Non-perturbative running of the coupling from four flavour lattice QCD with staggered quarks

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Using the Schrödinger functional (SF) with a single staggered fermion field we calculate the SF coupling in four-flavour QCD for a wide range of energies and lattice sizes up to $L/a = 16$. Preliminary results for the continuum extrapolation of the step-scaling function are presented. To reduce cutoff effects, one-loop $O(a)$ improvement has been implemented. Various cross checks are made possible by the use of two independent sets of lattices with either $T = L + a$ or $T = L - a$.  

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1. Introduction

The free parameters of QCD can be fixed by matching a corresponding number of hadronic observables at low energies. Then, predictions can in principle be made for any other observable both at low and high energies. A quantity of particular interest is the strong coupling constant $\alpha_s$. A commonly used reference value is the $\overline{\text{MS}}$ coupling of dimensional regularisation at the scale of the $Z$-boson mass. This poses a particular challenge for the lattice formulation, due to the large scale differences involved, which cannot be accommodated on presently affordable lattices. This difficulty can be overcome by using finite size techniques \cite{1,2}. The essential ingredient is the non-perturbative definition of a running coupling, $\bar{g}(L)$, which runs with the linear extent $L$ of the space-time volume. The Schrödinger functional provides a framework for such a definition, where $\bar{g}(L)$ is defined through the response of the system to a constant colour electric background field. See \cite{3} for a detailed explanation and \cite{4} for the definition of the SF for QCD both in the continuum and on the lattice with Wilson quarks.

Within this framework, the step scaling function, (SSF), plays a fundamental role. It can be regarded as a discretised version of the Callan and Symanzik $\beta$ function, and can be used to study the evolution of $\bar{g}(L)$ with energy. Such studies have been carried out for different numbers of flavours \cite{2,3,5-9}. We present here the step scaling function and the running coupling with four flavours of staggered quarks. In \cite{9} an analogous work using $O(a)$ improved Wilson quarks was presented. The agreement of the results in the continuum limit can thus be regarded as a test of universality.

This write-up is organised as follows. Section 2 reviews the basics of the SF on the lattice with staggered fermions, gives a definition for the renormalised running coupling, and revisits the basics on finite size techniques. In section 3, the $O(a)$ improvement for our setup is revisited. Section 4 presents the details of the simulations and the data analysis. In section 5, we present our results and we finish with an outlook to future work.

2. Schrödinger functional, coupling constant and finite size techniques

The SF is a useful tool to study the scaling properties of QCD. Here we will introduce it briefly. See \cite{3,4,10-12} for more details and \cite{13-15} for the set up of the SF with staggered fermions. It can be regarded as the Euclidean time evolution kernel for going from a state at time $x_0 = 0$ to another state at time $x_0 = T$. Using the transfer matrix formalism, it can be expressed as a path integral with fields satisfying periodic boundary conditions in space and Dirichlet boundary conditions in time. Homogeneous boundary conditions are imposed on the fermionic fields,

$$P_+ \psi \big|_{x_0=0} = 0 = \bar{\psi} P_+ \big|_{x_0=T}, \quad P_- \psi \big|_{x_0=T} = 0 = \bar{\psi} P_- \big|_{x_0=0},$$

with $P_\pm = \frac{1}{2}(1 \pm \gamma_0)$ and the spatial components of the gluon fields satisfy,

$$A_k(x) \big|_{x_0=0} = C_k, \quad A_k(x) \big|_{x_0=T} = C'_k. \quad (2.2)$$

The SF is then a functional of these boundary fields,

$$\mathcal{Z}[C',C] = \int \mathcal{D}[A,\psi,\bar{\psi}] e^{-S[A,\psi,\bar{\psi}]}. \quad (2.3)$$

The choice of the boundary fields is largely arbitrary. Following \cite{3} we choose Abelian and spatially constant fields such that the absolute minimum of the action is unique up to gauge transformations. A judicious choice of the boundary fields ensures that the absolute minimum of the
action is unique up to gauge transformations and yields small lattice artefacts in the renormalised coupling.

2.1 Definition of the coupling constant

The SF allows us to define a renormalised coupling constant $\bar{g}^2$ non-perturbatively, easily computable on the lattice and in perturbation theory and with reasonably small lattice artifacts. Since the induced background field is unique, it is possible to unambiguously define the effective action of the SF, i.e.,

$$\Gamma[B] = -\ln \mathcal{Z}[C,C'].$$

The boundary fields are parametrised by the scale $L$ and $\eta, \nu$, two dimensionless real parameters [5]. A renormalised coupling can be defined through,

$$\Gamma' = \left. \frac{\partial \Gamma}{\partial \eta} \right|_{\eta=\nu=0} = \frac{[\partial \Gamma_0/\partial \eta]_{\eta=0}}{\bar{g}^2(L)},$$

$\bar{g}^2(L)$ is going to run with the spatial box size $L$ which plays the role of the scale. The normalisation constant is chosen so that the renormalised coupling coincides with the bare coupling at tree level in the perturbative expansion.

2.2 SF with staggered fermions

The SF with staggered fermions requires lattices where the time extent $T/a$ is odd and the spatial extent $L/a$ is even. [13, 14]. This is illustrated in figure 1 in a two dimensional sketch, as well as one possible reconstruction of the staggered fermions. See [16] for a more detailed description on the fermionic reconstruction. The continuum limit for $\bar{g}^2$ is usually taken setting $T = L$ already for finite values of $a$. In order to define the continuum limit in our case, we are obliged to adopt modified conventions, [15]. Lattices with $T = L \pm a$ are interpreted as having physical time extent $T' = T + sa$ with $s = \pm 1$, so that the condition $T' = L$ provides us with 2 regularisations to our problem. This modification forces us to have the $O(a)$ improvement revisited.

![SF with staggered fermions, 2-dimensional sketch. Left, $T = L + a$ right, $T = L - a$. Thin (green) lines represent the lattice where the one-component staggered fermions live, thick (orange) lines represent the effective lattice for the reconstructed fermions and the brown dots stand for the sites where the reconstructed fermions live.](image-url)

2.3 Finite size techniques

We want to compute the scale evolution of the renormalised coupling. We introduce then the step scaling function in the continuum theory,

$$\sigma(u) = \left[ \bar{g}^2(2L) \right]_{u=\bar{g}^2(L)}.$$

On the lattice, it can be obtained as the continuum extrapolation from a sequence of pairs of lattices with sizes $L/a$ and $2L/a$. 
\[ \sigma(u) = \lim_{a \to 0} \Sigma(u,a/L). \] (2.7)

The procedure is repeated for a range of \( u \) values in \( [\bar{g}^2(L_{\text{min}}), \bar{g}^2(L_{\text{max}})] \),

\[ u_0 = \bar{g}^2(L_{\text{min}}), \quad u_k = \sigma(u_{k-1}) = g^2(2^k L_{\text{min}}), \quad k = 1, 2 \ldots \] (2.8)

After 7, 8 steps, energy differences of \( O(100) \) are bridged. At sufficiently large energies, perturbation theory can be applied to relate the SF coupling \( \bar{g}^2(L) \) with a perturbatively defined coupling, e.g. \( \bar{g}_{\text{MS}}^2 \). At low energies, the connection with physical units can be established through the computation of a hadronic quantity, e.g., \( F_\pi L_{\text{max}} \).

3. \( O(a) \) Improvement

Due to computer power limitations it is advisable to construct an action that is \( O(a) \) improved so that the dominating lattice artifacts are cancelled. Following Symanzik’s improvement programme [17], this can be done by adding irrelevant local counterterms to the action, monitored by adjustable coefficients. These coefficients admit an expansion in perturbation theory. In the SF framework additionally to the volume counterterms there exist boundary counterterms.

We want our observable, \( \Gamma' \) to be \( O(a) \) improved up to one loop in perturbation theory. The action is taken to be

\[ S[U, \chi, \bar{\chi}] = S_g[U] + S_f[U, \chi, \bar{\chi}], \]

\[ S_g[U] = \frac{1}{\bar{g}_0^2} \sum_p w(p) \text{tr} \{ 1 - U(p) \}, \] (3.1)

\[ S_f[U, \chi, \bar{\chi}] = a^4 \sum_{x_0 = a}^{T-a} \sum_{x,\mu} \frac{1}{2a} \eta_\mu(x) \bar{\chi}(x) \left[ \lambda_\mu U_\mu(x) \chi(x + a\hat{\mu}) - \lambda_\mu^* U_\mu(x - a\hat{\mu}) \chi(x - a\hat{\mu}) \right], \]

where the sum over the gauge fields runs over all the oriented plaquettes \( p \) and \( w(p) \) are weight factors that take the value 1 except for the boundary plaquettes, where they take the values \( c_i(g_0) \) for the time-like plaquettes attached to the boundaries and \( \frac{1}{2} c_s(g_0) \) for the spatial plaquettes. Concerning the fermionic part, \( \chi, \bar{\chi} \) represent the one-component fermionic fields, homogeneous boundary conditions have been assumed for the fermions, a constant phase factor \( \lambda_\mu \)\(^1\) has been included, and \( \eta_\mu = (-1)^{\Sigma_{x,\mu} x_\mu / a} \) are the usual phase factors of the staggered fermions.

There are no \( O(a) \) effects arising from the bulk, so that the staggered SF will be \( O(a) \) improved by including a couple of boundary counterterms. The only pure gauge counterterm relevant in our context takes the form

\[ c_i^f(g_0^2) \text{tr} \{ F_{0k} F_{0k} \}, \quad c_i^f(g_0^2) = c_i^{(0)i} + g_0^2 (c_i^{(1,0)i} + N f_i c_i^{(1,1)i}) + O(g_0^2), \] (3.2)

where the superscript \( s = \pm 1 \) stands for the two possible regularisations. The coefficients above have been calculated for our set up obtaining,

\[ c_i^{(0)i} = \frac{2}{2+s}, \quad c_i^{(0,1)i} = 0.0274(2), \quad c_i^{(1,0)i} = -0.4636(6), \quad c_i^{(1,1)i} = -0.0266(8). \] (3.3)

Concerning the fermionic part, there is also a boundary counterterm which, in terms of the single-component fields, takes the form \[ [16] \].

\(^1\)We have chosen \( \lambda_0 = 1, \lambda_k = e^{i\theta_k} = e^{i\frac{\pi}{2}} \). It leads to a smaller condition number of the free fermion matrix \[ [11] \].
\[ [d_s(g_0) - 1] \sum_{x,k} \left\{ \frac{1}{x^2} \eta_k(x) \lambda(x) \left[ \lambda U_k(x) \chi(x+a\hat{k}) - \lambda U_k(x-a\hat{k}) \chi(x-a\hat{k}) \right] \right\}_{x_0=a} \]
\[ [d_s(g_0^2) - 1] \sum_{x,k} \left\{ \frac{1}{x^2} \eta_k(x) \lambda(x) \left[ \lambda U_k(x) \chi(x+a\hat{k}) - \lambda U_k(x-a\hat{k}) \chi(x-a\hat{k}) \right] \right\}_{x_0=T-a} \]

The tree level value of \( d_s^{(0)} \) was found to be \( d_s^{(0)} = 1 + \frac{5}{4} \) [18].

4. Simulations and data analysis

In order to carry out our computations, we have made use of a customised version of the code offered by the MILC collaboration [19], where the \( O(a) \) improvement presented in the previous section was implemented. The simulations have been run for lattice sizes \( L/a = 4, 6, 8, 12, 16 \) and \( s = \pm 1 \). The statistics range from 60,000 measurements to 160,000 (the quantity \( \bar{v}, [2] \) has also been measured). The data analysis has been performed by using \( \text{uwerr.m} \) [20].

Instead of tuning the values of \( \beta = 2N_c/g_0^2 \) for different \( L/a \) so that they correspond to the same value of the renormalised coupling, we have followed the procedure proposed in [21]. We measure \( \bar{g}^2(L) \) for a set of values \( \beta, L/a \) and generate an interpolating function. This function is then used to tune \( \beta \). The interpolation function takes the form,
\[
\frac{1}{\bar{g}^2(\beta, L/a)} = \frac{\beta}{2N} + \sum_{i=1}^{r} x_i \left( \frac{2N}{\beta} \right)^{i-1}.
\]

The data have been fitted by making use of the least squares method. The interpolated data inherit two sources of errors, statistical and systematic.

5. Results

Since we have two regularisations at our disposal, it is possible to perform an analysis of the lattice artifacts of our data. A line of constant physics is defined by the coupling in one regularisation and we evaluate the coupling for the other regularisation at the same values of \( \beta \). One-loop perturbative cutoff effects can be subtracted, by defining the quantity,
\[
u_{\pm}^{(1)} = u_{\pm} \times \left[ 1 + u_{\pm}(m_1^\pm - m_0^\pm) \right]^{-1},
\]
where \( m_1^\pm \) is the coefficient in the perturbative expansion, \( \bar{g}_0^2 = g_0^2 + m_1^\pm g_0^4 \) and \( \pm \) stands for \( s = \pm 1 \).

In Figure 2 we show the lattice artifacts for \( u \) and \( u^{(1)} \). We have also measured the continuum extrapolation of the step scaling function. If we choose one regularisation to fix the physics, the lattice step scaling function can be computed in the two available regularisations. The continuum limit has to be shared. Perturbative effects can be subtracted, by defining \( \Sigma_{\pm}^{(1)} \),
\[
\Sigma^{(1)}(u, a/L) = \frac{\Sigma(u, a/L)}{1 + \delta_1(a/L)u}, \quad \delta = \frac{\Sigma(u, a/L) - \sigma(u)}{\sigma(u)} = \delta_1(a/L)u + \delta_2(a/L)u^2 + O(u^3).
\]

In figure 3 we can see the continuum extrapolation for some of our data. The fit has been done in the following way,
\[
\bar{\Sigma}_1(u, a/L) = \sigma_{\text{mixed}}(u_s) + A_1(a/L)^2, \quad \bar{\Sigma}_{-1}(u, a/L) = \sigma_{\text{mixed}}(u_s) + A_2(a/L)^2,
\]
where \( s \) stands for the regularisation chosen to fix the physics. The fit was performed excluding the data for \( L/a = 4 \). An analogous fit was done for \( \Sigma_{\pm}^{(1)}(u, a/L) \).

We interpolate the data of the continuum extrapolation of \( \sigma(u) \). In Figure 4 we present such interpolation, plotting \( \sigma(u)/u \) vs \( u \), together with the perturbative approximations to 1, 2 and 3 loop.
4-flavour running coupling

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Figure 2: Analysis of the lattice artifacts of our system. Diamond (blue) points are the values of $\bar{g}^2/(L/a)$. Dashed lines correspond to the fit to these data and asterisks (green), the continuum extrapolation. Circles, (magenta) are the values for the same data after performing the perturbative subtraction, and the dotted lines their fits. Squares (orange) represent their continuum limit (displaced from the origin). The solid horizontal (red) lines are the lines of constant physics, given also by a (red) triangle slightly displaced from the origin. $L/a = 4$ are not included.

Figure 3: Continuum limit extrapolation of the step scaling function. Diamond (blue) points are the values of the step scaling function using data from the same regularisation and the dashed lines represent the fits. Circles (red) represent the lattice step scaling function taking data from two regularisations and the solid lines their fits. Asterisks (magenta) are the continuum extrapolations $\sigma(u)$ of the lattice step scaling function. The renormalisation prescriptions, (values of $u$) are explicitly given in the plots. The graph on the right correspond to the regularisation $s = 1$ and the one on the left to $s = -1$.

in PT. Our fit function was a polynomial of degree 6 where the first coefficients where set to the perturbative coefficients up to 2 loop [12] in PT. The values corresponding to the largest couplings were not included in the fits. In the plot, we show the results obtained from the two different regularisations. They are correlated and therefore they can not be simultaneously used in a fit. The differences between the two can be regarded as systematic errors.

6. Conclusions and outlook

We have computed the SSF of the QCD coupling in the SF scheme with 4 flavours of massless staggered quarks. Unfortunately, the discretisation errors are fairly large. Some more effort will be put into the data analysis, and the $\Lambda$ parameter still needs to be computed. The results are in rough agreement with data obtained with Wilson quarks [9], but a detailed comparison is still needed.
4-flavour running coupling

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Figure 4: Step scaling function $\sigma(u)$. The dotted-dashed (red), dashed (blue) and solid (magenta) lines represent the perturbative 1-loop, 2-loop and 3-loop $\sigma(u)$. Diamonds (red) represent the extrapolated $\sigma(u)$ from the $s = 1$ regularisation and circles (green) from the $s = -1$. Their fits (largest value excluded) are given by the solid thick (black) lines.

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