



# Non-perturbative renormalization by decoupling

ALPHA Collaboration

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## ARTICLE INFO

### Article history:

Received 23 March 2020

Received in revised form 26 May 2020

Accepted 17 June 2020

Available online 23 June 2020

Editor: A. Ringwald

### Keywords:

QCD

Perturbation theory

Lattice QCD

## ABSTRACT

We propose a new strategy for the determination of the QCD coupling. It relies on a coupling computed in QCD with  $N_f \geq 3$  degenerate heavy quarks at a low energy scale  $\mu_{\text{dec}}$ , together with a non-perturbative determination of the ratio  $\Lambda/\mu_{\text{dec}}$  in the pure gauge theory. We explore this idea using a finite volume renormalization scheme for the case of  $N_f = 3$  QCD, demonstrating that a precise value of the strong coupling  $\alpha_s$  can be obtained. The idea is quite general and can be applied to solve other renormalization problems, using finite or infinite volume intermediate renormalization schemes.

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## 1. Introduction

Currently the best estimates of  $\alpha_s(m_Z)$  reach a precision below 1%, with lattice QCD providing the most precise determinations [1–8]. The main challenge in a solid extraction of  $\alpha_s$  by using lattice QCD is the estimate of perturbative truncation uncertainties, other power corrections, and finite lattice spacing errors which are present in all extractions (see also [9,10]).

A dedicated lattice QCD approach, known as step scaling [11], allows to connect an experimentally well-measured low-energy quantity with the high energy regime of QCD where perturbation theory can be safely applied, *without making any assumptions on the physics at energy scales of a few GeV*. It has recently been applied to three flavor QCD, yielding  $\alpha_s(m_Z)$  with very high precision by means of a non-perturbative running from scales of 0.2 GeV to 70 GeV [8,12,9] and perturbation theory above. Although new techniques [13,14] have recently made possible a significant improvement over older computations [15,3,16] a substantial further reduction of the overall error is challenging.

In this paper we propose a new strategy for the computation of the strong coupling. It is based on QCD with  $N_f \geq 3$  quarks.

We take the quarks to be degenerate, with an un-physically large mass,  $M$ . They then decouple from the low-energy physics, which predicts our basic relation

$$\frac{\Lambda_{\overline{\text{MS}}}^{(N_f)}}{\mu_{\text{dec}}} P \left( \frac{M}{\mu_{\text{dec}}} \frac{\mu_{\text{dec}}}{\Lambda_{\overline{\text{MS}}}^{(N_f)}} \right) = \frac{\Lambda_{\overline{\text{MS}}}^{(0)}}{\Lambda_s^{(0)}} \varphi_s^{(0)}(\sqrt{u_M}) + \mathcal{O}(M^{-2}), \quad (1)$$

as we will explain in detail. Here  $u_M = \bar{g}_s^2(\mu_{\text{dec}}, M)$  is the value of the coupling in a massive renormalization scheme at the scale  $\mu_{\text{dec}}$ . The function  $\varphi_s^{(0)}(\bar{g}(\mu_{\text{dec}})) = \Lambda_s^{(0)}/\mu_{\text{dec}}$  relates the same coupling and the renormalization scale  $\mu = \mu_{\text{dec}}$  in the zero-flavor theory and the function  $P$  gives the ratio  $\Lambda_{\overline{\text{MS}}}^{(0)}/\Lambda_{\overline{\text{MS}}}^{(N_f)}$ . As shown in [17,18]  $P$  is described very precisely by (high order) perturbation theory. The scale  $\mu_{\text{dec}}$  has to be small compared to  $M$  but is arbitrary otherwise. To make contact to physical units of MeV for the  $\Lambda$ -parameter,  $\mu_{\text{dec}}$  has to be related to a physical mass-scale such as  $\mu_{\text{phys}} = m_{\text{proton}}$  (at physical quark masses). The use of intermediate unphysical scales [19] is of course possible.

In essence the above formula relates the  $N_f$ -flavor  $\Lambda$  parameter to the pure gauge one by means of a massive coupling. Since perturbation theory is used only at the scale  $M$ , it can be controlled by making  $M$  sufficiently large.

The main advantage of this approach is that the non-perturbative running of  $\alpha_s$  from  $\mu_{\text{dec}}$  to high energies is needed only in the

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pure gauge theory, where high precision can be reached, see [20]. It is connected to the three flavor theory by a perturbative approximation for  $P$ , which is very accurate already for masses around the charm mass,  $M \approx M_{\text{charm}}$  [18].

Simulating heavy quarks on the lattice is a challenging multi-scale problem, but defining the intermediate scheme,  $s$ , in a finite volume allows us to reach large quark masses  $M \approx M_{\text{bottom}}$ .

## 2. Decoupling of heavy quarks

On general grounds, the effect of heavy quarks is expected to give small corrections to low energy physics [21]. Following [22], QCD with  $N_f$  heavy quarks of renormalization group invariant (RGI) mass  $M$  is well described by an effective theory at energy scales  $\mu \ll M$ . By symmetry arguments, this theory is just the pure gauge theory [17]. Thus, dimensionless low energy observables can be determined in the pure gauge theory – up to small corrections. In particular this holds true for renormalized couplings in massive renormalization schemes [23],

$$\bar{g}_s^{(N_f)}(\mu, M) = \bar{g}_s^{(0)}(\mu) + O(M^{-2}). \quad (2)$$

Here and below,  $O(M^{-k})$  stands for terms of  $O((\mu/M)^k)$ ,  $O((\Lambda/M)^k)$ . Parameterizing the fundamental ( $N_f$ -flavor) theory in a massless renormalization scheme such as  $\overline{\text{MS}}$ , eq. (2) also relates the values of the fundamental and effective couplings in the form [23]

$$[\bar{g}_{\overline{\text{MS}}}^{(0)}(m^*)]^2 = [\bar{g}_{\overline{\text{MS}}}^{(N_f)}(m^*)]^2 \times C(\bar{g}_{\overline{\text{MS}}}^{(N_f)}(m^*)). \quad (3)$$

In the chosen  $\overline{\text{MS}}$  scheme,  $C$  is perturbatively known including four loops [24–28] and with our particular choice of scale,<sup>1</sup>  $m^* = \bar{m}_{\overline{\text{MS}}}(m^*)$ , the one-loop term vanishes,

$$C(\bar{g}) = 1 + c_2(N_f)\bar{g}^4 + c_3(N_f)\bar{g}^6 + c_4(N_f)\bar{g}^8 + O(\bar{g}^{10}). \quad (4)$$

This relation between couplings provides a relation between the  $\Lambda$ -parameters in the fundamental and effective theories [18]. Given the  $\beta$ -function,

$$\beta_s(\bar{g}_s) = \mu \frac{d\bar{g}_s(\mu)}{d\mu}, \quad (5)$$

in a (massless) scheme  $s$ , the  $\Lambda$ -parameters are defined by<sup>2</sup>

$$\begin{aligned} \Lambda_s^{(N_f)} &= \mu \varphi_s^{(N_f)}(\bar{g}_s(\mu)), \\ \varphi_s^{(N_f)}(\bar{g}_s) &= (b_0 \bar{g}_s^{-2})^{-b_1/(2b_0^2)} e^{-1/(2b_0 \bar{g}_s^2)} \\ &\quad \times \exp \left\{ - \int_0^{\bar{g}_s} dx \left[ \frac{1}{\beta_s(x)} + \frac{1}{b_0 x^3} - \frac{b_1}{b_0^2 x} \right] \right\}. \end{aligned} \quad (6)$$

Thus,

$$\frac{\Lambda_{\overline{\text{MS}}}^{(0)}}{\Lambda_{\overline{\text{MS}}}^{(N_f)}} = P(M/\Lambda_{\overline{\text{MS}}}^{(N_f)}), \quad (8)$$

where

$$P(y) = \frac{\varphi_{\overline{\text{MS}}}^{(0)}(g^*(y) [C(g^*(y))]^{1/2})}{\varphi_{\overline{\text{MS}}}^{(N_f)}(g^*(y))}, \quad y \equiv M/\Lambda_{\overline{\text{MS}}}^{(N_f)}. \quad (9)$$

The function

<sup>1</sup> The running quark mass in scheme  $s$  is denoted  $\bar{m}_s$ .

<sup>2</sup> In our notation, the perturbative expansion of the  $\beta$ -function is  $\beta(x) = -x^3(b_0 + b_1 x^2 + \dots)$ .

$$g^*(M/\Lambda_{\overline{\text{MS}}}^{(N_f)}) = \bar{g}_{\overline{\text{MS}}}^{(N_f)}(m^*) \quad (10)$$

is easily evaluated as explained in [18]. High precision is achieved by using the five-loop renormalization group functions [29–33].

Finally, the combination of eqs. (6), (2), (8) results in

$$\rho P(z/\rho) = \frac{\Lambda_{\overline{\text{MS}}}^{(0)}}{\Lambda_s^{(0)}} \varphi_s^{(0)}(\sqrt{u_M}) + O(M^{-2}), \quad (11)$$

$$u_M = \bar{g}_s^2(\mu_{\text{dec}}, M), \quad (12)$$

written in terms of the dimensionless variables

$$\rho = \frac{\Lambda_{\overline{\text{MS}}}^{(N_f)}}{\mu_{\text{dec}}}, \quad z = M/\mu_{\text{dec}}. \quad (13)$$

The current perturbative uncertainty in  $P(M/\Lambda)$  is of  $O(\bar{g}^8(m^*))$ . It vanishes together with the power corrections of order  $M^{-2}$  as  $M$  is taken large. This completes the explanation of eq. (1).

When evaluating the above quantities by lattice simulations, a multitude of mass scales are relevant:

- $1/L$ , the inverse linear box size,
- $m_\pi$ , the pion mass,
- $\mu_{\text{phys}} \sim \mu_{\text{dec}} \sim m_{\text{proton}}$ , typical QCD mass scales,
- $M$ ,
- $a^{-1}$ , the inverse lattice spacing.

Small finite size effects require  $1/L \ll m_\pi$ , accurate decoupling is given when  $M \gg \mu_{\text{dec}}$  and all scales have to be small compared to  $a^{-1}$ . Such multi-scale problems are very challenging; they inevitably require very large lattices [18].

### 2.1. Ameliorating the multi-scale problem with a finite volume strategy

The multi-scale nature of the problem can be made manageable by using a finite volume coupling  $\bar{g}_s(\mu) = \bar{g}_{\text{FV}}(\mu)$  with [11]

$$\mu = 1/L. \quad (14)$$

The crucial advantages are:

1. There is no need for the volume to be large.
2. We can choose an intermediate value for the scale  $\mu_{\text{dec}}$ . With  $\mu_{\text{dec}} \approx 800$  MeV large quark masses  $M \approx 6000$  MeV can be simulated. Then the uncertainties in the perturbative evaluation of  $P$  are negligible and the power corrections  $(\mu_{\text{dec}}/M)^k$  are expected to be small [18].
3. One is free to choose a coupling definition that has a known non-perturbative running in pure gauge theory, e.g. a gradient flow coupling [12].

It remains that  $aM$  has to be small at large  $M/\mu_{\text{dec}}$ .

Most finite volume couplings used in practice are formulated with Schrödinger functional (SF) boundary conditions on the gauge and fermion fields [34,35] (i.e. Dirichlet boundary conditions in Euclidean time at  $x_0 = 0, T$ , and periodic boundary conditions with period  $L$  in the spatial directions). In this situation, the decoupling effective Lagrangian [18] contains terms with dimension four at the boundaries, which are suppressed by just one power of  $M$ . We have to generalize the  $O(M^{-2})$  corrections in eq. (11) to  $O(M^{-k})$  where  $k = 1$  if a boundary is present [36]. Finite volume schemes that preserve the invariance under translations, using either periodic [37] or twisted [38] boundary conditions, would show a faster decoupling with  $k = 2$ .

### 3. Testing the strategy

We now turn to a numerical demonstration of the idea for  $N_f = 3$ . Our discretisation employs non-perturbatively  $O(a)$  improved Wilson fermions, the same action as the CLS initiative [39]. The bare (linearly divergent) quark mass is denoted  $m_0$  and the pure gauge action has a prefactor  $\beta = 6/g_0^2$ . When connecting observables at different quark masses it is important to keep the lattice spacing constant up to order  $(aM)^2$ . This requires setting  $g_0^2 = \tilde{g}_0^2 / (1 + b_g(\tilde{g}_0)am_q)$ , where  $am_q = am_0 - am_{\text{crit}}$  and  $am_{\text{crit}}$  denotes the point of vanishing quark mass. The bare improved coupling  $\tilde{g}_0$  is independent of the quark mass [40,36]. We use the one-loop approximation to  $b_g$ .

#### 3.1. Choice of finite volume couplings

Several renormalized couplings can be defined in the SF using the Gradient Flow [14] (see [41] for a review of the topic). Our particular choice is based on

$$E_{\text{mag}}(t, x) = \frac{1}{4} G_{ij}^a(t, x) G_{ij}^a(t, x), \quad (t > 0; i, j = 1, 2, 3), \quad (15)$$

i.e. the spatial components of the field strength<sup>3</sup>

$$G_{\mu\nu}(t, x) = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu] \quad (16)$$

of the flow field defined by

$$\partial_t B_\mu(t, x) = D_\nu G_{\nu\mu}(t, x), \quad B_\mu(0, x) = A_\mu(x). \quad (17)$$

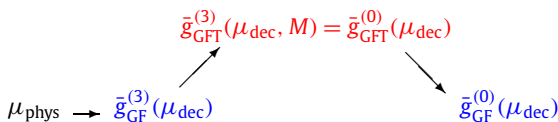
Composite operators formed from the smooth flow field  $B_\mu$  are finite [42] and thus

$$[\tilde{g}_{\text{GF}}^{(3)}(\mu)]^2 = \mathcal{N}^{-1} t^2 \langle E_{\text{mag}}(t, x) \rangle \Big|_{M=0, T=L}^{x_0=L/2, \mu=1/L, \sqrt{8t}=cL}, \quad (18)$$

is a finite volume renormalized coupling. Very precise results are available for  $\tilde{g}_{\text{GF}}^{(3)}$  in  $N_f = 3$  QCD [12] and in the Yang-Mills theory [20]. The constant  $\mathcal{N}$  is analytically known [14], we take  $c = 0.3$  and project to zero topology [43]; thus the coupling is exactly the one denoted  $\tilde{g}_{\text{GF}}$  in [12]. However, it is advantageous to apply decoupling to a slightly different coupling,

$$[\tilde{g}_{\text{GFT}}^{(3)}(\mu, M)]^2 = \mathcal{N}'^{-1} t^2 \langle E_{\text{mag}}(t, x) \rangle \Big|_{T=2L}^{x_0=L, \mu=1/L, \sqrt{8t}=cL}, \quad (19)$$

where  $E$  is inserted a factor two further away from the boundary and the  $M^{-1}$  effects are substantially reduced [44]. In contrast to large changes in the renormalization scale, changes of the scheme,  $\tilde{g}_{\text{GF}}^2 \leftrightarrow \tilde{g}_{\text{GFT}}^2$  are easily accomplished numerically; they do not contribute significantly to the numerical effort or the overall error. After choosing a precise value for  $\mu_{\text{dec}}$  by fixing the value of  $\tilde{g}_{\text{GF}}^{(3)}(\mu_{\text{dec}})$ , the use of the two schemes is schematically shown in the graph



and explained in detail in the following section.

**Table 1**

At each  $L/a$  the bare coupling  $\beta = 6/\tilde{g}_0^2$  and the bare mass  $am_0 = am_{\text{crit}}$  are fixed to have constant coupling, eq. (20), and vanishing quark mass [46,48].  $Z_m, b_m$  are determined by simulations with different  $am_q$  at fixed  $g_0$  [44].

$L/a$	$6/\tilde{g}_0^2$	$am_{\text{crit}}$	$\tilde{g}_{\text{GF}}^2$	$Z_m$	$b_m$
12	4.3020	-0.3234(3)	3.9533(59)	1.691(7)	-0.43(3)
16	4.4662	-0.3129(2)	3.9496(77)	1.726(8)	-0.50(3)
20	4.5997	-0.3043(3)	3.9648(97)	1.741(10)	-0.48(4)
24	4.7141	-0.2969(1)	3.959(50)	1.770(11)	-0.51(2)
32	4.90	-0.28543(4)	3.949(11)	1.814(16)	-0.63(5)

#### 3.2. Numerical computation

We fix a convenient value

$$[\tilde{g}_{\text{GF}}^{(3)}(\mu_{\text{dec}})]^2 = 3.95 \equiv u_0. \quad (20)$$

With the non-perturbative  $\beta$ -function of [12] and the relation to the physical scale  $\mu_{\text{phys}}$  of [8,45]<sup>4</sup> we deduce

$$\mu_{\text{dec}} = 789(15) \text{ MeV}. \quad (21)$$

For this choice, the bare parameters,  $\tilde{g}_0^2, am_0 = am_{\text{crit}}(\tilde{g}_0^2)$  are known rather precisely for several resolutions  $L/a$  [46], see Table 1.

In order to switch to massive quarks of a given RGI mass,  $M = z/L$ , we need to know  $am_q$  which is the solution of

$$z = \frac{L}{a} \frac{M}{\tilde{m}(\mu_{\text{dec}})} Z_m(\tilde{g}_0, a/L) \cdot (1 + b_m(\tilde{g}_0) am_q) am_q, \quad (22)$$

where  $Z_m$  is the renormalization factor in the SF scheme employed in [47] at scale  $\mu_{\text{dec}} = 1/L$ , the ratio  $\frac{M}{\tilde{m}(\mu_{\text{dec}})} = 1.474(11)$  in the same scheme is derived from the results of [47], and the term  $b_m am_q$  removes the discretisation effects of  $O(aM)$ . We have computed  $Z_m, b_m$ , listed in Table 1, by dedicated simulations [44].

As indicated above, the switch to massive quarks is accompanied by the switch to  $\tilde{g}_{\text{GFT}}$  in order to suppress linear  $1/M$  terms: we evaluate

$$\Psi^M(u_0, z) = \left[ \tilde{g}_{\text{GFT}}^{(3)}(\mu_{\text{dec}}, M) \right]_{[\tilde{g}_{\text{GF}}^{(3)}(\mu_{\text{dec}})]^2 = u_0}^2, \quad (23)$$

$$z = M/\mu_{\text{dec}}.$$

Here, with bare mass  $am_0$  set as explained, the condition  $[\tilde{g}_{\text{GF}}^{(3)}(\mu_{\text{dec}})]^2 = u_0$  fixes  $\tilde{g}_0^2$  to the values in Table 1.

We repeat the exercise for  $z = 1.972, 4, 6, 8$ , which correspond to  $M \approx 1.6, 3.2, 4.7, 6.3$  GeV.

It is left to perform continuum extrapolations of the function  $\Psi^M(u_0, z)$ , as illustrated in Fig. 1. They become more challenging at large values of  $z$ . We explore the systematics by imposing two mass cuts  $(aM)^2 < 1/8, 1/4$  and find compatible results, with the results with  $(aM)^2 < 1/8$  having significantly larger errors, at large values of  $M$ , where few points are left after the cut. We take the extrapolations using  $(aM)^2 < 1/8$  as our best estimates of the continuum values of  $\Psi^M(u_0, z)$  (see second column of Table 2).

The precise non-perturbative  $\beta$ -function  $\beta_{\text{GF}}^{(0)}$  of Ref. [20] determines  $\varphi_{\text{GF}}^{(0)}(\tilde{g}_{\text{GF}}^2)$  in the relevant range of  $\tilde{g}_{\text{GF}}^2 \gtrsim 4$ . We connect to it from the scheme GFT by extra simulations, which evaluate  $\tilde{g}_{\text{GFT}}^{(0)}(\mu)$  at the same parameters  $g_0^2, L/a$  where  $\tilde{g}_{\text{GF}}^{(0)}(\mu)$  is known. After con-

<sup>3</sup> Using only the magnetic components reduces the boundary  $O(a)$  effects [14].

<sup>4</sup> The physical scale is set by a linear combination of Pion and Kaon decay constants.

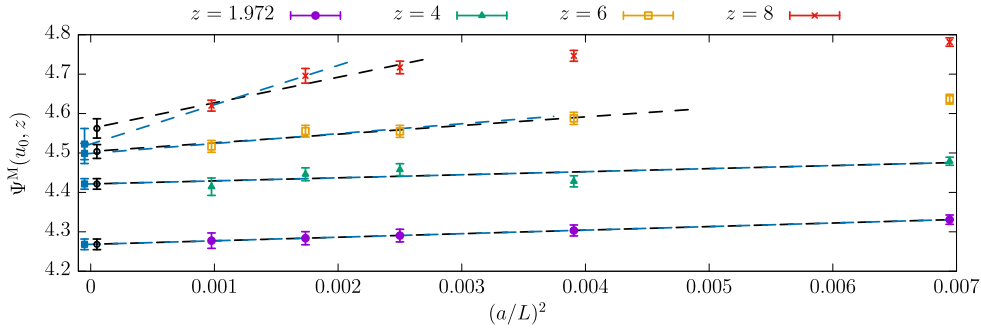


Fig. 1. Continuum extrapolation of the massive coupling  $\Psi^M(u_0, z)$ . We apply two cuts  $(aM)^2 < 1/8, 1/4$  in order to estimate the systematic uncertainty.

Table 2

Results for the massive coupling  $\Psi^M(u_0, z)$  at different values of  $M$  and fixed  $\mu_{\text{dec}} = 789(15)$  MeV. The perturbative factor  $P(M/\Lambda)$  is determined with five-loop running and including  $c_{l \leq 4}$  in eq. (4).  $\Delta_4$  shows the effect of  $c_4$  in  $\Lambda_{\overline{\text{MS}}}^{(3)}$ . The effect of  $c_3$  is larger by a factor 1.5 (for  $z = 1.972$ ) to 3 (for  $z = 8$ ).

$z$	$\Psi^M$	$\Lambda_{\overline{\text{MS}}}^{(0)}/\mu_{\text{dec}}$	$\frac{1}{P(M/\Lambda)}$	$\Lambda_{\overline{\text{MS}}}^{(3)}$ [MeV]	$\Delta_4$ [MeV]
1.972	4.268(13)	0.689(11)	0.8000(48)	434(12)	2.0
4.0	4.421(13)	0.725(11)	0.6865(28)	393(11)	0.7
6.0	4.499(26)	0.743(13)	0.6283(26)	368(10)	0.4
8.0	4.523(40)	0.749(14)	0.5889(27)	348(11)	0.3
$\infty$	FLAG19 (lattice) [1]			343(12)	

tinuum extrapolation of those data with  $L/a = 12, 16, 20, 24$  we find for  $3.8 \leq [\bar{g}_{\text{GF}}^{(0)}]^2 \leq 5.8$  [44]

$$[\bar{g}_{\text{GF}}^{(0)}]^{-2} - [\bar{g}_{\text{GF}}^{(0)}]^{-2} = p_0 + p_1[\bar{g}_{\text{GF}}^{(0)}]^2 + p_2[\bar{g}_{\text{GF}}^{(0)}]^4 \pm 7 \times 10^{-4},$$

with  $(p_0, p_1, p_2) = (2.886, -0.510, 0.056) \times 10^{-2}$ . For each of the values  $\Psi^M$  in Table 2 we obtain  $u_M = [\bar{g}_{\text{GF}}^{(0)}]^2$  from  $[\bar{g}_{\text{GF}}^{(0)}]^2 = \Psi^M$ , insert into eq. (11) (with scheme  $s = \text{GF}$ ) and solve (numerically) for  $\rho$ . The table includes  $\Lambda_{\overline{\text{MS}}}^{(3)}$  as well as the influence of the last known term of the series eq. (4) which demonstrates that perturbative uncertainties are negligible.

At present we have used a relatively modest amount of computer time. Our largest lattice is just  $64 \times 32^3$ . A significant improvement, simulating lattice spacings twice finer, is possible with current computing power.

### 3.3. Results

According to Eq. (1), the values obtained for  $\Lambda_{\overline{\text{MS}}}^{(3)}$  approach the true non-perturbative value as  $M \rightarrow \infty$ . We demonstrate this property in the plot of  $\rho$ , Fig. 2. While we see power corrections, these are small and the point with  $M \approx 6$  GeV is in agreement with the known number from [8] as well as with the FLAG average [1]. Rough extrapolations to the limit  $M \rightarrow \infty$  seem to make the agreement even better. This limit should be studied with even higher precision in the future.

## 4. Conclusions

In this letter we propose a new strategy to determine the strong coupling. It requires the determination of a renormalized coupling in an unphysical setup with degenerate massive quarks at some low energy scale. The second ingredient is the determination of the  $\Lambda$ -parameter in units of the low energy scale in the pure gauge theory defined in terms of the same coupling. The steps are

- i) Determination of a precise low energy scale, such as  $t_0$ , in physical units.

- ii) Definition of a suitable finite volume scheme  $s = \text{FV}$  with coupling  $\bar{g}_{\text{FV}}^{(3)}(\mu, M)$  in the theory with three massive, mass-degenerate, quarks. Determination of the coupling,  $\bar{g}_{\text{FV}}^{(3)}(\mu_{\text{dec}}, 0)$  in the massless case for  $\mu_{\text{dec}} = O(1 \text{ GeV})$ . The precise value of the decoupling scale  $\mu_{\text{dec}}$  is irrelevant, but its value has to be known precisely with the help of i).
- iii) Connection of  $\bar{g}_{\text{FV}}^{(3)}(\mu_{\text{dec}}, 0)$  and  $\bar{g}_{\text{FV}}^{(3)}(\mu_{\text{dec}}, M)$  for sufficiently massive quarks:  $z = M/\mu_{\text{dec}} = 3$  and larger.
- iv) Determination of  $\Lambda_{\overline{\text{MS}}}^{(0)}/\mu_{\text{dec}}$  as a function of  $\bar{g}_{\text{FV}}^{(0)}(\mu_{\text{dec}})$  for values  $\bar{g}_{\text{FV}}^{(0)}(\mu_{\text{dec}}) = \bar{g}_{\text{FV}}^{(3)}(\mu_{\text{dec}}, M)$  from the previous step.
- v) Application of decoupling of the three massive quarks in the form of eq. (1) with perturbative  $P$  to obtain  $\Lambda_{\overline{\text{MS}}}^{(3)}$ .

As we have shown, there is a clear advantage: the essential part of the multi-scale problem (i.e. the determination of  $\Lambda/\mu$  with  $\mu$  a low or intermediate energy scale) is done without fermions. The remaining problem, namely the limit of large  $M$  can be reached by two observations. First it is known that with a mass  $M$  of a few GeV, the perturbative prediction for  $P$  is very accurate [49,18]. Second we showed that with a suitable finite volume scheme one can reach masses of several GeV where the  $O(1/M^2)$  corrections can be controlled.

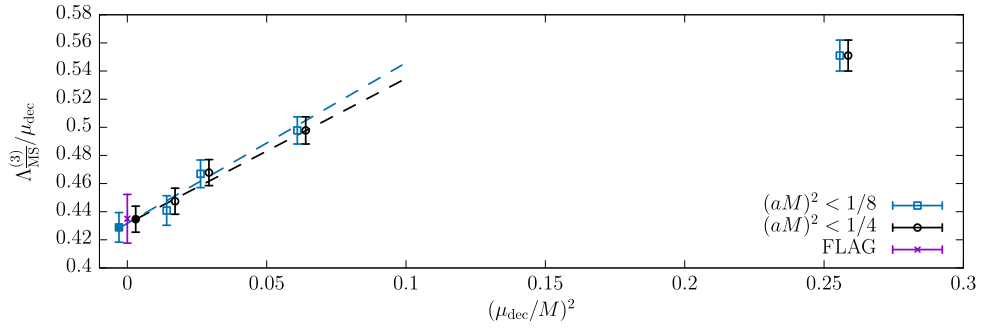
The result is in good agreement with the more standard step scaling approach, but promises a higher precision.

What improvement can we expect? The preliminary extrapolation in Fig. 2 shows an improvement of about a factor two compared to the FLAG number. The limits  $a \rightarrow 0$  at fixed  $M$  in iii) and  $M \rightarrow \infty$  in iv) still need to be made solid by investing a bit more than the present rather modest numerical effort. One can assume that the final error at  $z \rightarrow \infty$  will not be bigger than the present one, but will contain a sound estimate of the systematics. Further, the errors in the figure at finite  $z$  are dominated by an about 1.4% contribution from the pure gauge  $\Lambda_{\overline{\text{MS}}}^{(0)}/\mu_{\text{dec}}$  of step iv) [20]. Its reduction down to about 0.5% requires a modest effort. At that point there remains an, at present 2%, uncertainty due to the fixing of  $\mu_{\text{dec}}$  in physical units from steps i-ii), which we expect to reduce to about 1% by exploiting the newer CLS runs close to the physical point as well as more precise step scaling functions of  $\bar{g}_{\text{GF}}$  for  $\mu < \mu_{\text{dec}}$ . As a bottom line a factor two improvement of the accuracy of the present world average is in reach.

As mentioned, other definitions of the finite volume coupling with other boundary conditions may be chosen. We have already employed two somewhat different ones, GF and GFT to optimize our setup.

An alternative approach relies on the decoupling of  $t_0$  [13] or a different low energy scale (see also [17,18]),





**Fig. 2.** Values for  $\rho$  determined from the decoupling relation. As  $z = M/\mu_{\text{dec}}$  gets larger, the approximations for  $\rho = \Lambda_{\overline{\text{MS}}}^{(3)}/\mu_{\text{dec}}$  approach the FLAG result for  $\Lambda_{\overline{\text{MS}}}^{(3)}$  in units of  $\mu_{\text{dec}} = 789(15)$  MeV [1]. Filled symbols illustrate possible extrapolations  $M \rightarrow \infty$  (cf. Eq. (1)). The errors of these extrapolations show significantly smaller statistical uncertainties than the ones of the FLAG average ( $\mu_{\text{dec}}$  gives a negligible contribution to the uncertainty in  $\Lambda_{\overline{\text{MS}}}^{(3)}/\mu_{\text{dec}}$  from FLAG), and may be reduced further with a modest computational effort in the Yang-Mills theory. (Note: the data both at finite  $M$  and the extrapolations  $M \rightarrow \infty$  has been slightly shifted horizontally for a better visualization.)

$$[\Lambda_{\overline{\text{MS}}}\sqrt{t_0(M)}]^{(N_f)} P\left(\frac{M}{\Lambda_{\overline{\text{MS}}}^{(N_f)}}\right) = [\Lambda_{\overline{\text{MS}}}\sqrt{t_0}]^{(0)} + \mathcal{O}(M^{-2}).$$

The r.h.s. is known [20], so  $\Lambda_{\overline{\text{MS}}}^{(N_f)}$  can be determined once  $t_0(M)$  is computed with at least three degenerate quarks in physical units. This requires a set of massive large volume simulations. Controlling discretization errors, power corrections and perturbative corrections at the same time will require compromises but is worth exploring.

The idea presented here can easily be extended to other RGI quantities. A clear case is the determination of quark masses, where one can replace the running in the full theory by the one in the quenched approximation. On the other hand, four fermion operators will require to first study their perturbative decoupling relations and then to investigate the non-perturbative power corrections.

### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

### Acknowledgements

We are grateful to our colleagues in the ALPHA-collaboration for discussions and the sharing of code as well as intermediate unpublished results. In particular we thank Stefan Sint for many useful discussions and P. Fritzsche, J. Heitger, S. Kuberski for preliminary results of the HQET project [46]. We thank Matthias Steinhauser for pointing out that  $c_4$  is known [28]. RH was supported by the Deutsche Forschungsgemeinschaft in the SFB/TRR55. AR and RS acknowledge funding by the H2020 program in the *Europlex* training network, grant agreement No. 813942. Generous computing resources were supplied by the North-German Supercomputing Alliance (HLRN, project bep00072) and by the John von Neumann Institute for Computing (NIC) at DESY, Zeuthen.

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