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Results for α_s from the decoupling strategy

ALPHA collaboration

Mattia Dalla Brida,[a] **Roman Höllwieser,**[b,*] **Francesco Knechtli,**[b] **Tomasz Korzec,**[b] **Alessandro Nada,**[c] **Alberto Ramos,**[d] **Stefan Sint**[e,*] **and Rainer Sommer**[c,f]

[a] *Theoretical Physics Department, CERN, 1211 Geneva 23, Switzerland*
[b] *Deptartment of Physics, University of Wuppertal, Gaußstrasse 20, 42119 Germany*
[c] *John von Neumann Institute for Computing (NIC), DESY, Platanenallee 6, 15738 Zeuthen, Germany*
[d] *Instituto de Física Corpuscular (IFIC), CSIC-Universitat de Valencia, 46071, Valencia, Spain*
[e] *School of Mathematics and Hamilton Mathematics Institute, Trinity College Dublin, Dublin 2, Ireland*
[f] *Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany*

E-mail: hoellwieser@uni-wuppertal.de, sint@maths.tcd.ie

We present analysis details and new results for the strong coupling $\alpha_s(m_Z)$, determined by the decoupling strategy. We measure a massive gradient flow (GF) coupling defined in finite volume with Schrödinger functional (SF) boundary conditions in a theory with $N_\mathrm{f} = 3$ degenerate heavy quarks of mass M. The massive couplings are matched to effective couplings in pure gauge. Using the running in the pure gauge theory and the perturbative relation of the Lambda parameters, the Lambda parameter of the three flavor theory is obtained by an extrapolation to infinite M. Our final result is compatible both with the FLAG average and with the previous ALPHA result, albeit with a slightly smaller, yet still statistics dominated, error. This constitutes a non-trivial check, as the decoupling strategy is conceptually very different from the 3-flavor QCD step-scaling method, and so are most of its systematic errors. These include the uncertainties of the decoupling and continuum limits, which we discuss in some detail. Furthermore, by relying on decoupling once again, we could estimate the small $O(a)$ and $O(1/M)$ contaminations to the massive GF coupling stemming from the SF boundaries by means of pure gauge simulations.

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*Speaker

1. Introduction

The determination of the running coupling $\alpha_s = \bar{g}^2/(4\pi)$ of the strong force yields [1–12] with most precise results from lattice QCD based on finite volume renormalization schemes. In [13] we implement a new strategy to extract α_s from lattice QCD simulations based on the decoupling relation for a massive coupling

$$\bar{g}^2_{N_\mathrm{f}=3}(\mu, M) = \bar{g}^2_{N_\mathrm{f}=0}(\mu) + O((\Lambda/M)^2, (\mu/M)^2)\,. \tag{1}$$

Here $\bar{g}^2_{N_\mathrm{f}=3}(\mu, M)$ is a renormalized coupling in QCD with $N_\mathrm{f} = 3$ massive quarks of mass M[1] and $\bar{g}^2_{N_\mathrm{f}=0}(\mu)$ is the coupling in the pure gauge theory. The renormalization scale, μ, is the same in both theories. The result of Ref. [12] is based on the non-perturbative running of the coupling from low to high energies. Eq. (1) defers this computation to the pure gauge theory, where very high precision can be achieved [15, 16]. We computed a finite volume coupling in a setting with $N_\mathrm{f} = 3$ mass-degenerate heavy quarks for values of the quark mass ranging from charm to above the bottom and already provided a proof of principle that Eq. (1) can be used to extract α_s [13]. Here we present our latest results, confirming the world average of α_s with another independent method, and a good chance to further reduce its uncertainty.

2. Strategy

Decoupling [17, 18] applies to dimensionless, renormalized, low-energy, quantities which include suitably defined couplings at low renormalization scales. Eq.(1) holds when the two theories are matched, i.e. that the Λ-parameter of the $N_\mathrm{f} = 0$ theory is chosen such that

$$\Lambda^{(0)}_{\overline{\mathrm{MS}}} = \Lambda^{(3)}_{\overline{\mathrm{MS}}}\, P_{0,3}(M/\Lambda^{(3)}_{\overline{\mathrm{MS}}})\,. \tag{2}$$

$P_{0,3}$ is the matching factor between the two theories, which, if M is large enough, can be computed very accurately in perturbation theory [14, 19–24]. Equations (1), (2) can be exploited to determine the three flavor Λ-parameter following these steps:

- Choose a low energy renormalization scale μ, that is known in physical units (MeV) in the three flavor theory.
- Determine a massive coupling $\bar{g}^2 = \bar{g}^2_{N_\mathrm{f}=3}(\mu, M)$ on lattices with different lattice spacing a, and take the continuum limit.
- Determine the non-perturbative β-function of the coupling in the $N_\mathrm{f} = 0$ theory and compute the Λ-parameter in units of μ [15]

$$\frac{\Lambda^{(0)}}{\mu} = (b_0\bar{g}^2)^{-b_1/(2b_0^2)}\, e^{-1/(2b_0\bar{g}^2)}\, \exp\left\{-\int_0^{\bar{g}} \left[\frac{1}{\beta(x)} + \frac{1}{b_0x^3} - \frac{b_1}{b_0^2x}\right] dx\right\}\,. \tag{3}$$

  The Λ-parameter in the $\overline{\mathrm{MS}}$ scheme is then given *exactly* by a 1-loop relation. For more details on the exact procedure see [13].

[1] We follow the notation of [14] and denote by M the renormalization group invariant (RGI) quark mass, and by Λ the Lambda-parameter of QCD in the $\overline{\mathrm{MS}}$ scheme.

- Obtain the $N_\mathrm{f} = 3$ Λ-parameter in physical units as

$$\Lambda^{(3)}_{\overline{\mathrm{MS}}} = \mu \times \frac{\Lambda^{(0)}_{\overline{\mathrm{MS}}}}{\mu} \times \frac{1}{P_{0,3}(M/\Lambda^{(3)}_{\overline{\mathrm{MS}}})} + O(M^{-2})\,. \tag{4}$$

Finally, the result can be translated to the commonly used coupling constant $\alpha_s^{(5)}(M_Z)$, relying on the use of perturbation theory in the $\overline{\mathrm{MS}}$ scheme at the charm and bottom mass thresholds. In [13] we have shown, that this strategy is viable and able to reduce the uncertainty of the strong coupling. Several of the above steps were already carried out within different projects, *e.g.*, we know that in the three flavor theory $\bar{g}^2_\mathrm{GF}(\mu, M = 0) = 3.95$ implies $\mu = 789(15)$ MeV [12, 25], where $\bar{g}_\mathrm{GF}$ denotes the gradient-flow coupling, that runs with the box-size of the system $\mu = 1/L$ [26]. We denote this particular choice of renormalization scale by μ_dec from here on. It is the low-energy scale (low in the sense that $\mu \ll M$) at which decoupling in the form of eq. (1) is applied. Another important ingredient that has already been worked out, is the β-function of the $N_\mathrm{f} = 0$ gradient-flow coupling. It has been constructed non-perturbatively to a very high precision, such that Eq. (3) can be evaluated for a large range of couplings [15]. The other key ingredient is a precise determination of the *massive* coupling at scale μ for various M. These simulations have to follow so-called lines of constant physics which give the bare parameters of the discretized theory such that

$$\bar{g}^2_\mathrm{GF}(\mu_\mathrm{dec}, 0) = 3.95\,, \quad M/\mu_\mathrm{dec} \equiv z \in \{2, 4, 6, 8, 12\} \tag{5}$$

for various resolutions $a/L = a\mu_\mathrm{dec}$. In a B-physics project of our collaboration [27], bare couplings, $\tilde{g}_0^2$ and hopping parameters $\kappa = \kappa_\mathrm{crit}$ have been tuned such that the condition for the massless coupling is satisfied within less than 4‰ and such that indeed the quarks are massless to high accuracy. The chosen resolutions are $L/a = 12, 16, 20, 24, 32$ and 40, where the parameters of $L/a = 40$ can be inferred from [25]. For the massive coupling, fixed values of $z = ML$ determine aM and therefore the hopping parameter κ. Their relation is provided by the following renormalization

$$M = \frac{M}{\overline{m}(\mu)} \frac{Z_A(\tilde{g}_0)}{Z_P(\tilde{g}_0, \mu)} m_\mathrm{PCAC} \left(1 + (b_A - b_P) am_q\right)\,, \quad m_\mathrm{PCAC} = \hat{Z}(\tilde{g}_0) m_q (1 + \hat{b}\, am_q)\,, \tag{6}$$

where $am_q = 1/(2\kappa) - 1/(2\kappa_\mathrm{crit})$ is the bare subtracted quark mass. All parameters in the relation between PCAC mass and RGI quark mass are known from [28] and Z_A from [29]. We have carried out massless MC simulations to determine $\hat{Z}$ and $\hat{b}$ with an example depicted in Fig. 1 on the left. The knowledge of these parameters allows massive MC simulations of $L/a = 12, 16, 20, 24, 32, 40$ with $T = 2L$ and for the z-values in Eq. (5) we have $M \approx 1.6 \ldots 9.5$ GeV, see the right plot of Fig. 1 for an overview of massive simulations to be discussed below. The fine resolutions are crucial to fully control the continuum limit $a/L \to 0$ of

$$\bar{g}^2_{N_\mathrm{f}=3}(\mu, z) \quad \text{for} \quad \bar{g}^2_{N_\mathrm{f}=3}(\mu, 0) = 3.95,\ \mu = 1/L,\ z = LM\,, \tag{7}$$

which gives values for the massive coupling in the continuum limit. The second limit that needs to be controlled is $M \to \infty$ in eq. (4).

Before we discuss how we obtain numerical control over the double limit $\lim_{z\to\infty} \lim_{a/L\to 0}$, we need to explain some details on the simulations, in particular the definition of the non-perturbative coupling, associated systematic effects and how we control them.

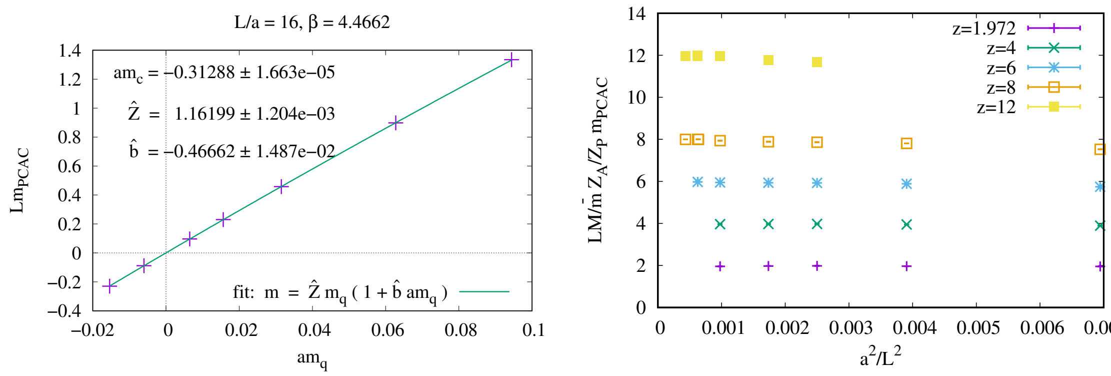

Figure 1: (left) Bare mass $m_{\rm PCAC}$ as a function of the bare subtracted mass $m_{\rm q} = 1/2\kappa - 1/2\kappa_c$ for various values of κ and g_0^2 fixed as explained. The fit determines $\kappa_c, \hat{Z}, \hat{b}$ for the resolution $L/a = 16$ and with Schrödinger Functional boundary conditions and $T = L$. (right) Renormalized PCAC masses of the massive simulations, giving an overview of simulated resolutions L/a and quark masses M, also providing a non-trivial check of our simulation parameters as simulated (intended) z values correspond to measured and renormalized LM values in the continuum limit.

3. Simulations and Analysis

For the Monte-Carlo simulations we use the open-source (GPL v2) `openQCD` package[2] [30] in plain C with MPI parallelization. The software has been successfully used in various large-scale projects and we use it in its version `openQCD-1.6` with additional implementation of

- the correct Schrödinger Functional boundary conditions for the Symanzik improved gauge action with SF boundary conditions precisely as in [25],
- on-the-fly measurements of gradient-flow observables using the Zeuthen flow [31], including measurements of the gradient flow coupling and the topological charge,
- on-the-fly measurements of Schrödinger Functional correlators, needed for the determination of the PCAC mass.

All simulations in this project use the Lüscher-Weisz improved gauge action with O(a) improvement for $N_{\rm f} = 3$ quarks tuned at and around zero quark mass in the first respectively quark masses $M \approx 1.6 \ldots 9.5$GeV in the second set of simulation runs.

We use a gradient flow coupling in a finite volume $T \times L^3$ with Schrödinger functional (SF) boundary conditions [13]. In this setting the formally leading corrections to decoupling are not $1/M^2$ but they are $1/M$. In the low energy effective field theory the $1/M$ term originates from only one operator, $\mathrm{tr}\, F_{0k} F_{0k}$ located at the two time-boundaries of the SF manifold. The exactly same term is responsible for $O(a)$ terms of the pure gauge SF. Its renormalization group improved perturbative expansion has recently been discussed [32]. In complete analogy we are able to treat the $1/M$ term and show that it is very small. Its smallness is due to a combination of 1) the smallness of the coefficient in the effective theory, which follows from [33], 2) the vanishing of

[2] `http://luscher.web.cern.ch/luscher/openQCD/`

the anomalous dimension of tr $F_{0k}F_{0k}$ at the boundary [32] and 3) our choice $T = 2L$. The latter was a precaution that we took in [13]. We are presently working out the coefficient of tr $F_{0k}F_{0k}$ to next to leading order in perturbation theory in $\bar{g}^2_{\overline{\rm MS}}(m_\star)$, where $\overline{m}_{\overline{\rm MS}}(m_\star) = m_\star$. The effect of the boundary operator can then be determined in the pure gauge theory. In summary, while $1/M$ terms are there, they can be estimated well and are negligible. Also $O(a)$ boundary lattice artifacts are suppressed by the choice $T = 2L$ and are very small due to the implemented one-loop boundary O(a) improvement.

The basis for the analysis of the continuum and decoupling limits is determined via first applying Symanzik EFT [34] and then performing a heavy quark mass expansion of that continuum EFT. The first step tells us that the only $\sim a^2$ cutoff effects accompanied by positive powers of the quark mass are of the form a^2M^2, once O(a) improvement is done. The second step yields a series in powers of $1/M^2$ of all terms in the Symanzik EFT, when we make the usual assumption that also the second level EFT is described by a local effective Lagrangian. Taking only the leading corrections, this argumentation yields

$$\bar{g}^2(z_i) = c_i + p_1\,[\alpha_s(a^{-1})]^{\hat{\Gamma}_1}\,(a/L)^2 + p_2\,[\alpha_s(a^{-1})]^{\hat{\Gamma}_2}\,(aM)^2, \tag{8}$$

as a fit function for performing the continuum limit. The presence of log-corrections of the form $[\alpha_s(a^{-1})]^{\hat{\Gamma}_i}$ is due to the anomalous dimensions of the operators in the EFTs. There is partial knowledge on them from Husung et al. [32, 35, 36], but it is not yet complete. We will vary the Γ_i to an extent suggested by [32, 35, 36], being aware that this is not the end of the story.

The combined, linear fit of our data using Eq. (8) is shown in Fig. 2. In order to get a good quality of the fit (min. χ^2), we only take data points with $z \geq 4$ and $aM \leq 0.4$ into account. We see in the right plot of Fig. 2 that the $z = 2$ data shows a very different slope in $(aM)^2$ compared to the other data sets. Further, varying the exponents $\hat{\Gamma}_i$ in the range $[-1\ldots1]$ gives a systematic error which is negligible in the final result of Λ. We use $\hat{\Gamma}_1 = \hat{\Gamma}_2 = 0$ for our central values.

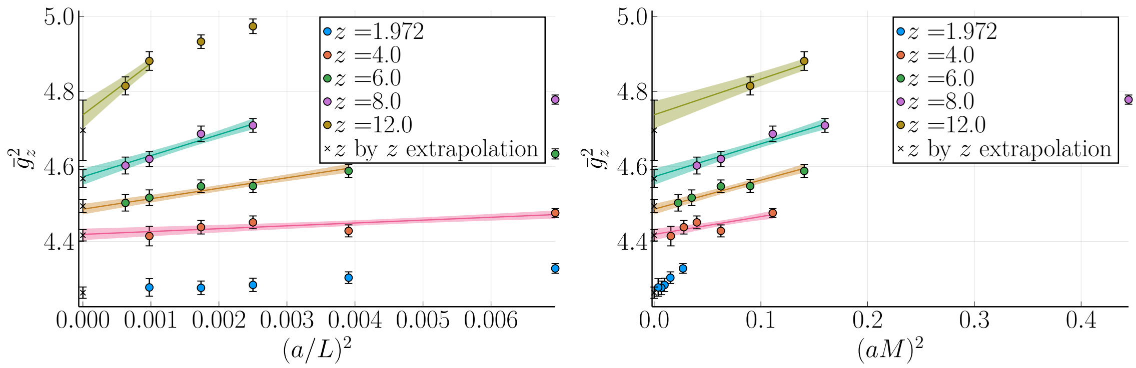

Figure 2: The gradient flow couplings $\bar{g}^2_z = \bar{g}^2(\mu, z\mu)$ of our massive simulations for $z = 2, 4, 6, 8, 12$ from bottom to top versus the leading discretization effects $(a/L)^2$ (left) and $(aM)^2$ (right), together with the combined, correlated, linear fit in Eq. (8), taking into account only data points with $z \geq 4$ and $aM \leq 0.4$. Note, the crosses on $a = 0$ axes stem from individual z extrapolations, not the combined fit.

Using Eqs. (3) and (4) we translate our continuum extrapolated couplings $\bar{g}^2_z = \bar{g}^2(\mu, z\mu)$ into $\Lambda^{(3)}_{\overline{\rm MS}}$-parameters in physical units. For the decoupling ($M \to \infty$) extrapolation we find the functional form

$$\Lambda^{(3)}_{\overline{\rm MS}}(z) = A + \frac{B}{z^2}\,[\alpha_s(m_\star)]^{\hat\Gamma} \qquad \text{with} \quad \overline{m}_{\overline{\rm MS}}(m_\star) = m_\star, \tag{9}$$

where again the fractional exponent $\hat\Gamma$ of the logarithmic correction is not known. In fig. 3 we fit Eq. (9) to the continuum extrapolated $\Lambda^{(3)}_{\overline{\rm MS}}$-parameters, omitting the data point with $z = 4$ which is clearly outside $1/z^2$ scaling, and present the extrapolated values for $\hat\Gamma \in [-1, 1]$ in the right plot.

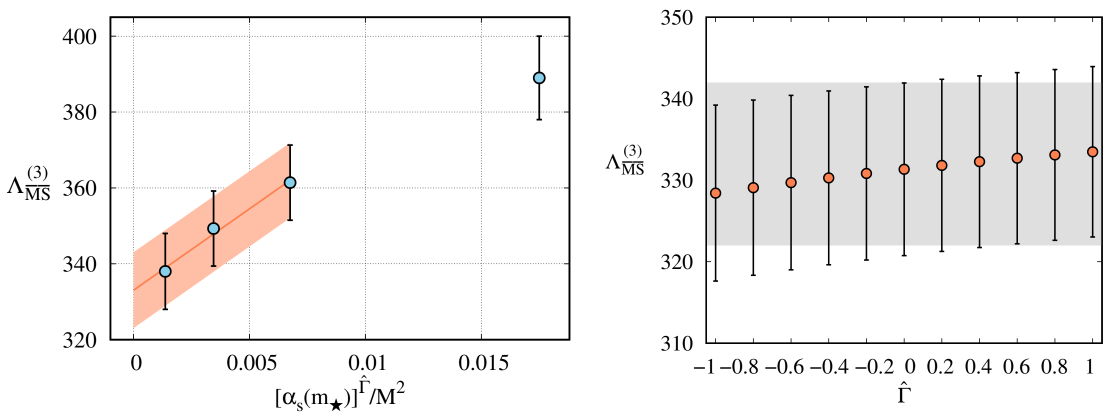

Figure 3: Values for $\Lambda^{(3)}_{\overline{\rm MS}}$ determined from the decoupling relation Eq. (4) and their extrapolation $M \to \infty$ using Eq. (9). In order to get a good quality of the fit (min. χ^2) we only take data points with $z \geq 6$ into account (left). The right plot shows different extrapolations for different exponents $\hat\Gamma \in [-1, 1]$ of the logarithmic corrections in Eq. (9), with the grey band indicating the preliminary result and error given below.

4. Conclusions and Outlook

With the present status of the simulations and their continuum (a/L resp. $aM \to 0$) and decoupling ($M \to \infty$) limits, we derive a preliminary value of

$$\Lambda^{(3)}_{\overline{\rm MS}} = 332(10)(2)\ \text{MeV}$$

where we add a systematic error of 2MeV for the variation with $\hat\Gamma$ in Eq. (9). The final value is about one standard deviation smaller, but in agreement with the previous result $\Lambda^{(3)}_{\overline{\rm MS}} = 341(12)$MeV [12], entirely performed in the $N_{\rm f} = 3$ theory. We want to stress that the present analysis is a largely independent computation, only the scale $\mu_{\rm dec}$ is in common, which contributes an overall $\sim 40\%$ to the error squared in the present analysis. The four-loop prediction for $\Lambda^{(5)}_{\overline{\rm MS}}/\Lambda^{(3)}_{\overline{\rm MS}}$ yields

$$\alpha_s(M_Z) = 0.1179(7)(1)(1) = 0.1179(7),$$

where the first two errors are the translations of the errors (10)(2) for $\Lambda^{(3)}_{\overline{\rm MS}}$ and the last one is the difference between using perturbation theory with all known orders and 2 orders less, respectively. In order to reduce the error further, we work on refining the analysis, *e.g.*, by fixing the exponents $\hat\Gamma_i$, and including more data points with increased statistics. Some simulations are still ongoing or yet to be analyzed and we may hope for a reduction of the error of the world average by a factor of two since at the same time, we will use the synergy with other projects of the ALPHA collaboration to reduce uncertainties in other elements which go into the analysis and final result. These are:

- The determination of $\mu_{\rm dec}$ in physical units [13] is based on 1) the scale setting of CLS [12, 37] and 2) the running of the massless GF coupling between $\mu_{\rm dec}$ and $\mu_{\rm dec}/4$. These will be improved by:

    1. Newer CLS ensembles reach down further in the light quark masses. This will allow for an improved scale setting [38].
    2. The ALPHA collaboration B-physics project performs extensive simulations in $L_0 = 1/\mu_{\rm dec}$ as well as $L_1 = 2L_0$, $L_2 = 4L_0$ volumes. The step scaling function of the massless GF coupling will be determined with higher precision and better resolution than in [25] exactly in the range of scales needed here.

- While the determination of the $N_{\rm f} = 0$ β-function in [15] is very precise, it does contribute a non-negligible amount to the overall uncertainty, which could be further reduced. Note that we are also performing further cross-checks on the determination of the pure gauge theory Λ-parameter.

For more details on our new procedure based on decoupling and an overview of past, present, and future of precision determinations of the QCD coupling from lattice QCD, please see [39–41].

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