hep-lat 1011.2332

arXiv:1011.2332v1 [hep-lat] 10 Nov 2010

Running of the SF-coupling with four massless flavours

DESY 10-192
SFB/CPP-10-102
HU-EP-10/72

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We discuss the status of different determinations of α_s, motivating a precise and reliable computation from lattice QCD. In order to suppress perturbative errors, the non-perturbative computation has to reach high energy scales μ. Such results already exist in the SF-scheme for $N_f = 0, 2$ [1, 2] and $N_f = 3$ [3]. We recently added the running with four massless flavours in a range of α from about 0.07 to 0.3 . It is based on our recent determination of the Sheikholeslami Wohlert coefficient in the four-flavour theory.

The XXVIII International Symposium on Lattice Field Theory, Lattice2010
June 14-19, 2010
Villasimius, Italy

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1. Introduction

The strong coupling, α_s, represents a fundamental parameter of the strong interactions. Its scale dependence in a suitable renormalization scheme teaches us about the connection between the strongly non-perturbative and the dominantly perturbative regions of QCD. Its value at high energy is needed for phenomenology, for example for the prediction of Higgs production cross sections for the LHC. The uncertainty on α_s is *not* negligible in this context [6].

For this conference we had compiled a plot of precise determinations of $\alpha \equiv \alpha_s$ with the renormalization scale set to the mass of the Z-boson and in the $\overline{\rm MS}$ scheme. It is shown in Fig. 1. We do not claim completeness but rather want to illustrate that the many determinations do not agree well within the estimated uncertainties.

Figure 1: Some recent precise numbers for $\alpha_s(M_Z)$ in the $\overline{\rm MS}$ scheme. From top to bottom: lattice QCD by HPQCD [4], hadronic τ decays (R_τ) [5], deep inelastic scattering [6], thrust [7], global electroweak fit [8], hadronic decays of the Z (R_Z) [9, 10] and the world average of [11].

Indeed, the spread of results in Fig. 1 is not that surprising, since a precision determination of $\alpha_s(M_Z)$ is difficult and so far compromises on various sources of errors had to be made despite an ever increasing sophistication in the analysis. Sources of errors are:

- Low energy: most determinations are not done from a process with an energy scale of order M_Z but at significantly lower energies and are then evolved perturbatively to $\mu = M_Z$. A prominent example is the determination from τ-decays, labeled R_τ.
- Sophisticated analysis involving simultaneous fits to $\alpha_s(\mu)$ and non-perturbative parameters of QCD, such as structure functions [6] and parameters of SCET [7].
- Global fits to many processes (EW fits) [8], which of course means that the correctness and theoretical mastering of the standard model enters in detail.
- The use of bare, unrenormalized, perturbation theory of Wilson loops at the cutoff scale in the lattice determination [4] shown in the figure. We discuss this further below.
- None of these applies to the extraction from the hadronic cross section on the Z-peak, R_Z, but this is experimentally more difficult, resulting in a larger quoted error.

The present world average by S. Bethke is dominated by the lattice determination [4]. We find this worrying due to several reasons. First there is the use of bare perturbation theory. There the problem is that successive terms do not show a convincing 'convergence' pattern. Either there are large coefficients of higher order terms (expansion in the original bare coupling) or the (modified) coupling itself "lives" at a quite low energy scale where it is large ("tadpole improved" coupling, coupling in "potential scheme"). In either case errors due to left out remainder terms are difficult to quantify. The continuum limit is in this way only reached at an asymptotic rate proportional to $1/|\ln a|$ and can in practise not be taken. Furthermore, rooted staggered quarks with their doubtful

theoretical status are employed. In spite of this, a phenomenological observation adds support to the analysis of [4]: there is agreement of results from several different variations of the theme.

The above mentioned difficulties have been a motivation for the ALPHA collaboration to work on a program which essentially is based only on the assumptions that the continuum limit of the lattice theory exists and asymptotic freedom is present non-perturbatively. The resulting errors in $\alpha_{\rm s}$ are dominantly statistical and also the systematic component can be reduced further when the overall precision is improved in the future. In particular, as has been explained many times [12–14],

- α is defined non-perturbatively in a physical (regularization independent) scheme,
- this running can be efficiently computed numerically by a finite size strategy,
- the continuum limit can be taken in individual steps free of multi-scale problems,
- renormalized perturbation theory is used only at large scales, where its precision is furthermore validated non-perturbatively.

These properties come with a price. Since a specific scheme had to be devised in order to make precise non-perturbative computations possible, the β-function at 3-loop order needed to be calculated [15–22]. The same perturbative calculations are also important to remove dominant parts of the discretization errors (see section II.2 of [14]). Furthermore a controlled non-perturbative running clearly has to include the strange and charm quarks; this step has only been carried out recently and we report on it here. Still, as will be discussed in the conclusions more work is needed before a numerical value for $\alpha_s(M_{\rm Z})$ can be given for phenomenology. It is also for these reasons that the ALPHA collaboration has so far not been able to publish a value of α in the physical theory with all quarks which we would like to be taken into account in the world average.

2. Computation of the step scaling function

In our finite size strategy, the coupling $\bar{g}^2$ is defined in a Euclidean space-time of size L^4 with Schrödinger functional boundary conditions [15, 16] and a renormalization scale $\mu = 1/L$. The discrete scale evolution defines the step scaling function σ via

$$\bar{g}^2(sL) = \sigma(s, \bar{g}^2(L)) = \lim_{a/L\to 0} \Sigma(s, \bar{g}^2(L), a/L),$$

which can be computed non-perturbatively as the continuum limit of the lattice approximant Σ as indicated. We chose a scale factor $s = 2$ for practical reasons and omit this argument from now on. In the Schrödinger functional, Dirichlet boundary conditions are imposed in Euclidean time and therefore the $\mathrm{O}(a)$ Symanzik improvement of the theory requires boundary terms. Their coefficients are taken from perturbation theory, exactly as in [23], where we determined the crucial bulk $\mathrm{O}(a)$ improvement coefficient $c_{\rm sw}$ non-perturbatively.

Figure 2: Interpolation eq. (2.1).

The computation of the lattice step scaling function, $\Sigma(u,a/L)$ requires to tune the bare mass and the bare coupling of the theory such that the PCAC mass (defined exactly as in [2, 24]) vanishes and $\bar{g}^2(L) = u$. At the same bare parameters one then computes $\Sigma(u,a/L) = \bar{g}^2(2L)$. An explicit 2-dimensional tuning is rather cumbersome. We therefore followed [25], picked a series of bare couplings $g_0^2 = 6/\beta$ and tuned the PCAC mass to zero. For those bare parameters we then compute $\bar{g}^2(\beta, L/a)$ and $\bar{g}^2(\beta, 2L/a)$ and interpolated to the desired values of u via

$$\bar{g}^2(\beta, L/a) = \frac{6}{\beta}\left[\sum_{m=0}^{M} c_{m,L/a}\left(\frac{6}{\beta}\right)^m\right]^{-1} \tag{2.1}$$

motivated by perturbation theory. We do not fix the known perturbative expansion coefficients, not even $c_{0,L/a}$. The interpolations for $L/a = 8$ are illustrated in Fig. 2. $\Sigma(u, 1/8)$ is given by the value of the upper curve at the β where the lower one passes through $\bar{g}^2(\beta, 8) = u$. Stability of the interpolations with respect to M was checked.

Using Σ from the interpolation, we form the 2-loop improved lattice step scaling function [26]

$$\Sigma^{(2)}(u,a/L) = \frac{\Sigma(u,a/L)}{1+\delta_1(a/L)u+\delta_2(a/L)u^2} \tag{2.2}$$

with δ_1, δ_2 known from [19–22, 27]. We expect $\Sigma^{(2)}$ to have smaller overall cutoff effects. Asymptotically, they still start at order $a \times u^4$ but terms of order $a^m \times u^n$ are removed for all m and for $n \leq 3$ (in fact non-perturbatively in a). As mentioned previously, the order $a \times u^4$ terms are due to the only perturbatively known boundary improvement terms. Their influence was explicitly checked for $N_\mathrm{f} = 2$ and found to be minor [2, 14] for our action, at least when c_t is known to 2-loop order. We therefore assume that the step scaling function converges *effectively* at a rate

Figure 3: Constant fit continuum extrapolation.

$$\Sigma^{(2)}(u,a/L) = \sigma(u) + \mathrm{O}(a^2). \tag{2.3}$$

To study the continuum limit and its uncertainty we carried out three different analysis.

- *Constant fit:* A fit of $\Sigma^{(2)}(u,a/L)$ for $L/a = 6, 8$ to a constant, for each u.
- *Global fit:* A fit $\Sigma^{(2)}(u,a/L) = \sigma(u) + \rho\, u^4\, (a/L)^2$, with a separate, independent parameter $\sigma(u)$ for each value u but a common parameter ρ modelling the cutoff-effects.
- $L/a = 8$ *data:* Using directly $\sigma(u) = \Sigma^{(2)}(u, 1/8)$.

The three different ansätze yield results which are in complete agreement with each other. The global fit returns $\rho = 0.007(85)$ which is a good indication that cutoff effects are negligible in the data for $L/a = 6, 8$. In order to have a safe error estimate on the continuum limit we chose just the $L/a = 8$ data as our present result.

3. The running of the coupling

A polynomial interpolation $\sigma(u) = u + s_0u^2 + s_1u^3 + 0.0036\,u^4 - 0.0005\,u^5$, with the coefficients up to u^3 fixed by perturbation theory represents $\sigma(u)$ in the range $0.9 \leq u \leq 2.7$ with negligible interpolation errors. The running of the coupling is then obtained by solving the recurrence

$$u_i = \sigma(u_{i+1}), \quad i = 0, \ldots, n, \quad u_0 = u_{\rm max} = \bar{g}^2\,(L_{\rm max}) \tag{3.1}$$

for $u_i = \bar{g}^2(L_i)$, $L_i = 2^{-i}L_{\rm max}$. As Fig. 4 shows, agreement with perturbative running at the 3-loop level is found at the highest scales in agreement with standard estimates of remainder terms. This allows us to relate u_9 to $L_9 \times \Lambda$ by using the 3-loop β-function [for couplings up to u_9 only]. Then with the non-perturbative $\sigma(u)$ used in eq. (3.1) we can connect to larger values of u, for example

$$\ln(\Lambda L_{\rm max}) = -2.294(83) \quad \text{ at } \bar{g}^2(L_{\rm max}) = u_{\rm max} = 3.45\,. \tag{3.2}$$

While a precise MeV value still has to be determined we clearly expect $L_{\rm max}$ to lie in the range of hadronic scales. The (uncorrelated) errors of our primary MC data for $\bar{g}^2(\beta, L/a)$ are propagated through all steps of the analysis as described in [24]. Note that some steps, in particular eq. (3.1), introduce correlations into the final results. The errors of the points Fig. 4 are therefore not independent.

4. Conclusions

At the present level of statistical errors, systematic errors from the continuum extrapolation are almost certainly negligible. In the future, in particular with further reduced statistical errors, data with larger L/a clearly have to be added. It will also be interesting to compare the efficiency of computations with different regularizations of the Schrödinger functional, such as chirally rotated boundary conditions [28, 29] and staggered quarks [30, 31].

Figure 4: Non-perturbative running coupling compared to perturbation theory.

We do observe a small but significant deviation from 3-loop perturbation theory at the largest coupling reached in Fig. 4. It is about 10% (three standard deviations) and the Schrödinger functional coupling has a value of $\alpha_{\rm SF} \approx 0.28$. For $N_{\rm f} = 2$ a similar effect was visible only for larger coupling [2]. These findings underline the necessity of going to weak coupling before applying perturbation theory.

We are now a good step closer to the computation of the Λ-parameter in 4-flavor QCD, which may then be perturbatively connected to e.g. the 5-flavor $\alpha_{\overline{\rm MS}}(M_{\rm Z})$. However the low energy scale $L_{\rm max}$ that was introduced for technical convenience, remains to be expressed in physical units through large volume 4-flavor simulations and we may want to improve the precision in Fig. 4.

Acknowledgements. We thank NIC and DESY for allocating computer time on the APE computers to this project and the APE group for its help. This work is supported by the Deutsche Forschungsgemeinschaft in the SFB/TR 09 and by the European community through EU Contract No. MRTN-CT-2006-035482, "FLAVIAnet".

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