$ and up to corrections $O(1/M^2)$.

3. Coupling from Decoupling

A valid nonperturbative matching relation is, that a *massive*² renormalized coupling has the same value in the fundamental and in the effective theory at some low energy scale μ_{dec}

$$\bar{g}_s^{(3)}(\mu_{\text{dec}}, M) \stackrel{!}{=} \bar{g}_s^{(0)}(\mu_{\text{dec}}). \quad (7)$$

Because the theories are now matched, eq. (6) holds up to corrections of $O(\Lambda^2/M^2)$ and $O(\mu_{\text{dec}}^2/M^2)$. This leads to the following strategy

- In $N_f = 3$ QCD: determine $\bar{g}_s^{(3)}(\mu_{\text{dec}}, M)$ at a known value of μ_{dec} and $M \gg \mu_{\text{dec}}$.
- Assume that eq. (7) holds and from $\bar{g}_s^{(0)}(\mu_{\text{dec}})$, equal to $\bar{g}_s^{(3)}(\mu_{\text{dec}}, M)$, obtain $\Lambda_s^{(0)}/\mu_{\text{dec}}$ (evaluate eq. (1)). This requires a precise determination of the β -function *in the pure gauge theory*.
- Translate $\Lambda_s^{(0)}$ to $\Lambda_{\overline{\text{MS}}}^{(0)}$ and then using eq. (6) to $\Lambda_{\overline{\text{MS},\text{eff}}}^{(3)}$. The subscript “eff” means that the value still contains residual $O(1/M^2)$ contaminations and the true three flavor Λ -parameter is obtained only after an $M \rightarrow \infty$ extrapolation.

²Mass-independent couplings are instead related to each other by decoupling relations.

Finally, the steps $\Lambda_{\overline{\text{MS}}}^{(3)} \rightarrow \Lambda_{\overline{\text{MS}}}^{(4)} \rightarrow \Lambda_{\overline{\text{MS}}}^{(5)} \rightarrow \alpha_{\overline{\text{MS}}}(M_Z)$ can be done perturbatively with charm and bottom quark and Z -boson masses as inputs. The advantage of this method is, that the part of the calculation that usually dominates the errors is completely moved to the pure gauge theory, where it can be computed with much better precision.

The first item is the main missing piece in this strategy. From related projects [30] the bare parameters g_0 and m_0 are known such that for a sequence of lattice resolutions $L/a \in \{12, 16, 20, 24, 32, 40, 48\}$ a line of constant physics (LCP) is realized where $L^{-1} = \mu_{\text{dec}} = 789(15)$ MeV and $M = 0$. We want to keep the same L , but turn on a mass such that $z \equiv M/\mu_{\text{dec}} \in \{1.972, 4, 6, 8, 10, 12\}$. For each z , the measured massive couplings can then be extrapolated to the continuum limit, as needed for step one. The details of the necessary mass renormalization and additional complications due to our chosen discretization of QCD are discussed below.

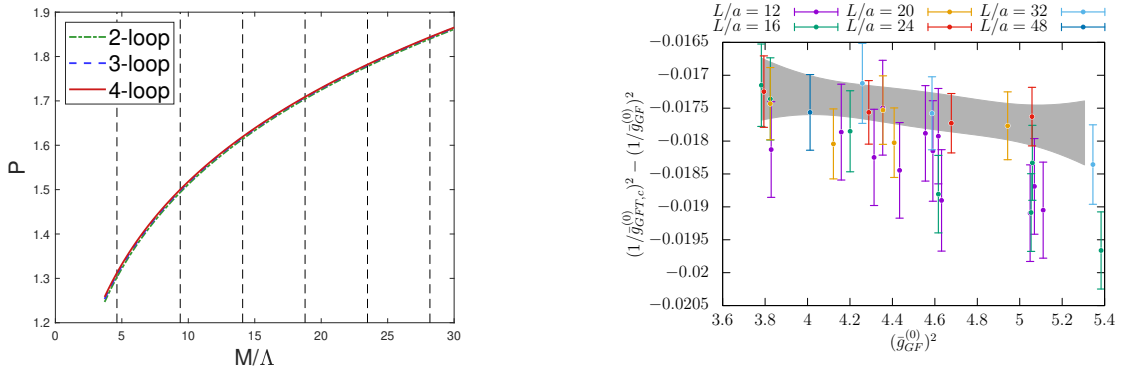


Figure 1: Left: The perturbatively determined translation factor P from eq. (6). Vertical lines correspond to our values of z , the loop order refers to the decoupling relation. Right: Matching of the GF and the GFT couplings in pure gauge theory. The gray band is the final result which is a continuum extrapolation of the colored data points.

4. Lattice Setup and Improvement

Our lattice discretization of QCD is the Lüscher-Weisz gauge action [31] paired with three flavors of non-perturbatively clover improved Wilson fermions [32, 33]. This coincides with the choice of CLS [34] and gives us access to the scale setting results [35]. The main disadvantage is that this discretization breaks chiral symmetry, which has several negative consequences for our project. The first is, that an additive mass renormalization is necessary, i.e. $M = Z_{\text{RGI}}(g_0^2)[m_0 - m_{\text{crit}}(g_0^2)] + O(a)$. The second is, that without explicit $O(a)$ -improvement many results come with errors linear in the lattice spacing. To eliminate the leading lattice artifact it is not enough to use the correct clover coefficient in the simulations. Other improvement coefficients are needed as well, that moreover become increasingly important when the masses are large. Given our massless LCP by a set of tuned $(L/a, g_0)$ pairs, such that $L = \mu_{\text{dec}}^{-1}$ and $M = 0$, in order to switch on a mass $M = z \mu_{\text{dec}}$ while keeping the lattice spacing constant up to $O(a^2)$, g_0 needs to be adjusted such that

$$\tilde{g}_0^2 = g_0^2 \left(1 + b_g(g_0^2) a [m_0 - m_{\text{crit}}(g_0^2)] \right). \quad (8)$$

remains constant. Here b_g is an improvement coefficient. The relation between bare and RGI mass also becomes more complicated

$$M = Z_{\text{RGI}}(g_0^2) [m_0 - m_{\text{crit}}(g_0^2)] \left(1 + ab_m(g_0^2) [m_0 - m_{\text{crit}}(g_0^2)] \right), \quad (9)$$

with the improvement coefficient b_m . These relations are used to move from a known massless LCP to the corresponding massive ones $(L/a, g_0, m_0)|_{L=\mu_{\text{dec}}^{-1}, M=0} \leftrightarrow (L/a, g'_0, m'_0)|_{L=\mu_{\text{dec}}^{-1}, M=z\mu_{\text{dec}}}$.

The main ingredient in our strategy is an appropriate definition of a finite volume coupling that is used in eq. (7). The most precisely known β -function in pure gauge theory [18] is based on a GF coupling defined in a Schrödinger functional. For this coupling, the boundary conditions are such that the spatial directions of length L are periodic (or periodic up to a phase $e^{i/2}$ for fermions, when defined in full QCD), and the temporal direction of size $T = L$ has Dirichlet boundaries for gauge fields and fermions. Boundary gauge fields are $U_k = 1$ and fermionic fields vanish. The family of GF couplings (one for each choice of c) is then defined by

$$\bar{g}_{\text{GF}}^2(\mu) = \mathcal{N}^{-1} \sum_{k,l=1}^3 \frac{t^2 \langle \text{tr} \{ G_{kl}(t, x) G_{kl}(t, x) \} \delta_{Q,0} \rangle}{\langle \delta_{Q,0} \rangle} \Bigg|_{\substack{x_0=T/2, c=\sqrt{8t}/L \\ \mu=1/L, T=L, M=0}}. \quad (10)$$

\mathcal{N} is a known normalization constant. $G_{\mu\nu}$ is the field strength tensor constructed from fields at finite flow time $t = (cL)^2/8$ and Q is the topological charge. Flowed fields are obtained as the solution of a flow equation

$$\begin{aligned} \partial_t B_\mu(t, x) &= D_\nu G_{\nu\mu}(t, x), & B_\mu(0, x) &= A_\mu(x), \\ D_\mu &= \partial_\mu + [B_\mu, \cdot], \\ G_{\mu\nu} &= \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu]. \end{aligned}$$

We used a continuum notation here. For the improved discretization of flow and action density we follow [36].

While this coupling has excellent statistical precision, can be computed non-perturbatively at zero mass and possesses a well defined perturbative expansion, the special choice of boundaries causes some additional challenges with respect to improvement and decoupling. For full $O(a)$ improvement of the SF, two additional boundary improvement coefficients are necessary: c_t and \tilde{c}_t [37]. Moreover, the explicit breaking of chiral symmetry by the boundaries leads to more possibilities for operators in the effective theory, so that decoupling will hold only up to $O(1/M)$ terms coming from boundary operators. To keep these to a minimum, we deviate slightly from eq. (10) for the definition of the coupling that will be used for eq. (7) and define the ‘‘GFT coupling’’ with a longer time extent. The definition is as eq. (10), but with $T = 2L$ and $M = z\mu_{\text{dec}}$.

Finally, the naive expectations based on effective theories (Symanzik and decoupling), that the corrections are powers in a or $1/M$, upon closer inspection get modified by powers of logarithms that are dictated by the anomalous dimensions of higher dimension operators in the effective theory [38]. Their impact on continuum and $M \rightarrow \infty$ extrapolations needs to be taken into account.

Items omitted from this proceeding due to size constraints, which were however studied in detail and can be reviewed in [22] are: The non-perturbative determination of Z_{RGI} and partially perturbative determination of b_m (using also results obtained in [39]), the impact and propagation

of errors $O(a)$ and $O(1/M)$ stemming from the SF boundaries and the non-perturbative matching of GF and GFT couplings in pure gauge theory. The result of this matching is shown in figure 1.

5. Results

Simulations at $L/a \in \{12, 16, 20, 24, 32, 40, 48\}$, $T = 2L$, $L = \mu_{\text{dec}}^{-1}$ and $M/\mu_{\text{dec}} \in \{1.972, 4, 6, 8, 10, 12\}$ were carried out and the GFT couplings with various c have been measured to high precision. To determine their values (for each M) in the continuum limit, various fits have been performed, e.g. a global fit of the form

$$\bar{g}_{\text{GFT}}^2(\mu_{\text{dec}}, M_i, a) = C_i + p_1 [\alpha_{\overline{\text{MS}}}(a^{-1})]^{\hat{\Gamma}} (a\mu_{\text{dec}})^2 + p_2 [\alpha_{\overline{\text{MS}}}(a^{-1})]^{\hat{\Gamma}'} (aM_i)^2, \quad (11)$$

where C_i are the desired continuum values, p_k are fitted coefficients for different $O(a^2)$ artifacts and $\hat{\Gamma}, \hat{\Gamma}'$ were varied to assess uncertainties due to only partial knowledge of logarithmic corrections. Various other fit functions were used as well, and different cuts on the data, e.g. $(aM)^2 < 0.25$, were applied. An example extrapolation is shown in figure 2. One of the bigger contributions to the error is the fact that b_g is known only perturbatively and we assume its error to be 100% of its value. This improvement coefficient plays a role in the determination of the massive simulation parameters, and its error is propagated into the error bands and final result of figure 2, but is left out of the individual error bars.

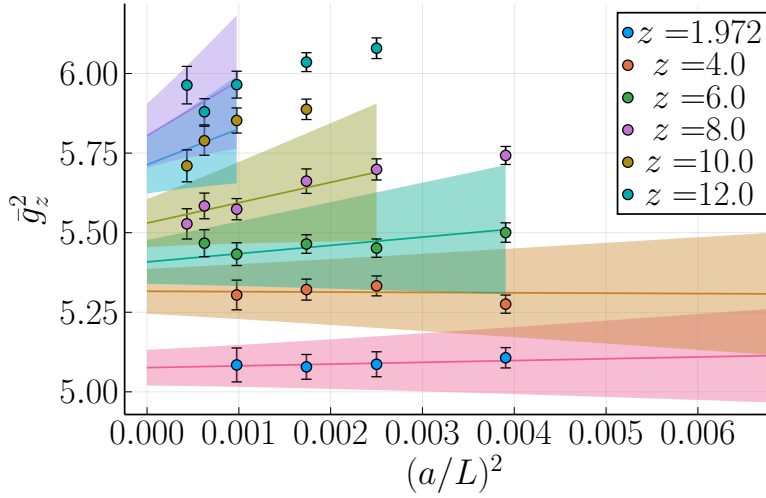


Figure 2: One of the continuum extrapolations according to eq. (11), here for the case $c = 0.36$ and $\hat{\Gamma} = \hat{\Gamma}' = 0$, omitting data with $aM > 0.4$.

As described in the previous section, each massive coupling C_i is used to obtain a value of $\Lambda_{\overline{\text{MS}},\text{eff}}^{(3)}$. These are extrapolated to $M \rightarrow \infty$ according to

$$\Lambda_{\overline{\text{MS}},\text{eff}}^{(3)} = A + \frac{B}{z^2} [\alpha_{\overline{\text{MS}}}(m_\star)]^{\hat{\Gamma}_m}. \quad (12)$$

A is the final result, B is a fit parameter and the fit is repeated with various values $\hat{\Gamma}_m$ (logarithmic corrections to decoupling). An example extrapolation is shown in figure 3.

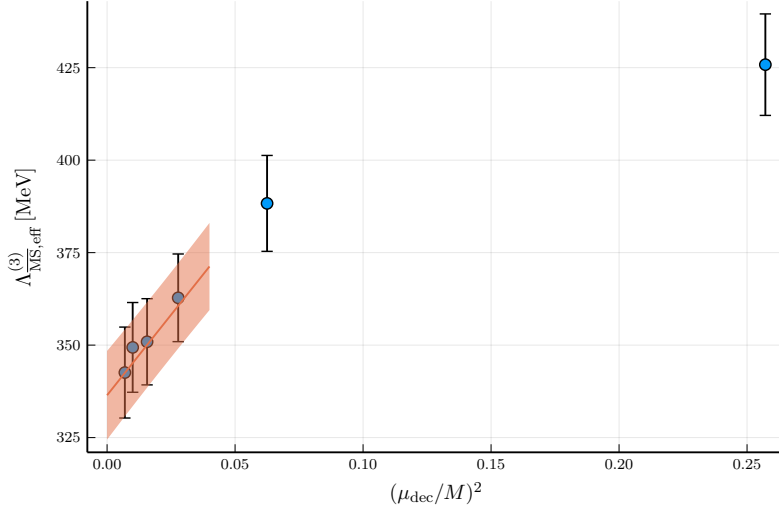


Figure 3: One of the $M \rightarrow \infty$ extrapolations according to eq. (12), here for the case of $c = 0.36$, $\hat{\Gamma}_m = 0$ and omitting the two lightest masses.

Our final result is

$$\Lambda_{\overline{\text{MS}}}^{(3)} = 336(10)(6)_{b_g} (3)_{\hat{\Gamma}_m} \text{ MeV} = 336(12) \text{ MeV} . \quad (13)$$

The first error is statistical, the second due to limited knowledge of b_g and the last due to the $M \rightarrow \infty$ extrapolations. This result is fully non-perturbative, as truncated PT is used only at scales $\sim M$ and becomes exact in the $M \rightarrow \infty$ limit. From this number one can perturbatively obtain

$$\Lambda_{\overline{\text{MS}}}^{(4)} = 294(12) \text{ MeV} , \quad (14)$$

$$\Lambda_{\overline{\text{MS}}}^{(5)} = 211.3(9.8) \text{ MeV} , \quad (15)$$

$$\alpha_{\overline{\text{MS}}}(m_Z) = 0.11823(84) . \quad (16)$$

The errors on these values contain uncertainties due to perturbative decoupling of charm and bottom quarks.

6. Conclusions

We can conclude that the decoupling strategy for computing the strong coupling works very well and offers the same advantages that traditional step-scaling methods do, but at a much reduced computational cost. In fact our final result is very close both in terms of value and error to our previous result [19]. Both calculations have the scale setting in common (value of μ_{dec}), but are completely independent otherwise.

To substantially reduce the error, the main contributors to the final error have to be addressed: The improvement coefficient b_g needs to be determined non-perturbatively, the precision of the $N_f = 0$ running needs to be increased and the scale setting for our action has to become more precise.

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