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The accuracy of QCD perturbation theory at high energies

(ALPHA Collaboration)

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We discuss the determination of the strong coupling $\alpha_{\overline{\rm MS}}(m_{\rm Z})$ or equivalently the QCD Λ-parameter. Its determination requires the use of perturbation theory in $\alpha_s(\mu)$ in some scheme, s, and at some energy scale μ. The higher the scale μ the more accurate perturbation theory becomes, owing to asymptotic freedom. As one step in our computation of the Λ-parameter in three-flavor QCD, we perform lattice computations in a scheme which allows us to non-perturbatively reach very high energies, corresponding to $\alpha_s = 0.1$ and below. We find that perturbation theory is very accurate there, yielding a three percent error in the Λ-parameter, while data around $\alpha_s \approx 0.2$ is clearly insufficient to quote such a precision. It is important to realize that these findings are expected to be generic, as our scheme has advantageous properties regarding the applicability of perturbation theory.

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INTRODUCTION

The fundamental parameter of the strong interactions, the coupling $\alpha_{\overline{\rm MS}}(\mu) = \bar{g}^2_{\overline{\rm MS}}(\mu)/(4\pi)$, is an essential input parameter for theory predictions of high energy processes in particular the physics at the LHC [1–3]. Conventionally the running $\alpha_{\overline{\rm MS}}(\mu)$ is quoted at the electroweak scale, $\mu = m_{\rm Z}$. There the coupling is weak, $\alpha = {\rm O}(1/10)$, perturbation theory (PT) is usually accurate. In particular $\alpha_{\overline{\rm MS}}(m_{\rm Z})$ is essentially equivalent to the renormalization group invariant Λ-parameter

$$\Lambda_{\overline{\rm MS}} = \varphi_{\overline{\rm MS}}(\bar{g}_{\overline{\rm MS}}(\mu)) \times \mu\,, \tag{1}$$

because the function

$$\varphi_s(\bar{g}_s) = (b_0\bar{g}_s^2)^{-b_1/(2b_0^2)}{\rm e}^{-1/(2b_0\bar{g}_s^2)} \times \exp\left\{-\int_0^{\bar{g}_s}{\rm d}x\,\left[\frac{1}{\beta_s(x)} + \frac{1}{b_0x^3} - \frac{b_1}{b_0^2x}\right]\right\} \tag{2}$$

is known precisely by replacing the renormalization group β-function by its perturbative expansion $\beta_s^{\rm pert}(g) = -g^3\sum_{n=0}^{l_{\rm b}-1} b_{n,s}g^{2n}$; in the $\overline{\rm MS}$-scheme $\beta_{\overline{\rm MS}}^{\rm pert}(g)$ is known up to $l_{\rm b} = 4$ loops [4, 5].

At lower energies, $\mu \ll m_{\rm Z}$, the perturbative uncertainty in approximating $\beta_s \approx \beta_s^{\rm pert}$ in eq. (2) is generally not negligible. It is $\Delta\Lambda_s/\Lambda_s = \Delta\varphi_s/\varphi_s = c_{l_{\rm b}}\alpha^{l_{\rm b}-1} + \ldots$ with coefficients $c_{l_{\rm b}}$, which are, for $l_{\rm b} \le 4$, of order one in the $\overline{\rm MS}$ scheme and expected to be so in "good" schemes in general.

While the $\overline{\rm MS}$ scheme makes sense only perturbatively, physical schemes defined beyond the perturbative expansion are easily derived from short-distance QCD observables $\mathcal{O}_s(\mu) = c_1^s\bar{g}^2_{\overline{\rm MS}}(\mu) + {\rm O}(\bar{g}^4_{\overline{\rm MS}}(\mu))$ via

$$\bar{g}_s^2(\mu) \equiv \mathcal{O}_s(\mu)/c_1^s = \bar{g}^2_{\overline{\rm MS}}(\mu) + {\rm O}(\bar{g}^4_{\overline{\rm MS}}(\mu))\,. \tag{3}$$

It is clear that high energies μ (small α_s) and at least $l_{\rm b} = 3$ are needed if one aims for a precision determination of $\alpha_{\overline{\rm MS}}(m_{\rm Z})$. Replacing high energy by just a larger $l_{\rm b}$ is dangerous because the perturbative expansion is only asymptotic, not convergent, and non-perturbative "corrections" can be large. In particular, whether one has lost control is difficult to detect because our knowledge of non-perturbative physics is very incomplete. Thus it is a challenge to reach an accuracy of a few percent in $\Lambda_{\overline{\rm MS}}$ equivalent to sub-percent accuracy in $\alpha_{\overline{\rm MS}}(m_{\rm Z})$.

Unfortunately, the determinations which quote the smallest uncertainties do typically not come from observables at large μ and uncertainties are dominated by systematics such as unknown higher order perturbative and non-perturbative terms. Both the Particle Data Group [6] and the Flavour Lattice Averaging Group [7] are therefore not just taking weighted averages of the individual determinations to arrive at their world averages.

Here we consider a family of observables (schemes) where lattice simulations allow one *simultaneously to reach high precision and high energy before using* PT. Then PT at $\mu = {\rm O}(m_{\rm Z})$ can be employed with confidence. In addition one can check its applicability at lower scales. This is the strategy of the ALPHA collaboration but so

far it was mostly restricted to unphysical models with an insufficient number of quark flavors [8–10]. For the interesting case of $N_{\rm f} = 3$ QCD, the strategy was applied by the CP-PACS collaboration [11]. We now have very precise results for $N_{\rm f} = 3$ which allow us to see important details previously hidden by uncertainties (see also [12]).

In this letter we discuss the most essential step: the accuracy of PT for couplings $\alpha \lesssim 0.2$ and our resulting precision for Λ. We will see that it is crucial to non-perturbatively reach $\alpha \approx 0.1$ to have confidence in PT at the 3-4 percent level in $\Lambda_{\overline{\rm MS}}$. This represents a general message for determinations of $\alpha_{\overline{\rm MS}}(m_{\rm Z})$.

Here we restrict ourselves to SF schemes (see below) and the region $\alpha < 0.2$. In the near future we will match the SF to a Gradient Flow scheme [13] at around $\alpha = 0.2$ and then connect that to the non-perturbative QCD scales defined in terms of decay constants of kaon and pion. This switch of scheme is advantageous because the Gradient Flow coupling can be computed with great precision when it is not too small. On the other hand, using it all the way to high energy does presently not allow for the extraction of $\Lambda_{\overline{\rm MS}}$ because only the leading order of its perturbative expansion is known. More details are found in [14].

THE SF SCHEME

We use a finite volume renormalization scheme [8, 15], derived from the so-called Schrödinger functional (SF) [16]. Dirichlet boundary conditions are imposed in Euclidean time,

$$A_k(x)|_{x_0=0} = C_k(\eta,\nu)\,, \quad A_k(x)|_{x_0=L} = C'_k(\eta,\nu)\,, \tag{4}$$

and the gauge potentials A_μ are taken periodic in space with period L.[1] The diagonal matrices LC_k, LC'_k depend only on the dimensionless parameters η, ν. With these boundary conditions the absolute minimum, $B_\mu^{\rm class}$, of the gauge action $S_{\rm G}$ corresponds to a constant color electric field [8]. A family of couplings [19], $\bar g_\nu$, at scale $\mu = 1/L$ is obtained by taking $\mathcal{O}_\nu$ to be the η-derivative of the effective action. This yields a simple path integral expectation value,

$$\langle \partial_\eta S|_{\eta=0}\rangle = \frac{12\pi}{\bar g_\nu^2}\,, \tag{5}$$

which is well suited for a Monte Carlo evaluation in the latticised theory. Small fluctuations around the background field generate the non-trivial orders in PT. It is worth pointing out that the whole one-parameter family of couplings can be obtained from numerical simulations at $\nu = 0$, as the ν-dependence is analytically known,

$$\frac{1}{\bar g_\nu^2} = \frac{1}{\bar g^2} - \nu\bar v\,, \tag{6}$$

in terms of the $\nu = 0$ observables $\bar g^2 \equiv \bar g^2_{\nu=0}$ and $\bar v$.

Advantageous properties of these couplings are:

1. $\Delta_{\rm stat}\bar g_\nu^2 = s(a/L)\bar g_\nu^4 + {\rm O}(\bar g_\nu^6)$, for $\Delta_{\rm stat}$ the statistical error at a given length of the Monte Carlo sample. This property makes it possible to maintain high precision at high energy.
2. The typical $\sim \mu^{-1}, \mu^{-2}$ renormalon contributions are absent since the finite volume provides an infrared momentum cutoff. Instead, the leading known non-perturbative contribution is due to a secondary stationary point of the action [20] at $g_0^2\,[S(B_{\rm sec}) - S(B_{\rm class})] = 32.9$. It generates corrections to PT of order
$$\exp(-2.62/\alpha) \sim (\Lambda/\mu)^{3.8}\,, \tag{7}$$
which evaluates to ${\rm O}(10^{-6})$ for $\alpha = 0.2$. At such values of α, fields with non-zero topology are *even further* suppressed given that $g_0^2\,[S_{|Q|\geq 1} - S(B_{\rm class})] \geq 6\pi^2$ [8, 16].
3. The β-function is known including its three-loop term,
$$(4\pi)^3 \times b_{2,\nu} = -0.06(3) - \nu \times 1.26\,,\ (N_{\rm f} = 3) \tag{8}$$
and for reasonable values of ν the three-loop term is of order one as it is in the $\overline{\rm MS}$ scheme.
4. As we will see discretisation effects are very small; at tree-level of perturbation theory they are ${\rm O}((a/L)^4)$. They are known to two-loop order in PT [21] and we can subtract those pieces [22].

The downside of the SF scheme is that the coefficient $s(a/L)$ diverges like $(L/a)^{1/2}$ for large L/a and is not that small in general. High statistics is needed and our computation is limited to $L/a \leq 24$. A second issue is the acceleration of the approach to the continuum limit through Symanzik improvement. With our Dirichlet boundary conditions the Symanzik effective Lagrangian contains terms located at the time-boundaries. These are responsible for ${\rm O}(a)$ effects. We cancel them by corresponding improvement terms with coefficients $c_{\rm t}$ and $\tilde c_{\rm t}$ known only in PT, see below.

STEP SCALING FUNCTIONS AND Λ-PARAMETER

The non-perturbative energy dependence of finite volume couplings is constructed from the step scaling function [15]

$$\sigma_\nu(u) = \bar g_\nu^2(1/(2L))\big|_{\bar g_\nu^2(1/L)=u, m=0}\,, \tag{9}$$

[1] Quark fields are included as described in [17]. Their periodicity angle, θ, introduced in [18], is set to $\theta = \pi/5$ and we use C_k, C'_k as in that reference.

where $m = 0$ ensures the quark mass independence of the scheme [23]. The step scaling function corresponds to a discrete version of the β-function and is computed as the continuum limit $a/L \to 0$ of its lattice approximants $\Sigma_\nu(u, a/L)$. The conditions $\bar{g}^2_\nu(1/L) = u$ and $m = 0$ then refer to a $(L/a)^4$ lattice and fix the bare coupling and bare quark mass of the theory. $\bar{g}^2_\nu(1/(2L))$ is to be evaluated for the same bare parameters on a $(2L/a)^4$ lattice.

We will use the $\nu = 0$ scheme for a reference, dropping the index ν. The scale L_0 is defined by a value u_0 and the condition

$$\bar{g}^2(1/L_0) = u_0\,. \tag{10}$$

The solution of the implicit equation

$$u_k = \sigma(u_{k+1}), \tag{11}$$

for u_{k+1}, $k = 0, 1, \ldots$ gives a series of couplings $u_k = \bar{g}^2(2^k/L_0)$. With a few steps one reaches $\mu = 1/L_n = 2^n/L_0 = \mathrm{O}(m_\mathrm{Z})$ and the perturbative φ at this high scale will give a good approximation to $L_0\Lambda$

$$L_0\Lambda = 2^n\varphi(\sqrt{u_n})\,. \tag{12}$$

Note that thanks to eq. (6) and the exact relation between Λ-parameters [8, 18]

$$r_\nu = \Lambda/\Lambda_\nu = \mathrm{e}^{-\nu\times 1.25516}\,, \tag{13}$$

the same combination $L_0\Lambda$ can be obtained in any scheme with $\nu \neq 0$. Whether different values of ν, number of steps (n) and perturbative orders (l_b) give consistent results is an excellent way to test the reliability of perturbation theory.

SIMULATIONS

We used the standard Wilson plaquette action and three massless O(a)-improved [24, 25] quarks simulated by a variant of the `openQCD` code [26, 27]. At eight couplings $\bar{g}^2(1/L)$ in the range $1.11-2.02$, we simulated pairs of lattices $L/a, 2L/a$ with $L/a = 4, 6, 8$ and at three couplings we also included $L/a = 12$.

Between 80k and 300k independent Monte Carlo measurements were taken on each lattice. As we have already noted, non-trivial topology is very suppressed in these small volumes [28]. Therefore topology freezing [29, 30] is irrelevant here.

A critical issue for any lattice computation is the removal of discretization effects. In preparation of our continuum extrapolations we apply both Symanzik improvement of the action and perturbative improvement of the step scaling function [22].

Improvement of the action

Apart from the bulk O(a) improvement term, the complete removal of linear (in a) discretization errors requires a boundary improvement coefficient c_t in the gluon action [16] and a coefficient $\tilde{c}_\mathrm{t}$ in the fermion action [24]. Regarding the former, the known two-loop accuracy [21],

$$\begin{aligned} c_\mathrm{t} = 1 &+ g_0^2(-0.0890 + 0.019141N_\mathrm{f}) \\ &+ g_0^4(-0.0294 + 0.002N_\mathrm{f} + 0.000(1)N_\mathrm{f}^2)\,, \end{aligned} \tag{14}$$

is expected to be sufficient [31] since we are in the weak bare coupling region. Still, we propagate the small deficit of O(a)-improvement into our errors. As an uncertainty in c_t we use the full two-loop term. The derivative of Σ with respect to c_t is obtained from a numerical estimate of $\delta_b(\bar{g}^2) \equiv \frac{L}{2a}\frac{1}{\bar{g}^2}\frac{\mathrm{d}\bar{g}^2}{\mathrm{d}c_\mathrm{t}}$, namely $\delta_b(2.02) = -2.15(5)$ for $L/a = 6, 8$ with negligible dependence on L/a and ν. Combined with $\delta_b(0) = -1$ we then use the interpolation $\delta_b(u) = -(1 + 0.57(3)\,u)$.

Similarly, for the coefficient $\tilde{c}_\mathrm{t}(g_0) = 1 - 0.01795g_0^2 + \mathrm{O}(g_0^4)$ [32] we use the full one-loop term as an error estimate. Its effect is much smaller than the one of the uncertainty in c_t, since it contributes only through quark loops.

Perturbative improvement of the step scaling functions

In addition, we can improve the observables at a given order i in perturbation theory but to all orders in a via

$$\Sigma^{(i)}(u, a/L) = \frac{\Sigma(u, a/L)}{1 + \sum_{k=1}^{i}\delta_k(a/L)\,u^k}\,, \tag{15}$$

with δ_1, δ_2 known [21].

CONTINUUM EXTRAPOLATIONS AND RESULTS

As the residual linear a effects are treated as an uncertainty, we can proceed with continuum extrapolations linear in a^2. First we look at the data in figure 1. They are statistically compatible with having no a-effects for $L/a \geq 6$; for $N_\mathrm{f} = 0$ this was found with similar precision for $L/a \geq 5$ (see Fig. 3 of [31]).

Both the continuum limit of the step scaling function and its cutoff effects are smooth functions of the coupling. This motivates global fits of the form

$$\Sigma^{(i)}_\nu(u, a/L) = \sigma_\nu(u) + \rho^{(i)}_\nu(u)\,(a/L)^2\,. \tag{16}$$

We performed various such fits in order to assess the systematic errors which result from the assumptions made in the fit functions. We parameterize the cutoff effects by a polynomial in u, with the correct asymptotics for small u,

$$\rho^{(i)}_\nu(u) = \sum_{k=1}^{n^{(i)}_\rho}\rho^{(i)}_{\nu,k}u^{i+1+k}\,, \tag{17}$$

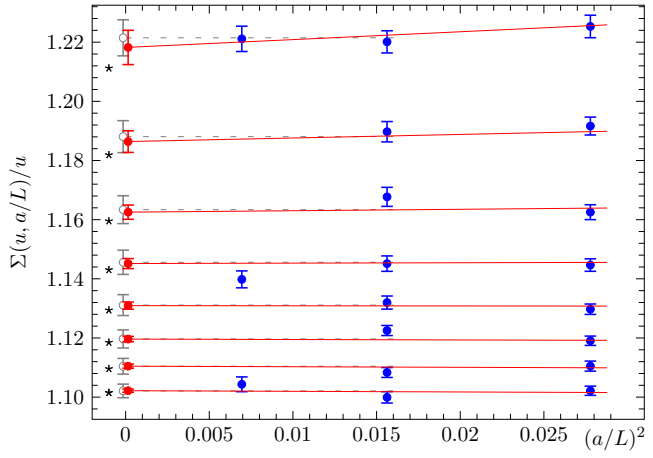

FIG. 1. Continuum limit of the step scaling function $\Sigma^{(i)}(u,a/L)/u$ with $i=2$ loop improvement. As an illustration a constant ($n_\rho=0$, dashed, fit G) and a linear ($n_\rho=2$, fit C) continuum extrapolation is shown. Continuum extrapolated results include the errors due to $c_{\rm t}$ and $\tilde{c}_{\rm t}$ (cf. text). The $\star$-symbols show the perturbative σ computed from the three-loop $\beta^{\rm pert}$.

where the case of neglecting cutoff effects is covered by $n_\rho^{(i)}=0$. The continuum step scaling function is naturally parameterized by a polynomial in u,

$$\sigma_\nu(u) = u + u^2\sum_{k=0}^{3} s_k u^k\,. \tag{18}$$

Lower order coefficients are fixed to their known perturbative values while s_3 ("$n_c=1$") or s_2, s_3 ("$n_c=2$") are fit parameters. A selection of such fits are illustrated in table I. Instead of the parameters of the continuum step scaling function the table shows directly the extracted $L_0\Lambda$, where L_0 is defined through eq. (10) and the value $u_0=2.012$. Recalling eq. (6) and using $\bar{v}=0.1199(10)$ (see next section) we have

$$\bar{g}^2_\nu(1/L_0) = 2.012\,(1-0.1199(10)\times 2.012\,\nu)^{-1}\,. \tag{19}$$

Apart from the form of the fit, $L_0\Lambda$ depends on the value of n where eq. (12) with $\beta_\nu=\beta_\nu^{\rm pert}$ is used. Since we insert $\beta_\nu^{\rm pert}$ at three-loop, the residual dependence on the coupling is $\mathrm{O}(\alpha^2(1/L_n))$.

The observed behavior, figure 2, is consistent with a dominatingly linear dependence of $L_0\Lambda$ on $\alpha^2(1/L_n)$. For $\nu=0$ the slope is not very significant and for $\nu=0.3$ it about disappears, but for $\nu=-0.5$ it is quite large and outside errors.

This suggests to perform alternative fits, where the continuum step scaling function is parameterized by an effective four-loop β-function, adding a term $b_3^{\rm eff}g^9$ to the known ones. The determined $L_0\Lambda$ are then automatically independent of n and we include $b_3^{\rm eff}$ instead of u_n in the table. For $\nu=-0.5$ the effective fit value is larger than it should be in a well-behaved perturbative expansion.

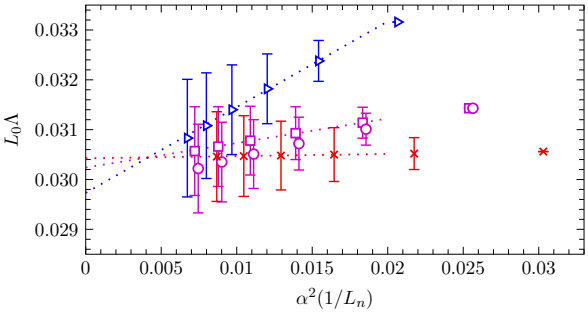

FIG. 2. From top to bottom the different symbols correspond to $\nu=-0.5,0,0.3$. We use $i=1$ loop improved data and fit B, for $\nu=0$ we also show $i=2$, fit C. Dotted lines show linear dependence in α^2 to guide the eye.

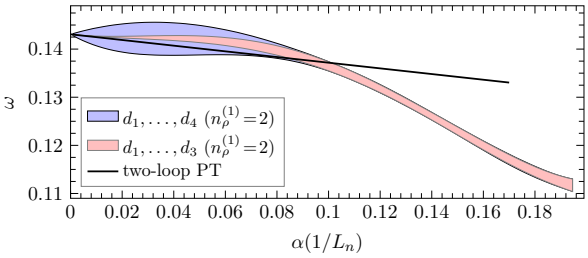

FIG. 3. The function $\omega(\bar{g}^2)$ after continuum extrapolation, covering the $\pm1\sigma$ band of two fits described in the text.

fit	u_n	i	$\frac{L}{a}\big\vert_{\rm min}$	$n_\rho^{(i)}$	n_c	$L_0\Lambda$ $\times100$	$b_3^{\rm eff}$ $\times(4\pi)^4$	χ^2	d.o.f.
A	1.193(4)	0	6	2	1	3.04(8)		14.7	16
B	1.194(4)	1	6	2	1	3.07(8)		14.2	16
C	1.193(5)	2	6	2	1	3.03(8)		14.5	16
D	1.192(7)	2	6	2	2	3.03(13)		14.5	15
E		2	6	2	1	3.00(11)	4(3)	14.6	16
F		2	8	1	1	3.01(11)	4(3)	12.7	9
G	1.191(11)	2	8	0	2	3.02(20)		13.0	9
H		1	6	2	1	3.04(10)	3(3)	14.1	16

fit	ν	i	$\frac{L}{a}\big\vert_{\rm min}$	$n_\rho^{(i)}$	n_c	$L_0\Lambda$ $\times100$	$b_{3,\nu}^{\rm eff}$ $\times(4\pi)^4$	χ^2	d.o.f
H	-0.5	1	6	2	1	3.03(15)	11(5)	10.4	16
H	0.3	1	6	2	1	3.04(10)	0(3)	20.0	16

TABLE I. Results for $\nu=0$ in the upper part.

We will come back to this issue shortly, but first we give our result for $L_0\Lambda$. We take the standard polynomial fit to σ (for $\nu=0$) with $\alpha_n\approx0.1$ ($u_n\approx1.2$). A typical perturbative error of size $\Delta(\Lambda L_n)=\alpha_n^2\,\Lambda L_n$ is then a factor 3 or more below our statistical errors. We further quote (with $\bar{g}^2(1/L_0)=2.012$)

$$L_0\Lambda = 0.0303(8)\,. \tag{20}$$

This is the result of fit C. It is in perfect agreement with all variations of the global fit, even with fit G, which

neglects all cutoff effects but uses only data with $L/a \geq 8$. It has a rather conservative error. If an even more conservative result is desired, one may take the one of fit D, $L_0\Lambda = 0.0303(13)$.

ACCURACY OF PERTURBATION THEORY

While $b_{3,\nu}^{\rm eff}$ is large for $\nu = -0.5$, it does have an error of around 50%. A much better precision can be achieved by considering directly the observable

$$\omega(u) = \bar{v}|_{\bar{g}^2(1/L)=u,m=0} = v_1 + v_2 u + \mathrm{O}(u^2)\,, \quad (21)$$

with known coefficients v_1, v_2 (cf. [10]). In contrast to the step scaling function $\omega(u)$ does not require pairs of lattices, so that the continuum extrapolation can be performed using data for the entire range of lattice sizes $L/a = 6, 8, 10, 12, 16, 24$. Improvement and fits for obtaining the continuum limit are carried out in analogy to those of Σ_ν. Figure 3 shows the result of two different fits with fit parameters d_k in $\omega(u) = v_1 + v_2 u + d_1 u^2 + d_2 u^3 + d_3 u^4$ and in $\omega(u) = v_1 + d_1 u^1 + d_2 u^2 + d_3 u^3 + d_4 u^4$. The overall band of the two fits may be taken as a safe estimate of the continuum limit. As an example we find $\omega(2.012) = 0.1199(10)$ for both fits, leading to eq. (19). In the above analysis we did not use data with $L/a = 6$. Including them yields only tiny changes and excellent χ^2 values.

A good measure of the deviation from two-loop perturbation theory is

$$(\omega(\bar{g}^2) - v_1 - v_2\bar{g}^2)/v_1 = -3.7(2)\,\alpha^2 \quad (22)$$

at $\alpha = 0.19$. It is quite large and statistically significant beyond any doubt. If one attempts to describe this by perturbation theory, the three-loop coefficient v_3 has to be too large for perturbation theory to be trustworthy at $\alpha = 0.2$. We come to the conclusion that $\alpha \approx 0.1$ needs to be reached non-perturbatively before perturbation theory becomes accurate.

SUMMARY AND CONCLUSIONS

Our chosen definition of $\alpha_s(\mu)$ allows us to compute it with very good precision through lattice Monte Carlo simulations. In particular we have controlled the errors due to the discretisation of the theory also at large μ. Known non-perturbative corrections are parametrically very small: $\mathrm{O}(\mathrm{e}^{-2.6/\alpha})$. In other words we have an excellent scheme to test the accuracy of PT in a given region of α.

In fact, we have a family of schemes, depending on ν. For small positive ν, the couplings follow perturbation theory very closely in the full investigated range $0.1 \leq \alpha \leq 0.2$ as illustrated by the flatness of Λ in figure 2 extracted from eq. (12) with the three-loop β-function.

However, for negative ν, e.g. $\nu = -0.5$, values of α just below 0.2 are not small enough to confirm perturbative behaviour. The observable $\bar{v}$, figure 3, shows that the α-dependence seen in figure 2 is not just a statistical fluctuation. We could take the continuum limit of $\bar{v}$ with very high precision and eq. (22) shows a clear deviation from the known perturbative terms, corresponding to $l_{\rm b} = 3$, at $\alpha = 0.19$.

We conclude that it is essential to reach $\alpha = 0.1$ in order to be able to achieve a precision around 3% for the Λ-parameter. Fortunately we have access to that region and can quote such an accuracy in eq. (20). While of course schemes exist where three-loop running holds accurately down to smaller energies – for example $\nu = 0.3$ produces flatness in figure 2 as far as we can tell – to know whether a chosen scheme possesses this property is difficult unless one has control also over the $\alpha \approx 0.1$ region. Once that is achieved larger α are not much needed any more.

What we reported in this letter is part of our determination of a precise value for $\Lambda_{\overline{\rm MS}}$. As our next step, we will soon connect L_0 to the decay constants of pion and kaon, as explained above and in [33].

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