We report on the latest results on the running coupling of two flavour QCD in the Schrödinger functional scheme. Results for the step scaling function are obtained from simulations on lattices $L/a = 8$ and $L/a = 16$ which confirm the first results from lattices $L/a = 4, 5, 6$ presented one year ago by the ALPHA collaboration. We also discuss some algorithmic aspects, in particular concerning the occurrence of metastable states. A modified sampling, in order to estimate the proper weight of these states in the path integral, is proposed and tested.

1. INTRODUCTION

The relation between the short distance regime of QCD and its low energy sector is a problem which can be addressed by lattice techniques. The $\Lambda$ parameter, characterizing the coupling at large energy, can be related to a hadronic quantity by a recursive finite–size technique, avoiding in such a way the multiple scale problem. This method has been successfully applied to the zero flavour approximation of QCD [1] and first results extending it to QCD with two massless flavours have been presented last year by our collaboration [2]. Here we report about more recent results which allow for a better estimate of systematic effects on our determination of the $\Lambda$ parameter in the two flavour theory. This result is essential also in the computation of the running quark mass [3].

We consider the Schrödinger functional (SF), defined as the Euclidean partition function of QCD on a cylinder of size $L^3 \times T$

$$ e^{-\Gamma} = \int_{T\times L^3} D[U, \psi, \bar{\psi}] e^{-S}, $$

with periodic (up to a phase) boundary conditions in the spatial directions and Dirichlet boundary conditions at $x_0 = 0, T$. The spatial links at $x_0 = 0, T$ are fixed to diagonal SU(3) matrices specified in terms of $L$ and one angle $\eta$ while the quark fields are given by Grassmann values $\rho, \bar{\rho}$ and $\rho', \bar{\rho}'$, which are used as sources and then set to zero.

We work with an $O(a)$ improved Wilson action and improved operators, employing the non–perturbative $c_{SW}$ [4] coefficient and one and two–loop values for the boundary coefficients $c_t$ and $c_L$ [5,6]. The improvement coefficient $c_A$ is also set to its one–loop value. It enters our definition of quark mass $m$ via the PCAC relation. The mass is required to be consistent with zero [2].

For $T = L$, the SF coupling $\bar{g}_2$ is defined [1,7]
\[
(\partial \Gamma/\partial \eta)|_{\eta=0} = (\partial S/\partial \eta)|_{\eta=0} = kg^{-2}(L) \tag{2}
\]

with \( k \) fixed by the condition \( \bar{g}^2 = g_b^2 + O(g_d^4) \). Here \( L \) plays the role of a renormalization scale.

2. NUMERICAL RESULTS

The main quantity in the present computation is the step scaling function (SSF)

\[
\sigma(u) = \bar{g}^2(2L)|_{\bar{g}(L)=u,m=0}, \tag{3}
\]

which can be viewed as a non-perturbative integrated form of the \( \beta \)-function. Once \( \sigma(u) \) has been computed in the continuum limit and for a large enough range of values, the equation

\[
\sigma(\bar{g}^2(L/2)) = \bar{g}^2(L) \tag{4}
\]

can be recursively solved \( n \) times (for explicit equations see e.g. [3]) starting from the hadronic scale \( L_{\text{max}} \) with \( \bar{g}^2(L_{\text{max}}) = u_{\text{max}} \). In this way we obtain values for \( \bar{g}^2(2^{-n}L_{\text{max}}) \). For large \( n \) this coupling is perturbative and we compute the \( \Lambda \) parameter in units of \( L_{\text{max}} \) making use of the three-loop \( \beta \)-function in the SF scheme [2,6]

\[
\Lambda L_{\text{max}} = 2^n(b_0 g_0)^{-b_1/2b_2} \exp \left\{ -\frac{1}{2b_0 g_0^2} \right\} 
\times \exp \left\{ -\int_0^\infty dx \left[ \frac{1}{\beta_0 x^3} + \frac{b_1}{b_0 x} - \frac{b_1}{b_0^2 x} \right] \right\} \tag{5}
\]

Later we will have to relate \( L_{\text{max}} \) to a physical scale, e.g. by determining \( L_{\text{max}} F_\pi \). Our new sim-

tulations and results are summarized in Table 1.

These allow for more reliable continuum limit extrapolations of the SSF.

\[
\begin{array}{cccc}
L/a & u & \Sigma & u & \Sigma \\
8 & 0.9807(17) & 1.0745(55) & 1.508(4) & 1.716(14) \\
8 & 1.1818(29) & 1.3338(58) & 2.014(10) & 2.475(31) \\
8 & 2.479(13) & 3.348(48) \\
4 & 3.334(11) & 5.513(42) \\
6 & 3.326(20) & 5.62(9) \\
\end{array}
\]

Table 1

New data for the lattice SSF \( \Sigma(u,a/L) \). \( c_t(g_0) \) was set to its one-loop value for the left part, and to two-loop for the two rightmost columns.

We extract the continuum limit values for the SSF using data for the two-loop improved observable \( \Sigma^{(2)}(u,a/L) \) [2] from \( L/a = 6 \) and \( L/a = 8 \). The scaling of \( \Sigma^{(2)} \) vs. \( (a/L)^2 \) is shown in Figure 1 for two different values of \( u \). For comparison we included in the plot the continuum results in the quenched case (black squares) for the same value of the couplings. The function \( \sigma(u) \)

\[
\begin{array}{cc}
\Sigma^{(2)}(u,a/L) & u=2.0142 \\
\Sigma^{(2)}(u,a/L) & u=1.1818 \\
\end{array}
\]

Figure 1. Scaling plot for \( \Sigma^{(2)} \). Black squares indicate the continuum limit extrapolation for \( N_f = 0 \).

is obtained interpolating the continuum limit estimates by a sixth-order polynomial with the first three coefficients constrained by perturbation theory. Starting from \( u_{\text{max}} = 3.3 \) or \( u_{\text{max}} = 5 \) we can then estimate the quantity \( \Lambda L_{\text{max}} \) as discussed above. Results are summarized in Table 2.

We use the difference between continuum values

\[
\begin{array}{ccc}
\bar{g}^2(L_{\text{max}}) = 3.3 & g^2(L_{\text{max}}) = 5 \\
\hline
n & c.l. & L/a = 5 \\
\hline
5 & 1.82(5) & 1.87 \\
6 & 1.84(6) & 1.89 \\
7 & 1.85(7) & 1.91 \\
\hline
\end{array}
\]

Table 2

Values for \(-\ln(\Lambda L_{\text{max}})\) for two choices of \( L_{\text{max}} \).

and data from \( L/a = 5 \) to estimate our systematic uncertainty, which we linearly add to the statistical errors. This yields

\[
\begin{align}
\ln(\Lambda L_{\text{max}}' &= -1.85(13) \quad \bar{g}^2(L_{\text{max}}) = 3.3 \\
\ln(\Lambda L_{\text{max}}' &= -1.26(11) \quad \bar{g}^2(L_{\text{max}}) = 5 \} \tag{6}
\end{align}
\]

\[\]
Comparing with the results in [2], we see that the systematic uncertainty on $\ln(\Lambda)$ is nearly halved, while the central values are fully consistent. The non-perturbative evolution of $\alpha(\mu) = \bar{g}^2(L)/4\pi$ ($\mu = 1/L$) starting from $\bar{g}^2 = 5$ is plotted in Figure 2. Statistical and systematical errors (difference between continuum limit and $L/a = 5$) are too small to be visible in the plot. The figure shows that differences between Monte Carlo results and three-loop perturbation theory become appreciable for large values of the coupling, while for high energies the perturbative approximation very closely reproduces the non-perturbative results.

### Figure 2. Running of $\alpha = \bar{g}^2/4\pi$ in the SF scheme.

#### 3. METASTABLE STATES

For the largest values of the coupling in our study ($\bar{g}^2 \simeq 3.3$ and $\bar{g}^2 \simeq 5.5$) we observed a long tail towards negative values in the distribution of $\partial S/\partial \eta$. In addition, measuring by a cooling procedure the pure gauge contribution to the action $S_G^{\text{cool}}$, and to the coupling $\partial S_G^{\text{cool}}/\partial \eta$, we observed occurrences of metastable states in our Monte Carlo histories. The action $S_G^{\text{cool}}$ for these states is consistent with the value for a secondary solution of the field equations [7], given our choice for the boundary fields. This solution appears to be a local minimum by numerical evidence.

In order to properly estimate the weight of these states we enhanced their occurrence through a modified sampling [1], adding to the HMC effective action a term

$$\frac{\partial S_G}{\partial \eta} \bigg|_{\eta=0} + \frac{1}{w_\gamma}(\gamma - \gamma_0)^2,$$

where $\gamma_0$ and $w_{\gamma}$ are fixed values, while $\gamma$ is a dynamical variable. The expectation values in the original ensemble are then obtained by reweighting properly the observables.

Defining a quantity $q$ whose value is 1 for metastable states and 0 otherwise (so that $\langle \delta q_1 \rangle + \langle \delta q_0 \rangle = 1$), for an observable $O$ one can write

$$\langle O \rangle = \langle \delta q_1 O \rangle + \langle \delta q_0 O \rangle = \langle \delta q_1 O \rangle + \langle O \rangle_1 (1 - \langle \delta q_1 \rangle),$$

where $\langle O \rangle_1 = \langle \delta q_0 O \rangle / \langle \delta q_0 \rangle$. If the main contribution to $\langle O \rangle$ comes from the $q = 0$ sector then a precise estimate of $\langle O \rangle$ just requires a precise estimate of $\langle O \rangle_1$, which can be obtained by an algorithm which samples only the $q = 0$ sector, together with rough estimates of $\langle \delta q_1 \rangle$ and $\langle \delta q_0 O \rangle$ which can be obtained by the modified sampling.

By a set of simulations on $L/a = 8$ and 12 using this approach we could estimate the effect of metastable states on $\bar{g}^2$ to be nearly 0.10(2)% for $\bar{g}^2 \simeq 3.3$. This result is independent, within errors, from $L/a$. Moreover, for this value of the coupling, we noticed a slightly better behavior for the PHMC algorithm in comparison with HMC (smaller values of $\gamma_0$ needed in order to generate a certain number of transitions from/to a metastable state).

For $\bar{g}^2 \simeq 5.5$, the effect of metastable states is much larger, as expected, resulting in a 4 to 5% contribution. However their sampling is also enhanced in this case using both PHMC or HMC already in the original ensemble. Indeed we repeated the $L/a = 12$ simulation for $\bar{g}^2 \simeq 5.5$ using ordinary PHMC as in Ref. [2] but disentangling the occurrence of metastable states. This turned out to be around 6% and the result for $\bar{g}^2$ was fully consistent with the number in Ref. [2].

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REFERENCES
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