

An $O(a)$ modified lattice set-up of the Schrödinger functional in $SU(3)$ gauge theory



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Abstract

The set-up of the QCD Schrödinger functional (SF) on the lattice with staggered quarks requires an even number of points L/a in the spatial directions, while the Euclidean time extent of the lattice, T/a , must be odd. Identifying a unique renormalisation scale, $L = T$, is then only possible up to $O(a)$ lattice artefacts. In this article we study such lattices in the pure $SU(3)$ gauge theory, where we can also compare to the standard set-up. We consider the SF coupling as obtained from the variation of an $SU(3)$ Abelian and spatially constant background field. The $O(a)$ lattice artefacts can be cancelled by the existing $O(a)$ boundary counterterm. However, its coefficient, c_t , differs at the tree-level from its standard value, so that one first needs to re-determine the induced background gauge field. The perturbative one-loop correction to the coupling allows to determine c_t to one-loop order. A few numerical simulations serve to demonstrate that residual cutoff effects in the step scaling function are small in both cases, $T = L \pm a$ and comparable to the standard case with $T = L$.

1 Introduction

Renormalisation schemes based on the Schrödinger functional [1–3] have come to play an important rôle in lattice QCD and in Technicolor inspired models of electroweak symmetry breaking. The Schrödinger functional (SF) is used to define a technically convenient, intermediate renormalisation scheme, where the scale is set by the finite space-time volume, and all fermion masses are taken to vanish. In SF schemes, the non-perturbative scale evolution of the running coupling or multiplicative renormalisation constants of composite operators can then be constructed recursively (see [4,5] for an introduction). Note that the scale evolution is eventually obtained in the continuum limit and thus universal. Hence, the choice of the lattice regularisation for this part of the calculation is merely a matter of practical considerations. In particular, in order to minimise computational costs it is advisable to use some variant of either Wilson or staggered quarks.

The Schrödinger functional in lattice QCD was originally obtained for Wilson type quarks [2]. Its formulation for staggered/Kogut-Susskind quarks has been initiated in [6] and further studied in [7]. For theories with a multiple of four massless fermion flavours¹, staggered quarks constitute an attractive alternative to Wilson quarks: no tuning is required to recover the chiral limit, and numerical simulations for a given lattice size are computationally less demanding. In fact, the SF coupling has already been studied with $N_f = 16$ [8] and $N_f = 8, 12$ [9] fermion flavours, and a four-flavour QCD study is in preparation [10–12]. A drawback, however, consists in the observation that staggered fermions require lattices with an even extent L/a in the spatial directions, whereas the time extent T/a must be odd [6,7]. As the renormalisation scale must be given by a unique scale, $\mu = L^{-1}$, the ratio T/L must be fixed and is usually set to $T/L = 1$. With staggered quarks, this can only be achieved up to corrections of $O(a)$ and the question arises how the ensuing $O(a)$ effects can be eliminated. For the running coupling, Heller proposed to take an average of observables on lattices with $T = L \pm a$, and he showed that this procedure is consistent to one-loop order of perturbation theory. The same recipe was then also applied in numerical simulations [8,9]. However, it is not obvious how this procedure can be generalised to fermionic correlation functions [13].

It is thus desirable to find an alternative to the averaging procedure. It is the purpose of the present paper to show how this is possible by slightly modifying the approach to the continuum limit. More precisely, the limit should be taken at fixed T'/L where T' is either set to $T + a$ or to $T - a$. Requiring $O(a)$ improvement of the pure gauge theory leads to modifications of the boundary $O(a)$ counterterm proportional to c_t already at the tree-level. This in turn affects the equations of motion for the gauge field and thus changes the minimum action configuration used to define the coupling in the SF scheme. We determine the new background gauge field and then perform a one-loop computation to calculate the boundary $O(a)$ improvement of the SF to this order for the pure gauge theory. A numerical simulation has been carried out to check for the size of residual cutoff effects in the step-scaling function for the SF coupling. Although our motivation for this work originates in the fermionic sector of the SF, we here only discuss the necessary modifications to the SF in the pure gauge theory [1]. The details and calculations pertaining to the fermionic sector with staggered quarks will be presented elsewhere [10,14].

¹For staggered quarks we here use the traditional term “flavour” rather than “taste”.

This paper is organised as follows: after a brief review of the continuum Schrödinger functional and the definition of the renormalised coupling, we discuss its lattice regularization and the origin of the constraint on lattice sizes with staggered fermions (Sect. 2). In Sect. 3, the background gauge field is found with c_t left as parameter, which is then determined such as to cancel $O(a)$ effects in the action. We then proceed with the one-loop calculation of the running coupling (Sect. 4), and determine c_t to this order, as well as the size of remaining lattice artefacts at one-loop order. In Sect. 5 we discuss the results of our numerical simulation at an intermediate value of the running coupling. Conclusions are presented in Sect. 6. For future reference, an appendix contains two tables with the raw data of our perturbative one-loop calculation.

2 A short reminder of the Schrödinger functional coupling

In this section we review some known facts and definitions which will be relevant for this paper. In the continuum the Schrödinger functional is formally defined as the Euclidean path integral,

$$\mathcal{Z}[C, C'] = \int D[A, \psi, \bar{\psi}] e^{-S_{\text{cont}}[A, \psi, \bar{\psi}]}, \quad (2.1)$$

with the Euclidean action

$$S_{\text{cont}} = \int_0^T dx_0 \int d^3\mathbf{x} \mathcal{L}(x), \quad (2.2)$$

$$\mathcal{L}(x) = -\frac{1}{2g_0^2} \text{tr}\{F_{\mu\nu}(x)F_{\mu\nu}(x)\} + \bar{\psi}(x)(\gamma_\mu D_\mu + m)\psi(x). \quad (2.3)$$

Here, g_0 denotes the bare coupling constant, $F_{\mu\nu}$ is the field tensor associated with the gauge field A_μ ,

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu], \quad (2.4)$$

and $D_\mu = \partial_\mu + A_\mu + i\theta_\mu/L$ denotes the covariant derivative acting on the quark fields (including a constant U(1) background field with $\theta_\mu = (1 - \delta_{\mu 0})\theta$). The space-time manifold is taken to be a hyper-cylinder. In the spatial directions periodic boundary conditions are imposed on all fields. At the time boundaries the conditions for the fermionic fields read

$$P_+ \psi|_{x_0=0} = 0 = P_- \psi|_{x_0=T}, \quad \bar{\psi} P_-|_{x_0=0} = 0 = \bar{\psi} P_+|_{x_0=T}, \quad (2.5)$$

with the projectors $P_\pm = \frac{1}{2}(1 \pm \gamma_0)$. For the gauge field one has

$$A_k|_{x_0=0} = C_k, \quad A_k|_{x_0=T} = C'_k, \quad k = 1, 2, 3, \quad (2.6)$$

with the boundary gauge field configurations C_k and C'_k . Of particular interest are spatially constant Abelian fields, which take the form,

$$C_k = \frac{i}{L} \phi, \quad C'_k = \frac{i}{L} \phi', \quad k = 1, 2, 3, \quad (2.7)$$

with traceless and diagonal $N \times N$ -matrices ϕ and ϕ' . For $N = 3$ colours we follow [15] and parameterise the diagonal elements by,

$$\begin{aligned}\phi_1 &= \eta - \frac{\pi}{3}, & \phi'_1 &= -\eta - \pi, \\ \phi_2 &= \eta \left(\nu - \frac{1}{2} \right), & \phi'_2 &= \eta \left(\nu + \frac{1}{2} \right) + \frac{\pi}{3}, \\ \phi_3 &= -\eta \left(\nu + \frac{1}{2} \right) + \frac{\pi}{3}, & \phi'_3 &= -\eta \left(\nu - \frac{1}{2} \right) + \frac{2\pi}{3},\end{aligned}\tag{2.8}$$

where η and ν are 2 real parameters. In the temporal gauge the field equations with these boundary conditions are solved by,

$$B_0 = 0, \quad B_k = C_k + \frac{x_0}{T} (C'_k - C_k), \quad k = 1, 2, 3.\tag{2.9}$$

which corresponds to a constant chromo-electric field,

$$G_{0k} = \partial_0 B_k = \frac{C'_k - C_k}{T} = \frac{i(\phi'_k - \phi_k)}{LT}, \quad k = 1, 2, 3,\tag{2.10}$$

all chromo-magnetic components of the field tensor being zero. The background field B is, up to gauge transformations, uniquely determined by the gauge boundary fields since it corresponds to the absolute minimum of the gauge action,

$$S_{\text{cont}}[B] = \frac{3}{\rho g_0^2} \sum_{\alpha=1}^3 (\phi'_\alpha - \phi_\alpha)^2 = \frac{18}{\rho g_0^2} \left(\eta + \frac{\pi}{3} \right)^2,\tag{2.11}$$

where $\rho = T/L$ is the aspect ratio. The effective action for the SF can thus be taken to be a function of the background field,

$$\Gamma[B] = -\ln \mathcal{Z}[C', C],\tag{2.12}$$

which admits a weak coupling expansion,

$$\Gamma[B] \stackrel{g_0 \rightarrow 0}{\sim} \frac{1}{g_0^2} \Gamma_0[B] + \Gamma_1[B] + \mathcal{O}(g_0^2),\tag{2.13}$$

with the lowest order term given by the classical action, $\Gamma_0[B] = g_0^2 S_{\text{cont}}[B]$. Setting $T = L$, one remains with a single external scale, L , and a renormalised coupling $\bar{g}(L)$ can now be defined through

$$\left. \frac{\partial \Gamma}{\partial \eta} \right|_{\eta=0} = k \left\{ \frac{1}{\bar{g}^2(L)} - \nu \bar{v}(L) \right\}, \quad k = \left. \frac{\partial \Gamma_0}{\partial \eta} \right|_{\eta=0} = 12\pi.\tag{2.14}$$

Here the η -derivative serves to eliminate any background field independent terms in the effective action. Moreover, it implies that the coupling is defined by an SF correlation function rather than by the SF itself, which renders it measurable by numerical simulations. In practice the parameter ν will be set to zero. However, its coefficient in Eq. (2.14), $\bar{v}$, defines a further observable, which can also be measured at $\nu = 0$, based on the relation,

$$\bar{v}(L) = -\frac{1}{k} \frac{\partial}{\partial \nu} \left\{ \left. \frac{\partial \Gamma}{\partial \eta} \right|_{\eta=0} \right\}_{\nu=0}.\tag{2.15}$$

In numerical simulations, the scale evolution for the coupling is constructed non-perturbatively by computing the continuum step-scaling function

$$\sigma(u) = \bar{g}^2(2L)|_{u=\bar{g}^2(L)}. \quad (2.16)$$

Prescribing a value for $u = \bar{g}^2(L)$ implicitly fixes the scale L , and thus the only free parameter in pure Yang-Mills theory. The coupling at the scale $2L$ or $\bar{v}(L)$ are then fixed and can be obtained by taking the continuum limit of the corresponding observables on the lattice. We will later use the deviation from their respective continuum limits $\sigma(u)$ and

$$\omega(u) = \bar{v}(L)|_{u=\bar{g}^2(L)}, \quad (2.17)$$

to obtain an impression of the cutoff effects for the different lattice regularisations considered here.

The SF coupling is gauge invariant and can be non-perturbatively defined on the lattice. For small volumes it can be related perturbatively to the $\overline{\text{MS}}$ scheme. This relation is known to two-loop order both for the pure SU(3) gauge theory [16] and QCD [17]. Setting $q = 1/L$ and $\alpha = \bar{g}^2/4\pi$, the result for pure SU(3) gauge theory is

$$\alpha_{\overline{\text{MS}}}(q) = \alpha(q) + c_1 \alpha^2(q) + c_2 \alpha^3(q) + \text{O}(\alpha^4), \quad (2.18)$$

with [16],

$$c_1 = 1.255621(2), \quad c_2 = c_1^2 + 1.197(10). \quad (2.19)$$

For the perturbative checks in this paper we will also need the one-loop result for the observable $\bar{v}(L)$ [15],

$$\omega(u) = \omega_1 + \omega_2 u + \text{O}(u^2), \quad \omega_1 = 0.0694603(1). \quad (2.20)$$

Finally, we recall that the step-scaling function to first non-trivial order is given by

$$\sigma(u) = u + 2b_0 \ln(2) \times u^2 + \text{O}(u^3), \quad b_0 = 11/(4\pi)^2. \quad (2.21)$$

Here, b_0 is the universal one-loop coefficient of the SU(3) β -function, which, for the SF coupling is known to 3-loop order [16].

3 Variants of the pure gauge Schrödinger functional on the lattice

We here summarise the basic definitions and properties of the SF in the SU(N) lattice gauge theory. The change at $\text{O}(a)$ motivated by staggered fermions has tree-level consequences which will be worked out in the remainder of this section.

3.1 The standard lattice framework

The lattice formulation of the SF for pure SU(N) gauge theories can be obtained from the transfer matrix formalism [1]. When written as a path integral it takes the form

$$\mathcal{Z}[C, C'] = \int D[U] e^{-S[U]}. \quad (3.1)$$

The pure gauge action is given by

$$S[U] = \frac{1}{g_0^2} \sum_p w(p) \text{tr}\{1 - U(p)\}, \quad (3.2)$$

where the sum runs over all oriented plaquettes p of the lattice and $U(p)$ denotes the parallel transporter around p . Assuming Abelian boundary gauge fields C_k and C'_k , the boundary conditions, Eq. (2.6) translate to

$$U(x, k)|_{x_0=0} = W(\mathbf{x}, k), \quad U(x, k)|_{x_0=T} = W'(\mathbf{x}, k), \quad (3.3)$$

with the boundary link variables,

$$W(\mathbf{x}, k) = \exp(aC_k), \quad W'(\mathbf{x}, k) = \exp(aC'_k). \quad (3.4)$$

Finally, the weight factor, $w(p)$, is set to

$$w(p) = \begin{cases} \frac{1}{2}c_s(g_0) & \text{for spatial plaquettes } p \text{ at } x_0 = 0, T, \\ c_t(g_0) & \text{for time-like plaquettes } p \text{ attached to the boundaries,} \\ 1 & \text{otherwise.} \end{cases} \quad (3.5)$$

In the continuum limit the plaquette terms multiplied by c_t and c_s respectively reduce to the only gauge invariant local boundary operators of dimension 4, which are allowed by the symmetries of the SF (repeated spatial Lorentz indices are summed over),

$$\text{tr}\{F_{0k}F_{0k}\}, \quad \text{tr}\{F_{kl}F_{kl}\}. \quad (3.6)$$

There are no other sources for lattice artefacts linear in a , and one may thus cancel $O(a)$ effects in any on-shell quantity by properly adjusting these coefficients. Moreover, while c_t contributes to all observables, the counterterm proportional to c_s vanishes for spatially constant Abelian boundary gauge fields. In this case, $O(a)$ improvement can be achieved with the appropriate choice of c_t alone. In perturbation theory, one has

$$c_t(g_0) = c_t^{(0)} + c_t^{(1)} g_0^2 + \dots \quad (3.7)$$

In the standard set-up of the SF one sets $L = T$ and tree-level $O(a)$ improvement is achieved by setting $c_t = 1$. With this choice the classical equations of motion which follow from the lattice action are equivalent to

$$d^*P(x, \mu) - d^*P(x, \mu)^\dagger - \frac{1}{N} \text{tr} \left\{ d^*P(x, \mu) - d^*P(x, \mu)^\dagger \right\} = 0, \quad (3.8)$$

where

$$d^*P(x, \mu) = \sum_{\nu=0}^3 \left\{ P_{\mu\nu}(x) - U_\nu^\dagger(x - a\hat{\nu}) P_{\mu\nu}(x - a\hat{\nu}) U_\nu(x - a\hat{\nu}) \right\}, \quad (3.9)$$

and the plaquette field is defined by

$$P_{\mu\nu}(x) = U_\mu(x) U_\nu(x + a\hat{\mu}) U_\mu^\dagger(x + a\hat{\nu}) U_\nu^\dagger(x). \quad (3.10)$$

A solution $V_\mu(x)$ to Eq. (3.8) which is unique up to gauge equivalence, is referred to as the lattice background gauge field. For spatially constant Abelian boundary fields, the lattice background field is obtained by simply exponentiating the continuum solution, Eq. (2.9),

$$V_\mu(x) = \exp(aB_\mu(x)), \quad \mu = 0, \dots, 3. \quad (3.11)$$

Moreover, a mathematical proof establishes that this solution corresponds to an absolute minimum of the action, provided the condition

$$TL/a^2 > (N-1)\pi^2 \max\{1, N/16\}, \quad (3.12)$$

is met [1]. For $N = 3$ colours, this means that $S[V]$ represents an absolute minimum for $TL/a^2 \geq 2\pi^2$, implying $L/a > 4$ on lattices with $L = T$. The action at the minimum,

$$S[V] = \frac{3TL^3}{g_0^2} \sum_{\alpha=1}^3 \left\{ \frac{2}{a^2} \sin \left[\frac{a^2}{2TL} (\phi'_\alpha - \phi_\alpha) \right] \right\}^2, \quad (3.13)$$

only differs at $O(a^4)$ from the continuum action, Eq. (2.11).

One should note, however, that these considerations depend on having set $c_t = 1$. As we will now explain, staggered fermions require a modified approach to the continuum limit, which will lead to a different choice of c_t . Consequently, the determination of the classical background field needs to be revisited.

3.2 A constraint from staggered quarks

A peculiarity in the formulation of the Schrödinger functional with staggered quarks has first been noticed in [6] and can also be traced back to the properties of the transfer matrix [18]: the lattice sizes needed in this case have even spatial extent L/a and odd temporal extent T/a . To understand this constraint, one needs to recall that the 4 flavours of Dirac (i.e. four-component) spinors are reconstructed from the staggered one-component fields living on the $2^4 = 16$ corners of the elementary hypercubes of the lattice. The reconstructed fields may be imagined to live on a coarse lattice with the doubled lattice spacing. The constraint arises from having to construct an integer multiple of four Dirac spinors from those staggered one-component fields which are integration variables in the functional integral (cf. the left panel of figure 1 for an illustration in 2 dimensions). Equivalently, the lattice geometry must be such that an integer number of hypercubes with dynamical field components is obtained. Note that the Dirichlet conditions for the one-component fields at $x_0 = 0$ and $x_0 = T$ naturally lead to a Dirichlet condition for half of the Dirac spinors living at the boundaries. This implicitly defines projectors in spin-flavour space, the form of which depends on the details of the reconstruction of the Dirac spinors. However, there is enough freedom to obtain four flavours of quarks satisfying the standard boundary conditions in terms of the projectors $P_\pm = \frac{1}{2}(1 \pm \gamma_0)$ [19,7]. The reconstructed four-spinors thus live on a coarser lattice with size $(L/2a)^3 \times (T/a - 1)/2$.

A slightly less intuitive option to reconstruct the four-component spinors is illustrated in the right panel of figure 1. It corresponds to an extension of the fine lattice by a time slice beyond each of the time boundaries. The part of the four-component spinors living on these added time-slices correspond to the non-Dirichlet components at the boundaries, which need not

be dynamical field components². To treat this second case we also consider the coarser lattice with size $(L/2a)^3 \times (T/a + 1)/2$, and, combining both options, we set

$$T' = T + sa, \quad s = \pm 1. \quad (3.14)$$

Note that in the absence of staggered quarks we may also set $s = 0$ to recover the standard framework for the pure gauge theory. In the following we will thus try to take the continuum limit at fixed ratio, $\rho = T'/L$. In particular, for the computation of the SF coupling we set $\rho = 1$ exactly. This redefines the approach to the continuum limit, and we are thus led to discuss on-shell $O(a)$ improvement for this modified set-up.

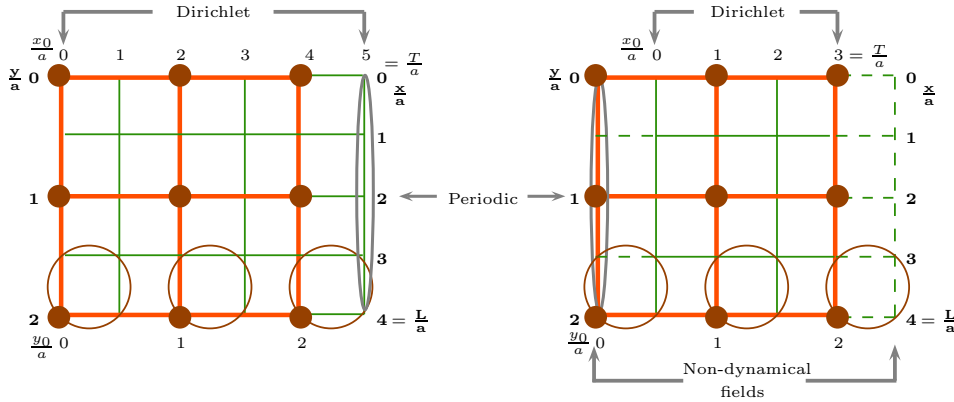


Figure 1: The figure shows a 2-dimensional section of the SF with staggered fermions with $L/a = 4$ and $T'/L = 1$. The left panel shows the case $T' = T - a$ ($s = -1$) the right panel corresponds to $T' = T + a$ ($s = 1$). Thin lines represent the lattice on which the one-component staggered fermions live. The Dirac spinors are reconstructed from those one-component fields residing inside the circles and live on the effective lattice depicted by the thick lines.

3.3 The equations of motion and the background field

The background field is the field configuration which minimises the lattice action. Since the latter depends on c_t , any change of this coefficient may modify the minimal action configuration. The equations of motion can easily be generalised to this case by simply including the weight factors $w_{\mu\nu}(x) \equiv w[P_{\mu\nu}(x)]$ in the definition of the covariant divergence, Eq. (3.9),

$$d_w^* P(x, \mu) = \sum_{\nu=0}^3 \left\{ w_{\mu\nu}(x) P_{\mu\nu}(x) - w_{\mu\nu}(x - a\hat{\nu}) U_\nu^\dagger(x - a\hat{\nu}) P_{\mu\nu}(x - a\hat{\nu}) U_\nu(x - a\hat{\nu}) \right\}. \quad (3.15)$$

The lattice action is stationary if and only if the traceless antihermitian part of $d_w^* P$ vanishes, i.e. the equations of motion read

$$d_w^* P(x, \mu) - d_w^* P(x, \mu)^\dagger - \frac{1}{N} \text{tr} \left\{ d_w^* P(x, \mu) - d_w^* P(x, \mu)^\dagger \right\} = 0. \quad (3.16)$$

²This is in fact the situation in the SF with Wilson quarks, where the non-Dirichlet components at the boundaries are completely decoupled from the dynamical field components [2].

In order to solve the equations we choose the temporal gauge, setting all temporal links to unity, $U_0(x) = 1$. Since the modification of the standard framework with $T' = T$ amounts to an $O(a)$ effect, it seems plausible that the solution of the equations of motion will again be Abelian and spatially constant, at least for large enough lattice sizes. Hence, we make the ansatz

$$V(x, k) = \exp[aB_k(x_0)], \quad (3.17)$$

and try to solve Eq. (3.8) for a colour diagonal and spatially constant field $B_k(x_0)$, subject to the boundary conditions

$$B_k(0) = C_k = i\phi/L, \quad B_k(T) = C'_k = i\phi'/L, \quad (3.18)$$

The coefficient c_t is left as a free parameter, which will be fixed later by demanding that the action is $O(a)$ improved. The field tensor associated with the plaquette field is defined by

$$P_{\mu\nu}(x)|_{U \rightarrow V} = \exp[a^2 G_{\mu\nu}(x_0)], \quad (3.19)$$

and is thus related to $B_k(x_0)$ by the forward lattice derivative,

$$G_{0k}(x_0) = \partial_0 B_k(x_0) = \frac{1}{a} [B_k(x_0 + a) - B_k(x_0)], \quad (3.20)$$

with all other components being zero. The boundary conditions are equal for all spatial indices $k = 1, 2, 3$, so that we introduce the notation

$$f(x_0) = G_{0k}(x_0). \quad (3.21)$$

Note that $f(x_0)$ is, for fixed x_0 , an anti-hermitian diagonal matrix in colour space with trace zero, i.e. its colour components $f_\alpha(x_0)$ are purely imaginary and must sum to zero. Eqs. (3.16) now reduce to T/a equations of the form,

$$M(x_0) - \frac{1}{N} \text{tr} [M(x_0)] = 0, \quad a \leq x_0 \leq T - a, \quad (3.22)$$

where the trace is over colour and the diagonal $N \times N$ -matrices $M(x_0)$ are given by

$$M(x_0) = \begin{cases} \sinh[a^2 f(a)] - c_t \sinh[a^2 f(0)] & \text{if } x_0 = a, \\ c_t \sinh[a^2 f(T - a)] - \sinh[a^2 f(T - 2a)] & \text{if } x_0 = T - a, \\ \sinh[a^2 f(x_0)] - \sinh[a^2 f(x_0 - a)] & \text{if } a < x_0 < T - a. \end{cases} \quad (3.23)$$

Expanding $f(x_0)$ in a power series in a ,

$$f(x_0) = \sum_{n=0}^{\infty} \left(\frac{a}{L}\right)^n f^{(n)}(x_0), \quad (3.24)$$

and inserting this expansion in the equations of motion (3.22), one may show by induction that, for all n ,

$$f^{(n)}(x_0) = \begin{cases} f^{(n)} + \Delta f^{(n)} & \text{if } x_0 = 0, T - a \\ f^{(n)} & \text{if } a \leq x_0 < T - a. \end{cases} \quad (3.25)$$

Hence one concludes that $f(x_0)$ is equal to the x_0 -independent constant matrix f except for a jump at the time boundaries by Δf . To proceed further one needs to go back to the background field $B_k(x_0)$ in the temporal gauge. One finds,

$$\begin{aligned} B_k(0) &= C_k \\ B_k(x_0) &= \left(x_0 - \frac{T}{2}\right) f + \frac{C_k + C'_k}{2} \quad \text{if } a \leq x_0 \leq T - a \\ B_k(T) &= C'_k, \end{aligned} \quad (3.26)$$

and the jump in the field tensor at the boundaries is given by

$$\Delta f = \frac{C'_k - C_k}{2a} - \frac{T}{2a} f. \quad (3.27)$$

Thus, for given boundary gauge fields and lattice geometry the background field and its field tensor are determined by the traceless and diagonal colour matrix f , which still needs to be computed.

We now specialise to $N = 3$ colours and insert the matrices f and Δf in Eq. (3.22). While $M(x_0) = 0$ for all $a < x_0 < T - a$, the 2 equations for $M(a)$ and $M(T - a)$ are identical and read, in terms of the colour components f_α ,

$$\begin{aligned} 0 &= \frac{1}{3} \sum_{\beta=1}^3 \left\{ c_t \sinh \left\{ a^2 f_\beta \left[1 + \frac{s}{2} - \frac{T'}{2a} \right] + ia \frac{\phi'_\beta - \phi_\beta}{2L} \right\} - \sinh \{ a^2 f_\beta \} \right\} \\ &\quad - c_t \sinh \left\{ a^2 f_\alpha \left[1 + \frac{s}{2} - \frac{T'}{2a} \right] + ia \frac{\phi'_\alpha - \phi_\alpha}{2L} \right\} + \sinh \{ a^2 f_\alpha \}, \end{aligned} \quad (3.28)$$

for $\alpha = 1, 2, 3$. Taking into account that $\phi'_1 - \phi_1 = -2(\phi'_2 - \phi_2) = -2(\phi'_3 - \phi_3)$ [cf. Eqs. (2.8)] one concludes that f_2 and f_3 satisfy the same equation and hence $f_2 = f_3$. Tracelessness of f then implies

$$f = f_2 \times \text{diag}(-2, 1, 1), \quad (3.29)$$

so that we are left with a single equation for f_2 . Introducing the real dimensionless variable φ through

$$f_2 = i\varphi/L^2, \quad (3.30)$$

the equation to be solved for φ is

$$c_t \sin \left\{ 2 \frac{a^2}{L^2} K(\varphi) \right\} + c_t \sin \left\{ \frac{a^2}{L^2} K(\varphi) \right\} - \sin \left\{ 2 \frac{a^2}{L^2} \varphi \right\} - \sin \left\{ \frac{a^2}{L^2} \varphi \right\} = 0, \quad (3.31)$$

with

$$K(\varphi) = \varphi \left[1 + \frac{s}{2} - \frac{\rho L}{2a} \right] + \frac{L}{2a} (\phi'_2 - \phi_2), \quad \rho = T'/L. \quad (3.32)$$

Next we expand φ in powers of a/L in analogy to Eq. (3.24) and solve Eqs. (3.31) order by order in a/L . For the first 3 coefficients, we find,

$$\varphi^{(0)} = \rho^{-1} (\phi'_2 - \phi_2) = \rho^{-1} \left(\eta + \frac{\pi}{3} \right) \quad (3.33)$$

$$\varphi^{(1)} = \varphi^{(0)} k_s, \quad k_s = \frac{(2+s)c_t - 2}{\rho c_t}, \quad (3.34)$$

$$\varphi^{(2)} = \varphi^{(0)} k_s^2. \quad (3.35)$$

Without further assumptions on c_t or s there are corrections to all orders in a/L . We note, however, that for the standard case with $s = 0$ and $c_t = 1$, Eq. (3.31) reduces to $K(\varphi) = \varphi$, which is exactly solved by $\varphi = \varphi^{(0)}$. In the general case one may obtain precise approximate solutions by pushing the Taylor expansion to higher orders. Alternatively, one may, for given numerical values of s , L/a , ρ , c_t and η , find a numerical solution for φ (and thus for f) by applying the Newton procedure to Eq. (3.31).

3.4 Choice of c_t

The free parameter c_t of the background field can now be determined by demanding that the classical action is $O(a)$ improved. This can be done analytically, as the dependence of the background field on c_t is known to $O(a)$ from Eq. (3.34). First we insert the background field (3.26) into the action, and set $T = T' - sa$,

$$S[V] = \frac{-3[T' - (2+s)a]L^3}{g_0^2} \sum_{\alpha=1}^3 \left\{ \frac{2}{a^2} \sinh \left[\frac{a^2}{2} f_\alpha \right] \right\}^2 - \frac{6aL^3 c_t}{g_0^2} \sum_{\alpha=1}^3 \left\{ \frac{2}{a^2} \sinh \left[\frac{a^2}{2} (f_\alpha + \Delta f_\alpha) \right] \right\}^2. \quad (3.36)$$

Then, using the relations (3.29,3.30), and

$$f + \Delta f = \frac{i}{L^2} K(\varphi) \times \text{diag}(-2, 1, 1), \quad (3.37)$$

the action can be written as a function of φ , viz.

$$S[V] = -\frac{24L^3}{g_0^2 a^3} \left\{ \left[1 + \frac{s}{2} - \frac{\rho L}{2a} \right] \left[\sin^2 \left(\frac{a^2}{L^2} \varphi \right) + 2 \sin^2 \left(\frac{a^2}{2L^2} \varphi \right) \right] - c_t \left[\sin^2 \left(\frac{a^2}{L^2} K(\varphi) \right) + 2 \sin^2 \left(\frac{a^2}{2L^2} K(\varphi) \right) \right] \right\} \quad (3.38)$$

Then, with

$$\varphi = \varphi^{(0)} \left[1 + \frac{a}{L} k_s + \frac{a^2}{L^2} k_s^2 + O(a^3) \right], \quad K(\varphi) = \frac{\varphi^{(0)}}{c_t} \left[1 + \frac{a}{L} k_s + O(a^2) \right], \quad (3.39)$$

and Taylor expanding in a/L , one obtains

$$S[V] = \frac{18\rho}{g_0^2} \left(\varphi^{(0)} \right)^2 \left\{ 1 + \frac{a}{L} k_s + O(a^2) \right\} = S_{\text{cont}}[B] \left\{ 1 + \frac{a}{L} k_s + O(a^2) \right\}. \quad (3.40)$$

In order to reduce the corrections to $O(a^2)$ the coefficient k_s , as defined in Eq. (3.34) must vanish, which is achieved by setting

$$c_t = \frac{2}{2+s} = \begin{cases} \frac{2}{3} & \text{if } s = 1, \\ 1 & \text{if } s = 0, \\ 2 & \text{if } s = -1. \end{cases} \quad (3.41)$$

Remarkably, with this choice for c_t , the action of the background field is not just $O(a)$ improved but cutoff effects only start at $O(a^4)$, in all three cases $s = \pm 1, 0$. In fact, the background field is only mildly distorted by lattice artefacts, as shown by the Taylor expansion,

$$\varphi|_{c_t=2/(2+s)} = \varphi^{(0)} + \left(\frac{a}{L}\right)^5 \varphi^{(5)} + \left(\frac{a}{L}\right)^9 \varphi^{(9)} + \left(\frac{a}{L}\right)^{10} \varphi^{(10)} + O(a^{13}), \quad (3.42)$$

where $\varphi^{(0)}$ is given in Eq. (3.33) and

$$\varphi^{(5)} = -\frac{(\phi'_2 - \phi_2)^3}{8\rho^4} s(s+4)(s+2), \quad (3.43)$$

$$\varphi^{(9)} = -\frac{(\phi'_2 - \phi_2)^5}{120\rho^6} s(s+4)(s+2) \left(\frac{79}{16}s^2 + \frac{79}{4}s + 17\right), \quad (3.44)$$

$$\varphi^{(10)} = \frac{3(\phi'_2 - \phi_2)^5}{2^6 \rho^7} s^2(s+4)^2(s+2)^2 = \frac{3}{\varphi^{(0)}} \left(\varphi^{(5)}\right)^2. \quad (3.45)$$

The expansion to this order yields rather precise approximations to the full solution of Eq. (3.31). For instance, with $\rho = 1$, we conclude that $\varphi/\varphi^{(0)}$ is obtained with double precision provided $L/a > 12$ and $L/a > 21$ for $s = -1$ and $s = 1$ respectively.

In Section 4 we will also need the η -derivative of the background field, i.e. of φ . Given φ , this can be obtained by differentiating Eq. (3.31) with respect to η . Alternatively one may obtain the a/L -expansion by differentiating the coefficients in Eqs. (3.43-3.45). Recalling that $\phi'_2 - \phi_2 = \eta + \pi/3$, the η -derivatives of the coefficients are given by

$$\partial_\eta \varphi^{(5)} = \frac{3\varphi^{(5)}}{\phi'_2 - \phi_2}, \quad \partial_\eta \varphi^{(9)} = \frac{5\varphi^{(9)}}{\phi'_2 - \phi_2}, \quad \partial_\eta \varphi^{(10)} = \frac{5\varphi^{(10)}}{\phi'_2 - \phi_2}. \quad (3.46)$$

3.5 A numerical check

The above solution of the classical field equations was obtained using the hypothesis that the background field is Abelian and spatially constant. While this can be rigorously established in the standard set-up, we here rely on the plausibility of the assumption that an $O(a)$ change in the set-up can only have a small impact, at least for large enough lattice sizes. To check the hypothesis on small size lattices ($L/a = 4-8$), we have tried to find the absolute minimum of the action numerically, by starting from a random gauge configuration. Sweeping through the lattice we minimised the plaquettes with respect to the $SU(3)$ link variables. In order to avoid getting trapped in secondary minima of the action we also used over-relaxation steps which change the configuration whilst leaving the action invariant. The obtained results agreed numerically very well with the expectation from the Abelian background field. Furthermore, the background field itself was found to be of the expected form after transformation to the temporal gauge. We take this as evidence that the true minimal action configuration is indeed the Abelian and spatially constant solution described above.

4 One-loop results

The perturbation expansion is analogous to the calculation in $SU(2)$ which has been described in the original paper [1] and we will be rather brief on the technical details. Given the one-

loop results we obtain the boundary improvement coefficients to this order and we can check remaining lattice artefacts in the step-scaling function for the coupling and in $\bar{v}(L)$.

4.1 The running coupling at one-loop order

So far our considerations have been purely classical. Dealing with quantum corrections the improvement coefficient c_t will become a function of the bare coupling, with an expansion of the form,

$$c_t(g_0) = c_t^{(0)} + g_0^2 c_t^{(1)} + O(g_0^4). \quad (4.1)$$

Our classical considerations in the previous section correspond to setting $g_0 = 0$ i.e. $c_t = c_t^{(0)}$, and $c_t^{(0)}$ is thus given by Eq. (3.41). The perturbative expansion of the effective action on the lattice takes the same form as in the continuum, Eq. (2.13), with the first 2 terms given by

$$\Gamma_0[B] = g_0^2 S[V]|_{c_t=c_t^{(0)}} \quad (4.2)$$

$$\Gamma_1[B] = c_t^{(1)} \Gamma_{0;c_t}[B] - \ln \det \Delta_0 + \frac{1}{2} \ln \det \Delta_1. \quad (4.3)$$

Here, the fluctuation operators Δ_0 and Δ_1 appear in the Gaussian parts of the action in the Faddeev-Popov ghost and the gluon fields, respectively. The counterterm $\propto c_t^{(1)}$ is specified by

$$\Gamma_{0;c_t}[B] = \frac{\partial}{\partial c_t} \Gamma_0[B]|_{c_t=c_t^{(0)}} = 24 \frac{L^3}{a^3} \left[\sin^2 \left(\frac{a^2}{L^2} K(\varphi) \right) + 2 \sin^2 \left(\frac{a^2}{2L^2} K(\varphi) \right) \right], \quad (4.4)$$

where φ is the solution of Eq. (3.31) with $c_t = c_t^{(0)}$. Setting $T' = L$ (i.e. $\rho = 1$) the definition of the SF coupling on the lattice

$$\bar{g}^2(L) = \frac{\partial_\eta \Gamma_0[B]}{\partial_\eta \Gamma[B]} \Big|_{\eta=\nu=0}, \quad (4.5)$$

is such that $\bar{g}(L) = g_0$ holds exactly at lowest order. Hence, the normalisation constant,

$$\partial_\eta \Gamma_0[B] = 12 \frac{L^2}{a^2} \left[\sin \left(\frac{a^2}{L^2} \varphi \right) + 2 \sin \left(2 \frac{a^2}{L^2} \varphi \right) \right], \quad (4.6)$$

must be computed including the lattice artefacts and differs from its value in the continuum limit, $k = 12\pi$ [cf. Eq. (2.14)], by terms of $O(a^4)$.

To one-loop order the perturbative relation to the bare coupling then reads,

$$\bar{g}^2(L) = g_0^2 + \left(m_1(L/a) - c_t^{(1)} \frac{\partial_\eta \Gamma_{0;c_t}[B]}{\partial_\eta \Gamma_0[B]} \Big|_{\eta=0} \right) g_0^4 + O(g_0^6), \quad (4.7)$$

where the coefficient $m_1(L/a)$ is a sum of two contributions,

$$m_1 = [h_0 - \frac{1}{2} h_1]_{\nu=0}. \quad (4.8)$$

which derive from the Fadeev-Popov ghost and gluon fluctuation operators,

$$h_j = \frac{\partial_\eta \ln \det \Delta_j}{\partial_\eta \Gamma_0[B]} \Big|_{\eta=0}, \quad j = 0, 1. \quad (4.9)$$

We have computed these contributions numerically for lattice sizes ranging from $L/a = 4$ to $L/a = 64$, using two completely different techniques. One of us has performed the computation along the lines of refs. [1,20], using recursion relations for the finite difference operators Δ_0 and Δ_1 , in order to compute their determinants in each sector of fixed spatial momentum and colour quantum numbers. In addition, an independent computation was carried out based on the automated perturbation theory described in refs. [21,22]. Perfect numerical agreement was found between the two methods, up to rounding errors. We also verified gauge invariance of $m_1(L/a)$ by computing it at different values of the gauge fixing parameter. For future reference the numerical results for $m_1(L/a)$ are collected in Tables 6 and 7 of Appendix A, for all three choices of $s = \pm 1, 0$. To estimate the numerical precision we have compared the two calculations and find agreement for 15 digits at $L/a = 4$ which reduces to about 12 digits at $L/a = 64$, due to the accumulation of rounding errors.

4.2 Determination of $c_t^{(1)}$

From Symanzik's analysis [23,24] of the cutoff dependence of Feynman diagrams on the lattice, one expects $m_1(L/a)$ to have an asymptotic expansion of the form

$$m_1(L/a) \stackrel{L/a \rightarrow \infty}{\sim} \sum_{n=0}^{\infty} (a/L)^n [r_n + s_n \ln(L/a)]. \quad (4.10)$$

The series is logarithmically divergent, since $m_1(L/a)$ relates a renormalised to a bare coupling. For the coefficient of the divergence one expects $s_0 = 2b_0$, where b_0 is the one-loop coefficient of the SU(3) β -function, Eq. (2.21). The divergence could be eliminated by renormalising the bare coupling g_0 e.g. by minimal subtraction of logarithms [25,26]. If one passes directly to the $\overline{\text{MS}}$ -scheme of dimensional regularisation, one finds that the coefficient c_1 in Eq. (2.18) is related to r_0 in Eq. (4.10) through

$$\begin{aligned} c_1 &= d_1(1)|_{N=3} - 4\pi r_0, \\ d_1(1) &= -\frac{\pi}{2N} + k_1 N, \quad k_1 = 2.135730074078457(2), \end{aligned} \quad (4.11)$$

where the coefficient $d_1(1)$ is taken from ref. [27]. Within the numerical precision we reproduce the known result for r_0 of ref. [15] in all three cases, $s = \pm 1, 0$.

The coefficient r_1 multiplies cutoff effects of order a/L which ought to be cancelled by correctly choosing $c_t^{(1)}$. Hence we need to evaluate the coefficient of $c_t^{(1)}$ in Eq. (4.7) to $\mathcal{O}(a)$. To this order, the c_t -dependence of Γ_0 can be inferred from Eq. (3.36) and is given by

$$\Gamma_{0;c_t}[B] = \partial_{c_t} [g_0^2 S[V]]_{c_t=c_t^{(0)}} = g_0^2 S_{\text{cont}}[B] \frac{a}{L} [\partial_{c_t} k_s]_{c_t=c_t^{(0)}} + \mathcal{O}(a^2), \quad (4.12)$$

and $\partial_{c_t} k_s = 2/(\rho c_t^2)$. This shows explicitly that this term is of $\mathcal{O}(a)$. Performing the η -derivative and requiring the absence of $\mathcal{O}(a)$ terms in the one-loop relation between the couplings, leads to the condition,

$$c_t^{(1)} = \rho \frac{r_1}{2} \left(c_t^{(0)} \right)^2. \quad (4.13)$$

Note that the coefficient s_1 of the term $(a/L) \times \ln(L/a)$ is expected to vanish, provided tree-level improvement is correctly implemented. Following the method presented in the appendix of [17],

the first few coefficients were extracted numerically. The outcome of this analysis for the cases $s = 0, \pm 1$ is shown in Table 1. In this table, coefficients shown with no errors have been assumed, entries $\times$ have also been fitted but are not listed here and the terms $\sim$ are included one at a time for the error analysis. As can be seen from the results, all expectations are confirmed within

	s_0	r_0	s_1	r_1	s_2	r_2	s_3	r_3
$s = -1$	0.13931(4)	0.3683(3)	-0.001(15)	-0.23(7)	$\times$	$\times$	$\sim$	$\sim$
	$22/(4\pi)^2$	0.368283(3)	-0.0004(10)	-0.230(6)	$\times$	$\times$	$\sim$	$\sim$
	$22/(4\pi)^2$	0.3682818(7)	0	-0.2318(3)	$\times$	$\times$	$\sim$	$\sim$
$s = 0$	0.13931(3)	0.3683(2)	-0.001(13)	-0.17(7)	$\times$	$\times$	$\sim$	$\sim$
	$22/(4\pi)^2$	0.368283(2)	-0.0003(9)	-0.176(6)	$\times$	$\times$	$\sim$	$\sim$
	$22/(4\pi)^2$	0.3682817(7)	0	-0.1779(3)	$\times$	$\times$	$\sim$	$\sim$
$s = 1$	0.13931(2)	0.3683(1)	0.001(7)	0.12(3)	$\times$	$\times$	$\sim$	$\sim$
	$22/(4\pi)^2$	0.368280(1)	0.0007(5)	0.120(3)	$\times$	$\times$	$\sim$	$\sim$
	$22/(4\pi)^2$	0.368283(1)	0	0.1232(4)	$\times$	$\times$	$\sim$	$\sim$

Table 1: Asymptotic expansion coefficients in $m_1(L/a)$, for $s = \pm 1, 0$.

the errors. In particular we confirm the known result for the case $s = 0$ [15], and the universal coefficients r_0 and s_0 agree for all choices of the parameter s . As expected, s_1 is found to be compatible with zero. Applying formula (4.13) with $\rho = 1$ we obtain

$$c_t^{(1)} = \frac{r_1}{2} \left(\frac{2}{2+s} \right)^2 = \begin{cases} 0.0274(1) & \text{if } s = 1, \\ -0.08895(15) & \text{if } s = 0, \\ -0.4636(6) & \text{if } s = -1, \end{cases} \quad (4.14)$$

The result for $s = 0$ agrees within errors with the more precise value $c_t^{(1)} = -0.08900(5)$ quoted in ref. [15]. Note that c_t is the coefficient of a local counterterm and thus cannot depend on global space-time properties such as the aspect ratio ρ . As a further check we also produced some data with $\rho = 1/2$. Within the numerical accuracy, the coefficient r_1 is found to be proportional to $1/\rho$, which cancels the explicit factor ρ in Eq. (4.13), and renders $c_t^{(1)}$ ρ -independent, as expected.

4.3 Residual cutoff effects in the step scaling function

In the previous subsection we have removed the $O(a)$ boundary lattice artefacts at one-loop order in perturbation theory. Nevertheless, higher order lattice artefacts are still present. We quantify these by studying the relative deviation of the lattice step scaling function, $\Sigma(u, a/L)$ from its continuum counterpart, $\sigma(u)$ [cf. Eq. (2.21)],

$$\delta(u, a/L) \equiv \frac{\Sigma(u, a/L) - \sigma(u)}{\sigma(u)} = \delta_1(a/L)u + \delta_2(a/L)u^2 + O(u^3). \quad (4.15)$$

Defining

$$\overline{m}_1(L/a) = m_1(L/a) - c_t^{(1)} \left. \frac{\partial_\eta \Gamma_{0; c_t}[B]}{\partial_\eta \Gamma_0[B]} \right|_{\eta=0}, \quad (4.16)$$

a one-loop computation yields

$$\delta_1(a/L) = \overline{m}_1(2L/a) - \overline{m}_1(L/a) - 2b_0 \ln(2), \quad (4.17)$$

which we here use to monitor higher order lattice artefacts. In practice, $\delta_1(a/L)$ can also be used to cancel *all* lattice artefacts to $O(u^2)$ in non-perturbative estimates of the step-scaling function. However, this implies that the c_t -counterterm must be evaluated exactly and not just in its asymptotic form as in Eq. (4.12). Using the field equation (3.31), the resulting formulae are surprisingly simple, and one obtains,

$$\frac{\partial_\eta \Gamma_{0;c_t}[B]}{\partial_\eta \Gamma_0[B]} = \frac{2}{c_t^{(0)}} \frac{a}{L} \left[\left(1 + \frac{s}{2} - \rho \frac{L}{2a} \right) \partial_\eta \varphi + \frac{L}{2a} \right] = \frac{a}{L} \frac{(2+s)^2}{2\rho} + O(a^5). \quad (4.18)$$

In the case $s = 0$ one has $\partial_\eta \varphi \equiv 1/\rho$ from Eq. (3.33) and the exact c_t -counterterm is thus found to coincide with its asymptotic a/L -term. For $s = \pm 1$ the numerical difference is very small, due to the mild cutoff effects in φ , Eq. (3.42), and hence in $\partial_\eta \varphi$. In Table 2 and in Fig. 2, we show two sets of data for $\delta_1(a/L)$, obtained by either setting $c_t^{(1)} = 0$ or by choosing the correct value for $c_t^{(1)}$ from Eq. (4.14). Asymptotically one expects $\delta_1(a/L)$ to approach zero with a rate $\propto a/L$ and $\propto (a/L)^2$, respectively. This is indeed observed in all cases. We also note that the data for all choices of the parameter s seem to behave similarly, i.e. there is no clearly superior choice.

	$\delta_1(a/L) _{c_t^{(1)}=0}$			$\delta_1(a/L)$		
L/a	$s = 1$	$s = 0$	$s = -1$	$s = 1$	$s = 0$	$s = -1$
4	-0.02036	0.01192	0.01575	-0.00489	-0.01033	-0.01302
6	-0.01224	0.01089	0.01519	-0.00195	-0.00394	-0.00409
8	-0.00876	0.00918	0.01252	-0.00105	-0.00194	-0.00196
10	-0.00686	0.00773	0.01041	-0.00069	-0.00117	-0.00117
12	-0.00564	0.00663	0.00887	-0.00050	-0.00079	-0.00079
14	-0.00479	0.00579	0.00771	-0.00039	-0.00057	-0.00057
16	-0.00416	0.00513	0.00682	-0.00031	-0.00043	-0.00043
18	-0.00368	0.00461	0.00610	-0.00025	-0.00034	-0.00033
20	-0.00329	0.00418	0.00553	-0.00021	-0.00027	-0.00027
22	-0.00298	0.00382	0.00505	-0.00018	-0.00022	-0.00022
24	-0.00272	0.00352	0.00464	-0.00015	-0.00019	-0.00018
26	-0.00250	0.00326	0.00430	-0.00013	-0.00016	-0.00016
28	-0.00232	0.00304	0.00400	-0.00012	-0.00013	-0.00013
30	-0.00216	0.00285	0.00375	-0.00010	-0.00012	-0.00012
32	-0.00202	0.00268	0.00352	-0.00009	-0.00010	-0.00010

Table 2: One-loop coefficients $\delta_1(a/L)$ for $s = 1, 0, -1$, without and with the one-loop counterterm $\propto c_t^{(1)}$. For $s = \pm 1$ we have used Eq. (4.14), for $s = 0$ we set $c_t^{(1)} = -0.089$ [15].

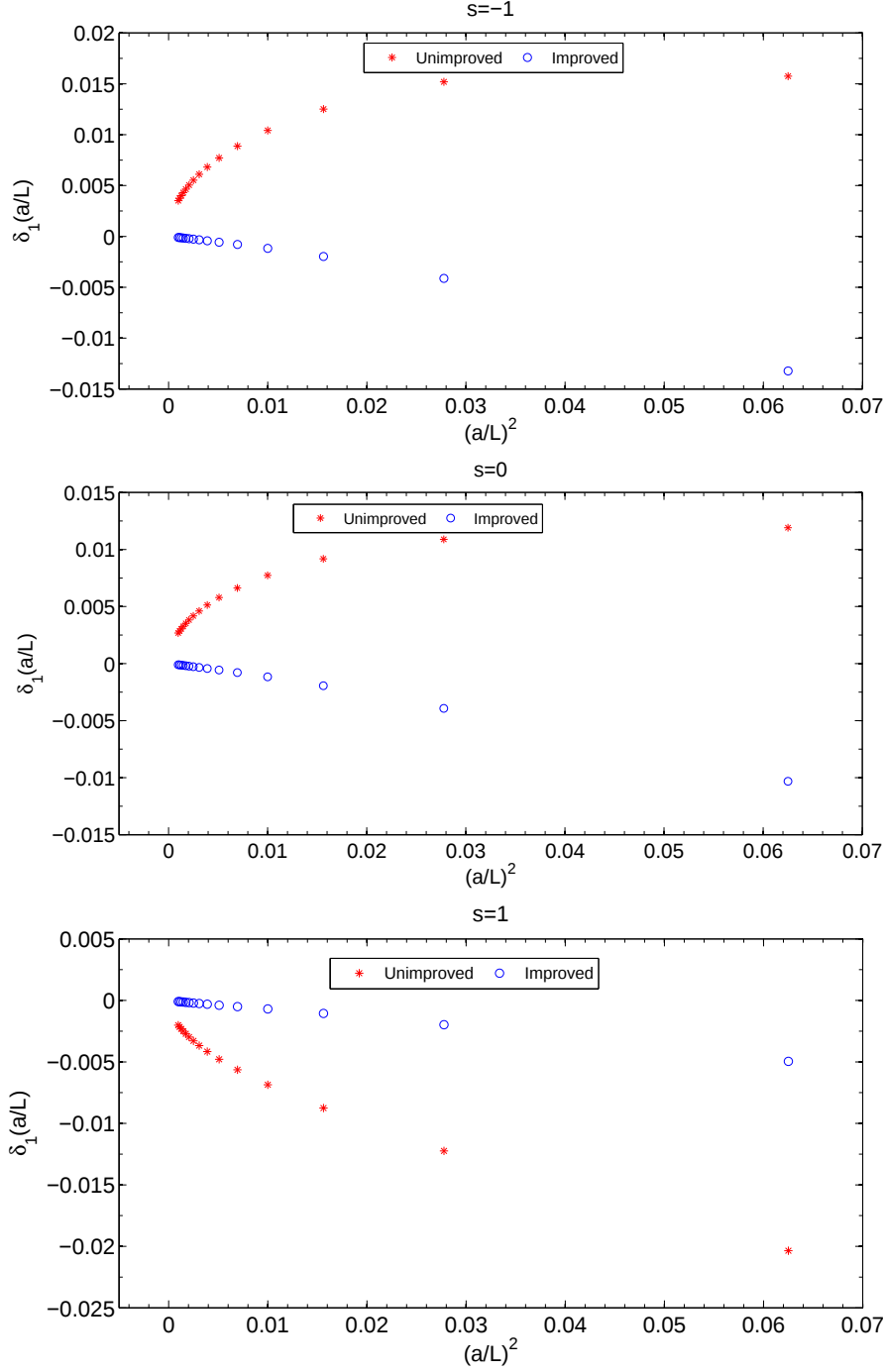


Figure 2: Discretisation effects in the step-scaling function for $s = -1, 0, 1$ from top to bottom, respectively. Stars show the result obtained before cancellation of the $O(a)$ part by the pure gauge boundary counterterm, $c_t^{(1)}$ and circles the results after the cancellation.

4.4 Residual cutoff effects in $\bar{v}(L)$

At fixed $u = \bar{g}^2(L)$ one may also study the lattice artefacts in the observable $\bar{v}(L)$ introduced in Section 2. On the lattice we define,

$$\Omega(u, a/L) = \bar{v}(L)|_{u=\bar{g}^2(L)} = \Omega_1(a/L) + \Omega_2(a/L)u + \mathcal{O}(u^2), \quad (4.19)$$

where $\Omega(u, a/L)$ converges to the universal function $\omega(u)$, Eq. (2.17) in the continuum limit. In order to compute the one-loop coefficient $\Omega_1(a/L)$ it is convenient to consider a finite difference in ν -values, rather than using Eq. (2.15). Both are equivalent since the ν -dependence is completely explicit in Eq. (2.14). Hence,

$$\bar{v}(L) = \frac{1}{(\nu_2 - \nu_1)\partial_\eta \Gamma_0[B]|_{\eta=0}} \left\{ \frac{\partial \Gamma[B]}{\partial \eta} \Big|_{\eta=0, \nu=\nu_1} - \frac{\partial \Gamma[B]}{\partial \eta} \Big|_{\eta=0, \nu=\nu_2} \right\}. \quad (4.20)$$

Choosing $\nu_1 = 0$ and $\nu_2 = 1$ one obtains

$$\Omega_1(a/L) = m_1^{\nu=1}(L/a) - m_1(L/a), \quad (4.21)$$

with the one-loop coefficient [cf. Eq. (4.9)],

$$m_1^{\nu=1} = [h_0 - \tfrac{1}{2}h_1]_{\nu=1}. \quad (4.22)$$

Note that the c_t -counterterm is ν -independent and does therefore not contribute in Eq. (4.21). We have computed $m_1^{\nu=1}$ for even lattice sizes up to $L/a = 64$. By combining with the $\nu = 0$ data we have checked that $\Omega_1(a/L)$ converges to the universal continuum value, ω_1 of Eq. (2.20) for all cases $s = \pm 1, 0$.

To study the cutoff effects we follow ref. [15] and define,

$$\epsilon(u, a/L) \equiv \frac{\Omega(u, a/L) - \omega(u)}{\omega(u)} = \epsilon_1(a/L) + \epsilon_2(a/L)u + \mathcal{O}(u^2). \quad (4.23)$$

At one-loop order we obtain

$$\epsilon_1(a/L) = \Omega(a/L)/\omega_1 - 1, \quad (4.24)$$

and we collect our numerical results in table 3. The continuum limit is always approached with a rate of $\mathcal{O}(a^2)$, as expected. While the cutoff effects in Ω_1 are sizeable, we do not observe a striking difference between the cases $s = 0, \pm 1$.

5 A non-perturbative check

In order to check our set-up non perturbatively, we have carried out numerical simulation to compute the step scaling function and the observable $\bar{v}$. To generate a representative ensemble of gauge configurations, we used an algorithm consisting in a combination of local heat bath sweeps (HB) with a number of over-relaxation sweeps (OR). Measurements are performed for every cycle, where a cycle is defined by,

$$1 \text{ cycle} = 1 \text{ HB} + N_{\text{OR}} \times \text{OR}, \quad (5.1)$$

L/a	$s = -1$	$s = 0$	$s = 1$
4	0.21001	0.18806	0.10209
6	0.06874	0.06773	0.04449
8	0.03365	0.03360	0.02419
10	0.02040	0.02039	0.01562
12	0.01380	0.01380	0.01104
14	0.00999	0.00999	0.00825
16	0.00758	0.00758	0.00641
18	0.00595	0.00595	0.00513
20	0.00480	0.00480	0.00420
22	0.00395	0.00395	0.00350
24	0.00331	0.00331	0.00297
26	0.00282	0.00282	0.00254
28	0.00243	0.00243	0.00221
30	0.00211	0.00212	0.00193
32	0.00185	0.00185	0.00171

Table 3: One-loop coefficients $\epsilon_1(a/L)$ for $s = -1, 0, 1$

with $N_{\text{OR}} = L/(2a)$. To study the evolution of the running coupling, pairs of lattices with sizes L/a and $2L/a$ have been simulated. The results are shown in Table 4. In order to extract the mean value of the observables, as well as their uncertainties and their integrated autocorrelation times, we have used the procedure advocated in ref. [28].

In Table 5 we show the results for the step scaling function at fixed $u = 2.1$. Figure 3 shows the cutoff dependence of the step scaling function at $u = 2.1$ and the continuum extrapolation. The results for $s = 0$ from ref. [15] are shown for comparison.

s	β	L/a	$\bar{g}^2$	τ_{int}	$\bar{v}$	τ_{int}	stat.
+1	7.2095	6	2.0966(31)	0.64(1)	0.0579(15)	1.49(4)	4700×16
		12	2.7191(96)	0.85(2)	0.0501(24)	1.89(8)	4500×16
-1	7.1214	6	2.0929(45)	0.58(1)	0.0610(16)	0.91(2)	29700×4
		12	2.739(15)	0.64(2)	0.0470(29)	0.98(4)	4700×16
+1	7.4218	8	2.0989(37)	0.68(1)	0.0602(17)	1.69(6)	5500×16
		16	2.725(17)	0.93(4)	0.0524(37)	1.74(10)	9500×4
-1	7.3632	8	2.0968(47)	0.58(1)	0.0587(16)	0.93(2)	39700×4
		16	2.747(18)	0.59(2)	0.0557(36)	0.95(4)	16700×4
+1	7.7447	12	2.0937(44)	0.77(2)	0.0578(20)	1.90(6)	7500×6
		24	2.715(15)	0.95(3)	0.0502(34)	1.90(9)	19500×4
-1	7.6985	12	2.1017(55)	0.61(1)	0.0579(19)	0.99(2)	49700×4
		24	2.772(19)	0.67(2)	0.0452(34)	0.97(4)	29700×4

Table 4: Simulation parameters and results for $\bar{g}^2$ and $\bar{v}$, and their autocorrelation time τ_{int} .

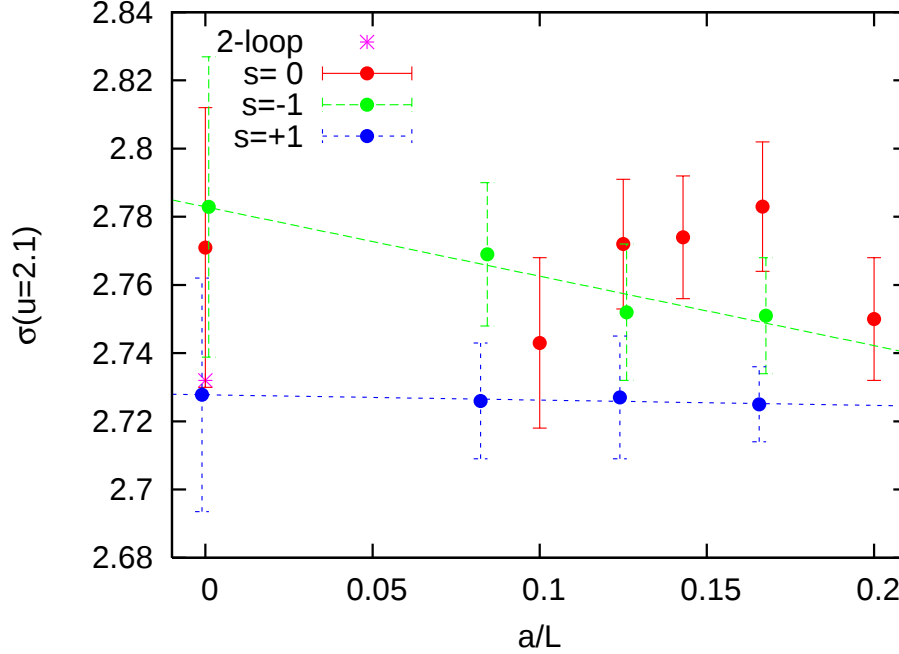


Figure 3: Cutoff dependence of the step scaling function at $u = 2.1$ and continuum extrapolation. For comparison, results for $s = 0$ taken from ref. [15] are also shown.

6 Conclusions

Motivated by applications to lattice theories with staggered fermions, we have defined an $O(a)$ modified lattice set-up for the Schrödinger functional in the $SU(3)$ gauge theory. Both perturbatively and non-perturbatively the cutoff effects in the step-scaling function for the coupling are comparable to the standard set-up. Note that our approach can be applied to the $SU(2)$ gauge theory with minor changes. However, for $SU(N)$ with $N \geq 4$ this may or may not be the case, depending on the choices made for the boundary gauge fields. More precisely, assuming that the induced lattice background field remains Abelian and spatially constant, one may need to solve coupled equations in two or more variables replacing the single equation for φ , Eq. (3.31) of the $SU(3)$ theory.

To extend this framework to four-flavour QCD and other QCD-like theories with staggered fermions, one needs to discuss $O(a)$ boundary improvement with staggered fermions [13,14]. While our motivation originates in applications using staggered fermions, we note that there are other potential applications: for instance, the SF with Wilson or Ginsparg-Wilson fermions and chirally rotated boundary conditions is, for technical convenience, constructed with an $O(a)$ offset in the orbifold construction [30,31]. This entails tree-level $O(a)$ artefacts in the fermionic propagator which could be avoided by keeping T'/L fixed when taking the continuum limit, with $T' = T \pm a$. In any case, the new framework increases the flexibility for applications of the SF scheme. Furthermore, it may help to improve control over the continuum limit, e.g. by performing constrained continuum extrapolations of data for step-scaling functions, computed at

L/a	s	$\sigma(u = 2.1)$
6	+1	2.725(11)
6	-1	2.751(17)
8	+1	2.727(18)
8	-1	2.752(21)
12	+1	2.726(17)
12	-1	2.769(21)
cont.	+1	2.728(35)
cont.	-1	2.783(44)

Table 5: Continuum extrapolated results for the step scaling function at $u = 2.1$. Central values and error are corrected by following the strategy in section 3.1 of ref. [29].

different values of the parameter s . This has already been attempted with staggered fermions [11, 12] and it can be applied more generally.

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A Raw one-loop data

L/a	$s = 1$	$s = 0$	$s = -1$
4	0.59867564635006385	0.52976131887602069	0.51922066331094546
6	0.64113765437070799	0.59321232599981455	0.58442701843014381
8	0.67488327354469054	0.63824441829314597	0.63153838271523941
10	0.70238903864308802	0.67280038634701944	0.66742121983892173
12	0.72546473348301643	0.70067317431899355	0.69618664881505825
14	0.74530462655573632	0.72398165609402260	0.72013453722120221
16	0.7626933877455524	0.74399271936483262	0.74062578372376441
18	0.77816541775427566	0.76151561542170611	0.75852242009405113
20	0.79209901867921951	0.77709645174594405	0.77440237357962767
22	0.80477118528362614	0.79112035275707051	0.78867107103739184
24	0.81639058776392414	0.80386875084304289	0.80162350146808351
26	0.82711823835863092	0.81555339356121976	0.81348080743360567
28	0.83708093056087357	0.82633751751530950	0.82441294090339149
30	0.84638026935694360	0.83634957239642928	0.83455327855159342
32	0.85509891481710033	0.84569242491756803	0.84400838361422786
34	0.86330500808698590	0.85444971446735487	0.85286472295855835
36	0.87105537841668160	0.86269035439316518	0.86119340950763814
38	0.87839791234295844	0.87047179120264344	0.86905362653451155
40	0.88537333426399287	0.87784241080234770	0.87649514951940602
42	0.89201656536325291	0.88484334593899240	0.88356023620527862
44	0.89835777515201167	0.89150985494698484	0.89028506544613721
46	0.90442320537524014	0.89787238814607281	0.89670084803647420
48	0.91023582290682148	0.90395742302994047	0.90283469523001835
50	0.91581584250088787	0.90978812583979161	0.90871030564770146
52	0.92118114931205926	0.91538488106299742	0.91434851426796011
54	0.92634764338015540	0.92076571925410400	0.91976773540748381
56	0.93132952274785759	0.92594666572356148	0.92498432332375374
58	0.93613951787157274	0.93094202701724371	0.93001286814371605
60	0.94078908704027068	0.93576462803843164	0.93486644054503752
62	0.94528858033171669	0.94042600966826691	0.93955679547364682
64	0.94964737799172085	0.94493659452353015	0.94409454285563946

Table 6: The one-loop coefficient, $m_1(L/a)$, Eq. (4.8) for $s = 1, 0, -1$. By comparing results of two independent calculations we estimate that the number of significant digits decreases due to rounding errors from 15 for $L/a = 4$ to about 12 for $L/a = 64$.

L/a	$s = 1$	$s = 0$	$s = -1$
5	0.62117136258700821	0.56468083125839683	0.55461713132090261
7	0.65893111142441375	0.61737811787009622	0.60974739393470162
9	0.68928647150162301	0.65654153428089878	0.65057003087364097
11	0.71439398959413626	0.68741301652316919	0.68252028857956904
13	0.73573276395961912	0.71280479111934452	0.70866242179288317
15	0.75426748654695955	0.73434096296455847	0.73074988732724165
17	0.77064247215528033	0.75302638176979129	0.74985728431314708
19	0.78530529883645214	0.76952176876897567	0.76668599155622038
21	0.79857842470262715	0.78428347860819714	0.78171762080518526
23	0.81070148601313597	0.79763941632436668	0.79529658268786343
25	0.82185727793917046	0.80983289063631291	0.80767742403345886
27	0.83218834749448024	0.82104930186717609	0.81905346010774183
29	0.84180796784671203	0.83143311025949667	0.82957488596710694
31	0.85080762207365805	0.84109903085829275	0.83936067325760364
33	0.85926224466335029	0.85013965596714345	0.84850663994188621
35	0.86723397937992463	0.85863078810432712	0.85709107745685024
37	0.87477492945292666	0.86663526032990589	0.86517876996699599
39	0.88192920731676446	0.87420573028207099	0.87282392619177697
41	0.88873448731299464	0.88138676139487858	0.88007235812526203
43	0.89522319912792745	0.88821639863152864	0.88696312708410143
45	0.90142345720374637	0.89472737905126752	0.89352980585123832
47	0.90735979318226442	0.90094807414573837	0.89980145942895982
49	0.91305373939615786	0.90690323216425240	0.90580341637673730
51	0.91852429830862484	0.91261456924592534	0.91155788213294810
53	0.92378832362922261	0.91810124483365024	0.91708443159609367
55	0.92886083231152201	0.92338024750431470	0.92240040837837180
57	0.93375526193982340	0.92846671072289073	0.92752125115677514
59	0.93848368458072277	0.93337417324448625	0.93246076251996867
61	0.94305698564346882	0.93811479540720059	0.93723133204075556
63	0.94748501439735390	0.94269953998217965	0.94184412261958892
65	0.95177671136930530	0.94713832432409256	0.94630922711111939

Table 7: Same as table 6 for lattices with odd L/a .