Normalization of the gradient-flow coupling in LQCD

Martin Lüscher January 2014, revised January 2016

1. Introduction

The Yang–Mills gradient flow provides interesting new opportunities for step-scaling studies of QCD and related theories [1,2]. Step scaling in lattice QCD requires a renormalized gauge coupling to be introduced that runs with the size of the lattice [3]. The couplings based on the gradient flow considered so far [4–6] are essentially all the same, but were proposed to be used together with various boundary conditions for the gauge and quark fields (periodic, Schrödinger functional (SF) and so-called twisted periodic boundary conditions).

In this note, SF boundary conditions are chosen, as in ref. [5], or open-SF boundary conditions, which may allow the infamous topology-freezing problem in numerical simulations to be bypassed [7,8]. The goal in both cases is to analytically compute the gradient-flow coupling to leading order of weak-coupling perturbation theory.

2. Lattice theory

The quark fields contribute to the gradient-flow coupling only at one-loop order of perturbation theory. Their presence is therefore ignored from the beginning and only the pure-gauge part of the theory is specified. For simplicity, the lattice spacing is set to unity and the gauge group is taken to be $\mathrm{SU}(N)$.

2.1 Lattice geometry and gauge field

The theory is set up on a hypercubic lattice of points x with Cartesian coordinates

$$
\begin{aligned}
&(x_0, x_1, x_2, x_3), \qquad x_\mu \in \mathbb{Z}, \\
&0 \leq x_0 \leq T, \qquad 0 \leq x_k < L \quad (k = 1, 2, 3),
\end{aligned}
\tag{2.1}
$$

where T and L are the lattice sizes in the time and space directions. In the space directions, periodic boundary conditions are imposed, i.e. the points x and $x+\hat{k}$ mod L (where $\hat{\mu}$ is the unit vector in direction μ) are considered to be nearest neighbours. The lattice is not periodically closed in time and instead has two boundaries, one at time 0 and the other at time T.

As usual, the gauge field is an assignment of matrices $U(x, \mu) \in \mathrm{SU}(3)$ to the links (x, μ) on the lattice, where x runs over all points in the range (2.1), $\mu = 0, \ldots, 3$ if $x_0 < T$ and $\mu = 1, 2, 3$ if $x_0 = T$. The active and static link variables $U(x, \mu)$ are, respectively, those integrated over in the QCD functional integral and the ones that have fixed values (see subsects. 2.3 and 2.4).

2.2 Gauge action

Let $\mathcal{S}_0$ and $\mathcal{S}_1$ be the sets of oriented plaquette and double-plaquette loops on the lattice (see fig. 1). The gauge actions considered are of the form

$$
S_{\mathrm{G}} = \frac{1}{g_0^2} \sum_{k=0}^{1} c_k \sum_{\mathcal{C} \in \mathcal{S}_k} w_k(\mathcal{C}) \, \mathrm{tr}\{1 - U(\mathcal{C})\},
\tag{2.2}
$$

where $U(\mathcal{C})$ denotes the ordered product of the link variables around the loop $\mathcal{C}$. The weight factor $w_k(\mathcal{C})$ depends on the choice of boundary conditions and differs from unity only near the boundaries of the lattice (see below).

In order to ensure the correct normalization of the bare coupling g_0, the coefficients c_k must be such that

$$
c_0 + 8c_1 = 1.
\tag{2.3}
$$

Moreover, the constraint $c_0 > 0$ is imposed as otherwise there may be fields with lowest action which are not locally pure gauge configurations [9].

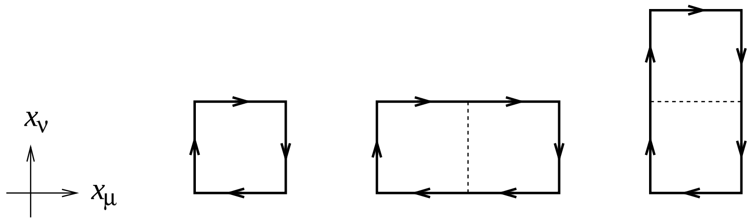

Fig. 1. Plaquette and planar double-plaquette loops in a (μ,ν)–plane of the lattice. The sums in eq. (2.2) run over all these loops, where loops differing by their orientation are considered to be different.

2.2 Schrödinger functional boundary conditions

The spatial link variables residing on the boundaries at time 0 and T are all static in this case and are taken to be of the form [10]

$$U(x,k)=\begin{cases}\exp\{C_k\} & \text{if } x_0=0,\\ \exp\{C'_k\} & \text{if } x_0=T,\end{cases} \tag{2.4}$$

$$C_k=\frac{i}{N_k}\mathrm{diag}\,(\phi_1,\ldots,\phi_N),\qquad C'_k=\frac{i}{N_k}\mathrm{diag}\,(\phi'_1,\ldots,\phi'_N), \tag{2.5}$$

for $k=1,2,3$. Subject to the constraints

$$\sum_{j=1}^{N}\phi_j=\sum_{j=1}^{N}\phi'_j=0, \tag{2.6}$$

the angles ϕ_j and ϕ'_j can be chosen arbitrarily.

For the form of the gauge action near the boundaries of the lattice, two choices, referred to as A and B, were proposed by Aoki, Frezzotti and Weisz [11]. Here another choice is made, which combines the advantages of choice A and B [12].

The sets of loops $\mathcal{C}$ summed over in the gauge action eq. (2.2) includes all loops that are fully contained in the range $0\le x_0\le T$ of time. In addition, the time-like double-plaquette loops that cross the boundaries of the lattice as shown in fig. 2 are included in the sum, the associated Wilson loops $U(\mathcal{C})$ being given by the square of the plaquette loops on the inner side of the boundary.

In view of the boundary conditions (2.4),(2.5), the space-like loops at time 0 and T do not contribute to the gauge action and their weights $w_k(\mathcal{C})$ can therefore be

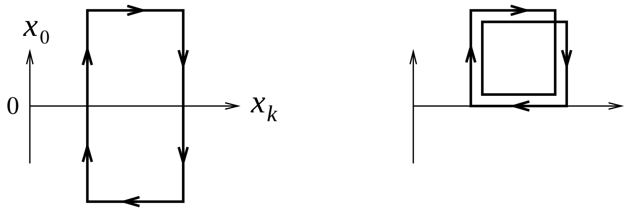

Fig. 2. At the boundaries of the lattice where SF boundary conditions are imposed, the double-plaquette loops $\mathcal{C}$ that cross the boundary are included in the gauge action (2.2), with weight $w_1(\mathcal{C}) = 1/2$ and $U(\mathcal{C})$ set to the product of the link variables around the loop shown on the right, which winds twice around the inner plaquette.

left unspecified. For the plaquette loops, the weights are then

$$w_0(\mathcal{C}) = \begin{cases} c_{\mathrm{G}} & \text{if } \mathcal{C} \text{ has exactly one link on a boundary,} \\ 1 & \text{otherwise,} \end{cases} \tag{2.7}$$

while for the planar double-plaquette loops they are given by

$$w_1(\mathcal{C}) = \begin{cases} \frac{1}{2} & \text{if } \mathcal{C} \text{ crosses a boundary as in fig. 2,} \\ 1 & \text{otherwise.} \end{cases} \tag{2.8}$$

Tree-level $\mathrm{O}(a)$-improvement is then guaranteed if $c_{\mathrm{G}} = 1$.

2.3 Open-SF boundary conditions

In this case, SF boundary conditions are imposed at time T only. The static link variables are then

$$U(x,k)|_{x_0=T} = \exp\{C'_k\}, \qquad C'_k = \frac{i}{N_k}\mathrm{diag}\,(\phi'_1,\ldots,\phi'_N), \tag{2.9}$$

while all other field variables are active. This amounts to imposing open boundary conditions at time 0 [7].

When these boundary conditions are chosen, the weights $w_k(\mathcal{C})$ are given by eqs. (2.7),(2.8), with c_{G} replaced by c'_{G}, for loops $\mathcal{C}$ near $x_0 = T$. At time $x_0 = 0$, the weights of the spatial plaquette and double-plaquette loops are instead

$$w_k(\mathcal{C}) = \tfrac{1}{2}c_{\mathrm{G}}, \tag{2.10}$$

all other loops having weight $w_k(\mathcal{C}) = 1$. Tree-level $\mathrm{O}(a)$-improvement is then again guaranteed if $c_{\mathrm{G}} = c'_{\mathrm{G}} = 1$, but at higher orders of perturbation theory improvement probably requires the coefficients c_{G} and c'_{G} to be different.

3. Expansion of the action

From now on the improvement coefficients c_{G} and c'_{G} are set to 1 and the boundary values C_k and C'_k to zero. In perturbation theory, the link variables are represented by a gauge potential $A_\mu(x)$ through

$$U(x,\mu) = \exp\{g_0 A_\mu(x)\}, \qquad A_\mu(x) = A_\mu^a(x) T^a, \tag{3.1}$$

where T^a, $a = 1, \ldots, N^2-1$, is a basis of orthonormal anti-hermitian generators of $\mathrm{SU}(N)$. The associated field tensor

$$F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) \tag{3.2}$$

is defined as in the continuum theory, with ∂_μ being the forward difference operator in direction μ.

3.1 Fourier representation

Both SF and open-SF boundary conditions go along with a natural Fourier representation of the gauge potential. The momentum space is however not the same in the two cases. While the space-like momentum components

$$p_k \in \left\{ n\frac{2\pi}{L} \,\middle|\, n = 0, 1, \ldots, L-1 \right\}, \quad k = 1, 2, 3, \tag{3.3}$$

run over the same set of values, the time component p_0 does not. Moreover, the Fourier representation looks slightly different.

(a) *SF boundary conditions.* In this case

$$p_0 \in \left\{ n\frac{\pi}{T} \,\middle|\, n = 0, 1, \ldots, T-1 \right\} \tag{3.4}$$

and the gauge potential is represented by

$$A_0(x) = \frac{2}{TL^3} \sum_p{}' \cos(p_0 x_0 + \tfrac{1}{2} p_0) \mathrm{e}^{i\boldsymbol{px}} \tilde{A}_0(p), \tag{3.5}$$

$$A_k(x) = \frac{2i}{TL^3} \sum_p{}' \sin(p_0 x_0) \mathrm{e}^{i\boldsymbol{px} + \frac{i}{2} p_k} \tilde{A}_k(p), \qquad \tilde{A}_k(p)\Big|_{p_0=0} = 0. \tag{3.6}$$

The primed momentum sums run over all values of the four-momentum $p = (p_0, \boldsymbol{p})$, the terms at $p_0 = 0$ being counted with weight 1/2.

Using the orthogonality relations

$$\sum_{x_0=0}^{T-1} \cos(p_0 x_0 + \tfrac{1}{2}p_0)\cos(q_0 x_0 + \tfrac{1}{2}q_0) = \tfrac{1}{2}T\delta_{p_0 q_0}(1 + \delta_{p_0 0}), \tag{3.7}$$

$$\sum_{x_0=1}^{T-1} \sin(p_0 x_0)\sin(q_0 x_0) = \tfrac{1}{2}T\delta_{p_0 q_0}(1 - \delta_{p_0 0}), \tag{3.8}$$

which hold for any momenta p_0, q_0 in the set (3.4), the representation (3.5),(3.6) is easily shown to hold when the gauge potential satisfies the boundary conditions, i.e. when $A_k(x)$ vanishes at $x_0 = 0$ and $x_0 = T$.

The Fourier representation of the field tensor derives from the one of the gauge potential and is given by

$$F_{0k}(x) = \frac{2i}{TL^3}\sum_p{}' \cos(p_0 x_0 + \tfrac{1}{2}p_0)\mathrm{e}^{i\boldsymbol{px}+\frac{i}{2}p_k}\big(\hat{p}_0\tilde{A}_k(p) - \hat{p}_k\tilde{A}_0(p)\big), \tag{3.9}$$

$$F_{kl}(x) = -\frac{2}{TL^3}\sum_p{}' \sin(p_0 x_0)\mathrm{e}^{i\boldsymbol{px}+\frac{i}{2}(p_k+p_l)}\big(\hat{p}_k\tilde{A}_l(p) - \hat{p}_l\tilde{A}_k(p)\big), \tag{3.10}$$

where

$$\hat{p}_\mu = 2\sin(\tfrac{1}{2}p_\mu) \tag{3.11}$$

as usual.

(b) *Open-SF boundary conditions.* In this case

$$p_0 \in \Big\{(n + \tfrac{1}{2})\frac{\pi}{T} \;\Big|\; n = 0, 1, \ldots, T-1\Big\} \tag{3.12}$$

and the gauge potential is represented by

$$A_0(x) = \frac{2i}{TL^3}\sum_p \sin(p_0 x_0 + \tfrac{1}{2}p_0)\mathrm{e}^{i\boldsymbol{px}}\tilde{A}_0(p), \tag{3.13}$$

$$A_k(x) = \frac{2}{TL^3}\sum_p \cos(p_0 x_0)\mathrm{e}^{i\boldsymbol{px}+\frac{i}{2}p_k}\tilde{A}_k(p). \tag{3.14}$$

The existence and uniqueness of the representation again follows from the orthogonality relations

$$\sum_{x_0=0}^{T-1} \sin(p_0x_0+\tfrac{1}{2}p_0)\sin(q_0x_0+\tfrac{1}{2}q_0)=\tfrac{1}{2}T\delta_{p_0q_0}, \tag{3.15}$$

$$\sum_{x_0=0}^{T}{}' \cos(p_0x_0)\cos(q_0x_0)=\tfrac{1}{2}T\delta_{p_0q_0}, \tag{3.16}$$

where the primed summation symbol indicates that the terms at $x_0=0$ and $x_0=T$ are given the weight 1/2. The Fourier representation of the field tensor is given by

$$F_{0k}(x)=-\frac{2}{TL^3}\sum_p \sin(p_0x_0+\tfrac{1}{2}p_0)\mathrm{e}^{i\boldsymbol{p}\boldsymbol{x}+\frac{i}{2}p_k}\bigl(\hat{p}_0\tilde{A}_k(p)-\hat{p}_k\tilde{A}_0(p)\bigr), \tag{3.17}$$

$$F_{kl}(x)=\frac{2i}{TL^3}\sum_p \cos(p_0x_0)\mathrm{e}^{i\boldsymbol{p}\boldsymbol{x}+\frac{i}{2}(p_k+p_l)}\bigl(\hat{p}_k\tilde{A}_l(p)-\hat{p}_l\tilde{A}_k(p)\bigr), \tag{3.18}$$

for these boundary conditions.

3.2 Quadratic part of the action

In the following, the gauge potential $A_\mu(x)$ is considered to be defined at all points x with integer coordinates through its Fourier representation. In the vicinity of the boundary at $x_0=0$, for example, this amounts to setting

$$A_0(\tilde{x}-\hat{0})=sA_0(x), \qquad \tilde{x}=(-x_0,\boldsymbol{x}), \tag{3.19}$$

$$A_k(\tilde{x})=-sA_k(x), \quad k=1,2,3, \tag{3.20}$$

where $s=+1$ ($s=-1$) when SF (open-SF) boundary conditions are imposed. The analogous rules hold, with $s=+1$, at $x_0=T$. In particular,

$$F_{0k}(x)=sF_{0k}(x-\hat{0}) \quad \text{at} \quad x_0=0,T. \tag{3.21}$$

Clearly, the extension of the fields beyond the range $0\leq x_0\leq T$ of time is purely a matter of notational convenience and no additional degrees of freedom are introduced.

For both choices of boundary conditions, the gauge action is now given by

$$S_{\mathrm{G}} = \tfrac{1}{2}c_0 \sum_{\boldsymbol{x}} \Bigg\{ \sum_{x_0=0}^{T-1} \big[F_{0k}^a(x)\big]^2 + \sum_{x_0=0}^{T}{}' \tfrac{1}{2}\big[F_{kl}^a(x)\big]^2 \Bigg\}$$

$$+ \tfrac{1}{2}c_1 \sum_{\boldsymbol{x}} \Bigg\{ \sum_{x_0=0}^{T}{}' \big[F_{0k}^a(x) + F_{0k}^a(x-\hat{0})\big]^2 + \sum_{x_0=0}^{T-1} \big[F_{k0}^a(x) + F_{k0}^a(x-\hat{k})\big]^2$$

$$+ \sum_{x_0=0}^{T}{}' \big[F_{kl}^a(x) + F_{kl}^a(x-\hat{k})\big]^2 \Bigg\} + \mathrm{O}(g_0) \qquad (3.22)$$

(repeated indices group and space indices are to be summed over in this formula). In terms of the Fourier components of the gauge field, this expression may be written in the form†

$$S_{\mathrm{G}} = \frac{1}{2TL^3} \sum_p{}' \sum_{\mu,\nu} \big(1 - c_1(\hat{p}_\mu^2 + \hat{p}_\nu^2)\big) \big|\hat{p}_\mu \tilde{A}_\nu^a(p) - \hat{p}_\nu \tilde{A}_\mu^a(p)\big|^2 + \mathrm{O}(g_0), \qquad (3.23)$$

or, equivalently, as

$$S_{\mathrm{G}} = \frac{1}{TL^3} \sum_p{}' \sum_{\mu,\nu} \tilde{A}_\mu^a(p)^* \Delta_{\mu\nu}(p) \tilde{A}_\nu^a(p) + \mathrm{O}(g_0), \qquad (3.24)$$

$$\Delta_{\mu\nu}(p) = \delta_{\mu\nu}\hat{p}^2 - \hat{p}_\mu\hat{p}_\nu - c_1 \left\{ \delta_{\mu\nu} \left[\hat{p}^4 + \tfrac{1}{2}\hat{p}^2 \left(\hat{p}_\mu^2 + \hat{p}_\nu^2\right)\right] - \hat{p}_\mu^3\hat{p}_\nu - \hat{p}_\mu\hat{p}_\nu^3 \right\}, \quad (3.25)$$

$$\hat{p}^2 = \sum_\mu \hat{p}_\mu^2, \quad \hat{p}^4 = \sum_\mu \hat{p}_\mu^4. \qquad (3.26)$$

Through the Fourier transformation, the diagonalization of the leading-order action is thus achieved.

† Note that primed and ordinary momentum sums are the same in the case of open-SF boundary conditions, since $p_0 = 0$ is excluded from the momentum spectrum (3.12).

4. Gauge fixing

With respect to the discussion of the lattice Schrödinger functional in ref. [10], the gauge modes are here treated slightly differently so as to ensure that the leading-order part of the gauge-fixed action is diagonal in momentum space. The gauge-fixing is sensitive to the choice of boundary conditions. Open-SF and SF boundary conditions are therefore considered separately and in this order, since the latter give rise to some additional complications.

4.1 Open-SF boundary conditions

Infinitesimal gauge transformations are in this case described by fields

$$\omega(x) \in \mathfrak{su}(N), \quad 0 \le x_0 \le T, \tag{4.1}$$

satisfying the boundary condition

$$\omega(x)\big|_{x_0=T} = 0. \tag{4.2}$$

The momentum-space representation of these fields is of the form

$$\omega(x) = \frac{2}{TL^3} \sum_p \cos(p_0 x_0) \mathrm{e}^{i\boldsymbol{p}\boldsymbol{x}} \tilde{\omega}(p), \tag{4.3}$$

where the sum runs over the same set of momenta as in the case of the gauge potential [cf. eqs. (3.12)–(3.14)]. For any two fields $\omega(x)$ and $\nu(x)$,

$$(\omega, \nu) = {\sum_{x_0=0}^{T}}' \sum_{\boldsymbol{x}} \omega^a(x)\nu^a(x) = \frac{2}{TL^3} \sum_p \tilde{\omega}(p)^* \tilde{\nu}(p) \tag{4.4}$$

is then a natural choice of scalar product.

To leading order in the gauge coupling, an infinitesimal gauge transformation amounts to changing the gauge potential according to

$$A_\mu(x) \to A_\mu(x) + \partial_\mu \omega(x), \quad 0 \le x_0 < T. \tag{4.5}$$

In momentum space, this is equivalent to

$$\tilde{A}_\mu(p) \to \tilde{A}_\mu(p) + i\hat{p}_\mu \tilde{\omega}(p). \tag{4.6}$$

For the gauge fixing term, a possible choice is thus

$$S_{\mathrm{gf}} = \tfrac{1}{2}\lambda_0(\eth A, \eth A), \qquad \lambda_0 > 0, \tag{4.7}$$

$$(\eth A)(x) = (1 + c_1 \partial_\mu^* \partial_\mu)\partial_\mu^* A_\mu(x), \tag{4.8}$$

where ∂_μ^* denotes the backward difference operator and, as explained at the beginning of subsect. 3.2, the gauge potential $A_\mu(x)$ is assumed to be defined at all integer points x through its Fourier representation. In particular,

$$(\eth A)(x) = \frac{2i}{TL^3}\sum_p \cos(p_0 x_0)\mathrm{e}^{i\boldsymbol{px}}(\hat{p}_\mu - c_1\hat{p}_\mu^3)\tilde{A}_\mu(p), \tag{4.9}$$

so that the addition of the gauge-fixing term to the action amounts to changing its quadratic part by

$$\Delta_{\mu\nu}(p) \to \Delta_{\mu\nu}(p) + \lambda_0(\hat{p}_\mu - c_1\hat{p}_\mu^3)(\hat{p}_\nu - c_1\hat{p}_\nu^3) \tag{4.10}$$

[cf. eqs. (3.23)–(3.25); note that $1 - c_1\hat{p}_\mu^2 > 1/2$ for all momenta p and directions μ in view of the constraint (2.3) and $c_0 > 0$]. To leading order in the gauge coupling, the associated Faddeev–Popov operator is diagonal in momentum space too and equal to $\hat{p}^2 - c_1\hat{p}^4$.

4.2 SF boundary conditions

The infinitesimal gauge transformations (4.1) must in this case satisfy the boundary conditions

$$\partial_k\omega(x)|_{x_0=0} = 0, \quad k = 1, 2, 3, \tag{4.11}$$

$$\omega(x)|_{x_0=T} = 0, \tag{4.12}$$

i.e. $\omega(x)$ must be constant at time $x_0 = 0$. Any such field can be represented by

$$\omega(x) = (1 - x_0/T)\omega(0) + \hat{\omega}(x), \tag{4.13}$$

$$\hat{\omega}(x) = \frac{2i}{TL^3}{\sum_p}' \sin(p_0 x_0)\mathrm{e}^{i\boldsymbol{px}}\tilde{\omega}(p), \quad \tilde{\omega}(p)|_{p_0=0} = 0, \tag{4.14}$$

where p_0 runs over the set (3.4) of momenta. Clearly, the scalar product

$$(\omega,\nu) = TL^3\omega^a(0)\nu^a(0) + \sum_{x_0=1}^{T-1}\sum_{\boldsymbol{x}}\hat{\omega}^a(x)\hat{\nu}^a(x)$$

$$= TL^3\omega^a(0)\nu^a(0) + \frac{2}{TL^3}{\sum_p}'\tilde{\omega}^a(p)^*\tilde{\nu}^a(p) \tag{4.15}$$

is positive definite and therefore an acceptable choice in what follows†.

Under infinitesimal gauge transformations, the gauge potential transforms according to eq. (4.5), as before, but in momentum space

$$\tilde{A}_\mu(p) \to \tilde{A}_\mu(p) + i\hat{p}_\mu\tilde{\omega}(p) - L^3\delta_{\mu0}\delta_{p0}\omega(0) \tag{4.16}$$

there is an extra term at $p=0$ that derives from the first term in eq. (4.13). The gauge fixing term is then again given by eq. (4.7) with

$$(\eth A)(x) = (1-x_0/T)\frac{1}{T^2L^3}\sum_{y_0=0}^{T-1}\sum_{\boldsymbol{y}}A_0(y) + (1+c_1\partial_\mu^*\partial_\mu)\partial_\mu^*A_\mu(x). \tag{4.17}$$

In momentum space, the addition of the gauge-fixing term to the action amounts to replacing

$$\Delta_{\mu\nu}(p) \to \Delta_{\mu\nu}(p) + \frac{\lambda_0}{T^2}\delta_{\mu0}\delta_{\nu0}\delta_{p0} + \lambda_0(\hat{p}_\mu - c_1\hat{p}_\mu^3)(\hat{p}_\nu - c_1\hat{p}_\nu^3) \tag{4.18}$$

in eq. (3.23).

An extra term also appears in the Faddeev–Popov ghost action

$$S_{\rm FP} = \frac{L^3}{T}\bar{c}^a(0)c^a(0) - \sum_{x_0=1}^{T-1}\sum_{\boldsymbol{x}}\hat{\bar{c}}^a(x)(1+c_1\partial_\mu^*\partial_\mu)\partial_\mu^*\partial_\mu\hat{c}^a(x) + {\rm O}(g_0). \tag{4.19}$$

The ghost fields $c(x)$ and $\bar{c}(x)$ are fermion fields but otherwise of the same kind as the infinitesimal gauge transformations, with a Fourier representation of the form

† The gauge-fixing term and the associated Faddeev–Popov ghost action depend on the choice of the scalar product in the space of infinitesimal gauge transformations. The scalar product must be real, symmetric and positive definite, but can otherwise be chosen arbitrarily. In particular, contrary to what is suggested in ref. [13], the scalar product does not need to be invariant under the (adjoint) action of the gauge group.

(4.13),(4.14). In the vicinity of the boundaries of the lattice, the latter allows the fields to be defined beyond the range $0 \leq x_0 \leq T$. This rule amounts to extending $\partial_\mu c(x)$ in exactly the same way as the gauge potential. The action of the lattice derivatives in eq. (4.19) near the boundaries is defined through the extension as usual. In particular, the ghost action

$$S_{\rm FP} = \frac{L^3}{T}\bar{c}^a(0)c^a(0) + \frac{2}{TL^3}\sum_p{}' \tilde{\bar{c}}^a(\tilde{p})(\hat{p}^2 - c_1\hat{p}^4)\tilde{c}^a(p), \qquad \tilde{p} = (p_0, -\boldsymbol{p}), \tag{4.20}$$

is diagonal in momentum space.

5. Gauge propagator

With the gauge-fixing term in place, the quadratic part of the total action is easily shown to have no zero modes. The gauge propagator is thus well-defined and can be worked out explicitly in momentum space.

5.1 Propagator in momentum space

In the case of SF boundary conditions, the spatial Fourier components $\tilde{A}_k(p)$ of the gauge field vanish at $p_0 = 0$. The gauge propagator at zero and non-zero p_0 must therefore be considered separately.

For any $p_0 \neq 0$ (and thus in all cases when open-SF boundary conditions are chosen), the inverse propagator in momentum space,

$$(D^{-1})_{\mu\nu}(p) = \Delta_{\mu\nu}(p) + \lambda_0(\hat{p}_\mu - c_1\hat{p}_\mu^3)(\hat{p}_\nu - c_1\hat{p}_\nu^3), \tag{5.1}$$

is a non-degenerate 4×4 matrix. The propagator, $D_{\mu\nu}(p)$, is hence unambiguously determined. Its dependence on the gauge parameter λ_0 can be worked out by noting that

$$\frac{\partial}{\partial\lambda_0} D_{\mu\nu} = -(Du)_\mu(Du)_\nu, \qquad u_\mu = \hat{p}_\mu - c_1\hat{p}_\mu^3, \tag{5.2}$$

$$(D^{-1}\hat{p})_\mu = \lambda_0(u\hat{p})u_\mu, \tag{5.3}$$

and thus

$$D_{\mu\nu}(p) = D_{\mu\nu}(p)|_{\lambda_0=1} + (\lambda_0^{-1} - 1)\frac{\hat{p}_\mu\hat{p}_\nu}{(u\hat{p})^2}. \tag{5.4}$$

For the non-gauge part of the propagator, a few lines of algebra quickly lead to the expression

$$D_{\mu\nu}(p)|_{\lambda_0=1} = \frac{\delta_{\mu\nu}}{r_\mu} - \frac{v_\mu v_\nu}{1+\sum_\rho v_\rho^2 r_\rho}, \tag{5.5}$$

$$r_\mu = \hat{p}^2 - c_1(\hat{p}^4 + \hat{p}^2\hat{p}_\mu^2), \qquad v_\mu = c_1\hat{p}_\mu^3/r_\mu. \tag{5.6}$$

Note that the second term in eq. (5.5) is of order a^4 in the continuum limit and that r_μ is positive.

At all momenta with $p_0 = 0$, on the other hand, the gauge action depends on the time component $\tilde{A}_0(p)$ only. For notational convenience, it is helpful to set

$$D_{\mu\nu}(p)\big|_{p_0=0} = 0 \quad \text{if } \mu \neq 0 \text{ or } \nu \neq 0. \tag{5.7}$$

The non-trivial component of the propagator is then

$$D_{00}(p)\big|_{p_0=0} = \begin{cases} \lambda_0^{-1}T^2 & \text{if } p = 0, \\ (\hat{p}^2 - c_1\hat{p}^4)^{-1} & \text{otherwise.} \end{cases} \tag{5.8}$$

As already mentioned, this case only occurs if SF boundary conditions are chosen.

5.2 Two-point function

To leading order in the gauge coupling, and for SF boundary conditions, the two-point function of the gauge potential is given by [cf. eq. (7.10)]

$$\langle A_0^a(x)A_0^b(y)\rangle = \frac{2\delta^{ab}}{TL^3}\sum_p{}' \cos(p_0x_0 + \tfrac{1}{2}p_0)\cos(p_0y_0 + \tfrac{1}{2}p_0)\mathrm{e}^{i\boldsymbol{p}(\boldsymbol{x}-\boldsymbol{y})}D_{00}(p), \tag{5.9}$$

$$\langle A_0^a(x)A_k^b(y)\rangle = -\frac{2i\delta^{ab}}{TL^3}\sum_p{}' \cos(p_0x_0 + \tfrac{1}{2}p_0)\sin(p_0y_0)\mathrm{e}^{i\boldsymbol{p}(\boldsymbol{x}-\boldsymbol{y})-\frac{i}{2}p_k}D_{0k}(p), \tag{5.10}$$

$$\langle A_k^a(x)A_0^b(y)\rangle = \frac{2i\delta^{ab}}{TL^3}\sum_p{}' \sin(p_0x_0)\cos(p_0y_0 + \tfrac{1}{2}p_0)\mathrm{e}^{i\boldsymbol{p}(\boldsymbol{x}-\boldsymbol{y})+\frac{i}{2}p_k}D_{k0}(p), \tag{5.11}$$

$$\langle A_k^a(x)A_l^b(y)\rangle = \frac{2\delta^{ab}}{TL^3}\sum_p{}' \sin(p_0x_0)\sin(p_0y_0)\mathrm{e}^{i\boldsymbol{p}(\boldsymbol{x}-\boldsymbol{y})+\frac{i}{2}(p_k-p_l)}D_{kl}(p). \tag{5.12}$$

The momenta with $p_0 = 0$ do not contribute in these equations except in the case of the correlation function (5.9) of the time component of the gauge field.

When open-SF boundary conditions are chosen, the two-point functions assume the form

$$\langle A_0^a(x)A_0^b(y)\rangle = \frac{2\delta^{ab}}{TL^3}\sum_p \sin(p_0x_0+\tfrac{1}{2}p_0)\sin(p_0y_0+\tfrac{1}{2}p_0)\mathrm{e}^{i\boldsymbol{p}(\boldsymbol{x}-\boldsymbol{y})}D_{00}(p), \quad (5.13)$$

$$\langle A_0^a(x)A_k^b(y)\rangle = \frac{2i\delta^{ab}}{TL^3}\sum_p \sin(p_0x_0+\tfrac{1}{2}p_0)\cos(p_0y_0)\mathrm{e}^{i\boldsymbol{p}(\boldsymbol{x}-\boldsymbol{y})-\frac{i}{2}p_k}D_{0k}(p), \quad (5.14)$$

$$\langle A_k^a(x)A_0^b(y)\rangle = -\frac{2i\delta^{ab}}{TL^3}\sum_p \cos(p_0x_0)\sin(p_0y_0+\tfrac{1}{2}p_0)\mathrm{e}^{i\boldsymbol{p}(\boldsymbol{x}-\boldsymbol{y})+\frac{i}{2}p_k}D_{k0}(p), \quad (5.15)$$

$$\langle A_k^a(x)A_l^b(y)\rangle = \frac{2\delta^{ab}}{TL^3}\sum_p \cos(p_0x_0)\cos(p_0y_0)\mathrm{e}^{i\boldsymbol{p}(\boldsymbol{x}-\boldsymbol{y})+\frac{i}{2}(p_k-p_l)}D_{kl}(p), \quad (5.16)$$

where p_0 here runs over the set (3.12).

6. Integration of the flow equation

6.1 Flow equation

The Yang–Mills gradient flow evolves the active link variables as a function of the flow time, while the static link variables are held fixed. When the lattice has boundaries, as is the case here, some care needs to be taken to ensure that the flow equation does not introduce $\mathrm{O}(a)$ lattice effects.

Let S_w be the tree-level $\mathrm{O}(a)$-improved Wilson plaquette action, i.e. the gauge action S_G with $c_0 = 1$, $c_1 = 0$ and $c_\mathrm{G} = 1$. The gauge field $V_t(x,\mu)$ at flow time t is determined by the boundary condition

$$V_t(x,\mu)|_{t=0} = U(x,\mu) \quad (6.1)$$

and the flow equation

$$\partial_t V_t(x,\mu)V_t(x,\mu)^{-1} = -w_{x,\mu}g_0^2\{\partial_{x,\mu}^a S_\mathrm{w}(V_t)\}T^a, \qquad 0 \le x_0 < T, \quad (6.2)$$

where $\partial^a_{x,\mu} S_{\rm w}(U)$ denotes the partial derivative of the action with respect to the link variable $U(x,\mu)$ in direction of the SU(N) generator T^a.

The weight factor $w_{x,\mu}$ in eq. (6.2) depends on the chosen boundary conditions. For SF boundary conditions

$$w_{x,\mu} = \begin{cases} 0 & \text{if } x_0 = 0 \text{ and } \mu > 0, \\ 1 & \text{otherwise,} \end{cases} \tag{6.3}$$

while for open-SF boundary conditions

$$w_{x,\mu} = \begin{cases} 2 & \text{if } x_0 = 0 \text{ and } \mu > 0, \\ 1 & \text{otherwise.} \end{cases} \tag{6.4}$$

As will made clear below, assigning weight 2 to the spatial links at time 0 is required for O(a) improvement [14].

6.2 Gauge damping

In perturbation theory, the link variables $U(x,\mu)$ are close to unity, but the link variables $V_t(x,\mu)$ obtained by integrating the flow equation need not have this property since the gradient flow does not damp the gauge degrees of freedom. Gauge damping allows this problem to be avoided through the addition of a term to the flow equation that has no effect on the time evolution of gauge-invariant observables.

Let $\Lambda_t(x)$ be a gauge transformation that depends on the flow time t and that satisfies

$$\Lambda_t(x)|_{t=0} = 1, \tag{6.5}$$

$$\Lambda_t(x)|_{x_0=T} = 1, \tag{6.6}$$

and additionally

$$\partial_k \Lambda_t(x)|_{x_0=0} = 0, \quad k = 1,2,3, \tag{6.7}$$

if SF boundary conditions are chosen. The transformed field

$$\tilde{V}_t(x,\mu) = \Lambda_t(x) V_t(x,\mu) \Lambda_t(x+\hat{\mu})^{-1} \tag{6.8}$$

is then a solution of the modified flow equation

$$\partial_t \tilde{V}_t(x,\mu) \tilde{V}_t(x,\mu)^{-1} = -w_{x,\mu} g_0^2 \{\partial^a_{x,\mu} S_{\rm w}(\tilde{V}_t)\} T^a - \tilde{D}_\mu \omega_t(x), \tag{6.9}$$

$$\omega_t(x) = \partial_t \Lambda_t(x) \Lambda_t(x)^{-1}, \tag{6.10}$$

$$\tilde{D}_\mu \omega_t(x) = \tilde{V}_t(x,\mu)\omega_t(x+\hat{\mu})\tilde{V}_t(x,\mu)^{-1} - \omega_t(x), \tag{6.11}$$

with the same boundary value (6.1) as $V_t(x,\mu)$.

In perturbation theory

$$\tilde{V}_t(x,\mu) = \exp\{g_0 B_\mu(t,x)\}, \qquad B_\mu(t,x)|_{t=0} = A_\mu(x), \tag{6.12}$$

and the damping of the gauge modes can be achieved by setting

$$\omega_t(x) = -g_0\alpha_0 \left\{ (1 - x_0/T) \frac{1}{T^2 L^3} \sum_{y_0=0}^{T-1} \sum_{\boldsymbol{y}} B_0(t,y) + \partial_\mu^* B_\mu(t,x) \right\} \tag{6.13}$$

in the case of SF boundary conditions and

$$\omega_t(x) = -g_0 \alpha_0 \partial_\mu^* B_\mu(t,x) \tag{6.14}$$

for open-SF boundary conditions. In these formulae, $\alpha_0 > 0$ denotes an adjustable "gauge damping parameter" and the divergence of the gauge potential $B_\mu(t,x)$ at the boundaries is to be evaluated by extending the potential to all points x in the same way as $A_\mu(x)$ (cf. discussion at the beginning of subsect. 3.2). The gauge transformation $\Lambda_t(x)$ is then determined through the differential equation (6.10) and the boundary condition (6.5).

6.3 Solution of the flow equation to leading order in g_0

Up to higher-order corrections, the flow equation reads

$$\begin{aligned} \partial_t B_\mu(t,x) = \{&\partial_\rho^* \partial_\rho \delta_{\mu\nu} + (\alpha_0 - 1)\partial_\mu \partial_\nu^*\} B_\nu(t,x) \\ &- \delta_{\mu 0} \frac{\alpha_0}{T^3 L^3} \sum_{y_0=0}^{T-1} \sum_{\boldsymbol{y}} B_0(t,y), \end{aligned} \tag{6.15}$$

where the last term is absent in the case of open-SF boundary conditions. As usual, the action of the derivatives near the boundaries of the lattice is defined by extending the fields beyond the range $0 \leq x_0 \leq T$. Equation (6.15) was derived taking the weight factors (6.3),(6.4) into account and it would look different if different weights were chosen.

In momentum space, the flow equation assumes the form

$$\partial_t \tilde{B}_\mu(t,p) = -\{\hat{p}^2\delta_{\mu\nu} + (\alpha_0 - 1)\hat{p}_\mu\hat{p}_\nu\}\tilde{B}_\nu(t,p) - \delta_{p0}\delta_{\mu 0}\frac{\alpha_0}{T^2}\tilde{B}_0(t,0), \qquad (6.16)$$

and for any non-zero momentum p its solution given by

$$\tilde{B}_\mu(t,p) = \frac{\mathrm{e}^{-t\hat{p}^2}}{\hat{p}^2}(\hat{p}^2\delta_{\mu\nu} - \hat{p}_\mu\hat{p}_\nu)\tilde{A}_\nu(p) + \frac{\mathrm{e}^{-\alpha_0 t\hat{p}^2}}{\hat{p}^2}\hat{p}_\mu\hat{p}_\nu\tilde{A}_\nu(p). \qquad (6.17)$$

At $p = 0$ (and thus for SF boundary conditions),

$$\tilde{B}_\mu(t,0) = \delta_{\mu 0}\mathrm{e}^{-\alpha_0 t/T^2}\tilde{A}_0(0) \qquad (6.18)$$

is the only non-vanishing Fourier component of the field.

7. Running coupling

7.1 Definition

Let $G_{\mu\nu}(t,x)$ be the standard clover lattice representation of the gauge-field tensor at flow time t. The running coupling introduced in ref. [5] is then given by

$$\bar{g}^2 = k\left\{t^2\langle E(t,x)\rangle\right\}_{\sqrt{8t}=cL}, \qquad (7.1)$$

$$E(t,x) = \tfrac{1}{4}G^a_{\mu\nu}(t,x)G^a_{\mu\nu}(t,x), \qquad (7.2)$$

where c is an adjustable constant that is part of the definition of the scheme. The normalization constant k is to be chosen such that

$$\bar{g}^2 = g_0^2 + \mathrm{O}(g_0^4) \qquad (7.3)$$

in the weak-coupling limit.

With SF or open-SF boundary conditions, the renormalized coupling (7.1) depends on the lattice sizes T and L, the proportionality constant c and the time x_0. Setting $x_0 = T/2$ is a natural choice, but in the following x_0 may assume any integer value in the range $0 < x_0 < T$. Of course, the coupling also depends on the theory and the parameters of the lattice action.

7.2 Leading-order expression for the field tensor

In position space,

$$G_{\mu\nu}(t,x) = \frac{g_0}{4}\left\{F_{\mu\nu}(t,x) + F_{\mu\nu}(t,x-\hat{\mu}) + F_{\mu\nu}(t,x-\hat{\nu}) + F_{\mu\nu}(t,x-\hat{\mu}-\hat{\nu})\right\} \tag{7.4}$$

up to terms of order g_0^2, where

$$F_{\mu\nu}(t,x) = \partial_\mu B_\nu(t,x) - \partial_\nu B_\mu(t,x). \tag{7.5}$$

Recalling eqs. (6.17),(6.18), one then obtains

$$G_{0k}(t,x) = \frac{2ig_0}{TL^3}\sum_p{}' \cos(p_0x_0)\mathrm{e}^{i\boldsymbol{px}}\mathrm{e}^{-t\hat{p}^2} \\ \times \cos(\tfrac{1}{2}p_0)\cos(\tfrac{1}{2}p_k)\{\hat{p}_0\tilde{A}_k(p) - \hat{p}_k\tilde{A}_0(p)\}, \tag{7.6}$$

$$G_{kl}(t,x) = -\frac{2g_0}{TL^3}\sum_p{}' \sin(p_0x_0)\mathrm{e}^{i\boldsymbol{px}}\mathrm{e}^{-t\hat{p}^2} \\ \times \cos(\tfrac{1}{2}p_k)\cos(\tfrac{1}{2}p_l)\{\hat{p}_k\tilde{A}_l(p) - \hat{p}_l\tilde{A}_k(p)\}, \tag{7.7}$$

for SF boundary conditions and

$$G_{0k}(t,x) = -\frac{2g_0}{TL^3}\sum_p \sin(p_0x_0)\mathrm{e}^{i\boldsymbol{px}}\mathrm{e}^{-t\hat{p}^2} \\ \times \cos(\tfrac{1}{2}p_0)\cos(\tfrac{1}{2}p_k)\{\hat{p}_0\tilde{A}_k(p) - \hat{p}_k\tilde{A}_0(p)\}, \tag{7.8}$$

$$G_{kl}(t,x) = \frac{2ig_0}{TL^3}\sum_p \cos(p_0x_0)\mathrm{e}^{i\boldsymbol{px}}\mathrm{e}^{-t\hat{p}^2} \\ \times \cos(\tfrac{1}{2}p_k)\cos(\tfrac{1}{2}p_l)\{\hat{p}_k\tilde{A}_l(p) - \hat{p}_l\tilde{A}_k(p)\}, \tag{7.9}$$

for open-SF boundary conditions. All terms depending on the gauge-damping parameter α_0 drop out in these equations. In particular, the term (6.18) does not contribute, since the right-hand side of eq. (7.6) vanishes at $p = 0$.

7.3 Normalization factor

Noting

$$\langle \tilde{A}^a_\mu(p)\tilde{A}^b_\nu(q)^*\rangle = \frac{TL^3}{2}\delta_{pq}(1+\delta_{p_0 0})\delta^{ab}D_{\mu\nu}(p) + \mathrm{O}(g_0^2), \tag{7.10}$$

the expectation value on the right of eq. (7.1) is now easily evaluated to leading order. As a result one obtains an analytic expression for the normalization factor k. To be able to write it down in a compact form, it is helpful to introduce the symmetric tensor

$$S_{\mu\nu}(p) = (1-\tfrac{1}{4}\hat{p}_\mu^2)(1-\tfrac{1}{4}\hat{p}_\nu^2)\left\{\hat{p}_\mu^2 D_{\nu\nu}(p) + \hat{p}_\nu^2 D_{\mu\mu}(p) - 2\hat{p}_\mu\hat{p}_\nu D_{\mu\nu}(p)\right\}. \tag{7.11}$$

The normalization factor is then given by

$$k^{-1} = \frac{N^2-1}{TL^3}\sum_p{}' \left\{t^2 \mathrm{e}^{-2t\hat{p}^2}\right\}_{\sqrt{8t}=cL} \times \left\{\cos(p_0x_0)^2\sum_{l=1}^3 S_{l0}(p) + \sin(p_0x_0)^2 \sum_{l>j=1}^3 S_{lj}(p)\right\} \tag{7.12}$$

for SF boundary conditions and by

$$k^{-1} = \frac{N^2-1}{TL^3}\sum_p \left\{t^2 \mathrm{e}^{-2t\hat{p}^2}\right\}_{\sqrt{8t}=cL} \times \left\{\sin(p_0x_0)^2\sum_{l=1}^3 S_{l0}(p) + \cos(p_0x_0)^2 \sum_{l>j=1}^3 S_{lj}(p)\right\} \tag{7.13}$$

for open-SF boundary conditions. Equations (7.12) and (7.13) are very similar, but the momentum p_0 runs over different sets of values in the two cases. There is no dependence on the gauge-fixing parameter λ_0, since the gauge term in eq. (5.4) and the term at $p=0$ in eq. (5.8) both drop out when the tensor $S_{\mu\nu}(p)$ is formed.

7.4 Special cases

(1) *Open-SF boundary conditions, $x_0 = T/2$.* In this particular case,

$$\cos(p_0x_0)^2 = \sin(p_0x_0)^2 = \frac{1}{2} \tag{7.14}$$

for all momenta p_0 so that

$$k^{-1} = \frac{N^2-1}{2TL^3}\sum_p \left\{t^2 \mathrm{e}^{-2t\hat{p}^2}\right\}_{\sqrt{8t}=cL} \sum_{\mu>\nu=0}^{3} S_{\mu\nu}(p). \tag{7.15}$$

In the continuum limit,

$$\sum_{\mu>\nu=0}^{3} S_{\mu\nu}(p) \to 3, \tag{7.16}$$

and the normalization factor converges to a product

$$k^{-1} = \frac{3(N^2-1)}{4TL^3} t^2 \vartheta_2(0)\vartheta_3(0)^3, \tag{7.17}$$

$$\vartheta_2(0) = \sum_{n=-\infty}^{\infty} \exp\left\{-\frac{2t\pi^2}{T^2}(n+\tfrac{1}{2})^2\right\}, \tag{7.18}$$

$$\vartheta_3(0) = \sum_{n=-\infty}^{\infty} \exp\left\{-\frac{8t\pi^2}{L^2}n^2\right\}, \tag{7.19}$$

of Jacobi theta-functions (here and below it is understood that $\sqrt{8t}$ is set to cL). Using the Poisson summation formula

$$\sum_{n=-\infty}^{\infty} f(2\pi n) = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} \tilde{f}(n), \qquad \tilde{f}(n) = \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{inx} f(x), \tag{7.20}$$

(which holds for any smooth and rapidly decaying function $f(x)$), the theta-functions can be written in the form

$$\vartheta_2(0) = \frac{T}{\sqrt{2\pi t}} \sum_{n=-\infty}^{\infty} (-1)^n \exp\left\{-\frac{T^2}{2t}n^2\right\}, \tag{7.21}$$

$$\vartheta_3(0) = \frac{L}{\sqrt{8\pi t}} \sum_{n=-\infty}^{\infty} \exp\left\{-\frac{L^2}{8t}n^2\right\}. \tag{7.22}$$

In this special case, the finite-volume corrections are thus exponentially suppressed. For $T = L$ and $c = 0.3$, for example, the normalization factor is equal to its infinitevolume value,

$$k^{-1} \underset{L^2/t\to\infty}{=} \frac{3(N^2-1)}{128\pi^2}, \tag{7.23}$$

within a relative deviation of less than 10^{-4}.

(2) *Wilson plaquette action.* For all $p \neq 0$ and $\mu \neq \nu$, the tensor (7.11) is given by

$$S_{\mu\nu}(p) = (1 - \tfrac{1}{4}\hat{p}_\mu^2)(1 - \tfrac{1}{4}\hat{p}_\nu^2)\frac{\hat{p}_\mu^2 + \hat{p}_\nu^2}{\hat{p}^2} \tag{7.24}$$

in this case. The tensor vanishes when $p = 0$. Equation (7.12) is then found to agree with the result obtained in ref. [5] †.

(3) *Continuum limit.* For fixed T/L, x_0/T and c, the normalization factor k converges to its continuum value as $L \to \infty$ with a rate proportional to $1/L^2$ (cf. tables in appendix A).

8. Alternative running couplings

The definition (7.1),(7.2) of the running coupling may be varied in several ways. The clover expression for the square of the field tensor can be replaced by the plaquette definition, for example, or the sum over the Lorentz indices in eq. (7.2) may be restricted to the spatial and time-like components.

8.1 Definitions considered

In the following, the subscripts cs,ct,ps and pt distinguish different lattice expressions for the space- and time-like parts of the square of the field tensor. Explicitly,

$$E_{\rm cs}(t,x) = \tfrac{1}{4}G_{kl}^a(t,x)G_{kl}^a(t,x), \tag{8.1}$$

$$E_{\rm ct}(t,x) = \tfrac{1}{2}G_{0k}^a(t,x)G_{0k}^a(t,x), \tag{8.2}$$

† In the formula quoted in this paper, it is understood that any terms involving the momentum p_i are to be summed over the index i from 1 to 3. The (ill-defined) summand at $p = 0$ should be omitted.

while $E_{\rm ps}$ and $E_{\rm pt}$ stand for the corresponding symmetric expressions constructed using the plaquette loops passing through x (cf. subsect. 8.3).

The associated running couplings, $\bar{g}_{\rm cs},\ldots,\bar{g}_{\rm pt}$, are again given by eq. (7.1), with E replaced by $E_{\rm cs},\ldots,E_{\rm pt}$, respectively, and the proportionality constant k by constants $k_{\rm cs},\ldots,k_{\rm pt}$ so that all couplings coincide with g_0^2 to lowest order in perturbation theory.

8.2 Computation of $k_{\rm cs}$ and $k_{\rm ct}$

These two constants may be calculated following the lines of subsect. 7.2. In the case of SF boundary conditions,

$$k_{\rm cs}^{-1}=\frac{N^2-1}{TL^3}{\sum_p}'\left\{t^2{\rm e}^{-2t\hat{p}^2}\right\}_{\sqrt{8t}=cL}\sin(p_0x_0)^2\sum_{l>j=1}^{3}S_{lj}(p), \tag{8.3}$$

$$k_{\rm ct}^{-1}=\frac{N^2-1}{TL^3}{\sum_p}'\left\{t^2{\rm e}^{-2t\hat{p}^2}\right\}_{\sqrt{8t}=cL}\cos(p_0x_0)^2\sum_{l=1}^{3}S_{l0}(p), \tag{8.4}$$

while for open-SF boundary conditions the result

$$k_{\rm cs}^{-1}=\frac{N^2-1}{TL^3}\sum_p\left\{t^2{\rm e}^{-2t\hat{p}^2}\right\}_{\sqrt{8t}=cL}\cos(p_0x_0)^2\sum_{l>j=1}^{3}S_{lj}(p), \tag{8.5}$$

$$k_{\rm ct}^{-1}=\frac{N^2-1}{TL^3}\sum_p\left\{t^2{\rm e}^{-2t\hat{p}^2}\right\}_{\sqrt{8t}=cL}\sin(p_0x_0)^2\sum_{l=1}^{3}S_{l0}(p), \tag{8.6}$$

is obtained.

8.3 Computation of $k_{\rm ps}$ and $k_{\rm pt}$

To leading order in the gauge coupling,

$$E_{\rm ps}(t,x)=\frac{g_0^2}{16}\sum_{k,l=1}^{3}(2-\partial_k^*)(2-\partial_l^*)\{F_{kl}^a(t,x)F_{kl}^a(t,x)\}, \tag{8.7}$$

$$E_{\rm pt}(t,x)=\frac{g_0^2}{8}\sum_{k=1}^{3}(2-\partial_0^*)(2-\partial_k^*)\{F_{0k}^a(t,x)F_{0k}^a(t,x)\}, \tag{8.8}$$

where $F_{\mu\nu}(t,x)$ is given by eq. (7.5). For SF boundary conditions,

$$F_{0k}(t,x) = \frac{2i}{TL^3} {\sum_p}' \mathrm{e}^{-t\hat{p}^2} \cos(p_0 x_0 + \tfrac{1}{2}p_0) \mathrm{e}^{i\boldsymbol{px} + \frac{i}{2}p_k} \big(\hat{p}_0 \tilde{A}_k(p) - \hat{p}_k \tilde{A}_0(p)\big), \quad (8.9)$$

$$F_{kl}(t,x) = -\frac{2}{TL^3} {\sum_p}' \mathrm{e}^{-t\hat{p}^2} \sin(p_0 x_0) \mathrm{e}^{i\boldsymbol{px} + \frac{i}{2}(p_k + p_l)} \big(\hat{p}_k \tilde{A}_l(p) - \hat{p}_l \tilde{A}_k(p)\big), \quad (8.10)$$

which leads to the expressions

$$k_{\mathrm{ps}}^{-1} = \frac{N^2-1}{TL^3} {\sum_p}' \left\{ t^2 \mathrm{e}^{-2t\hat{p}^2} \right\}_{\sqrt{8t}=cL} \sin(p_0 x_0)^2 \sum_{l>j=1}^{3} R_{lj}(p), \quad (8.11)$$

$$k_{\mathrm{pt}}^{-1} = \frac{N^2-1}{TL^3} {\sum_p}' \left\{ t^2 \mathrm{e}^{-2t\hat{p}^2} \right\}_{\sqrt{8t}=cL}$$

$$\times \tfrac{1}{2} \left\{ \cos(p_0 x_0 + \tfrac{1}{2}p_0)^2 + \cos(p_0 x_0 - \tfrac{1}{2}p_0)^2 \right\} \sum_{l=1}^{3} R_{l0}(p), \quad (8.12)$$

$$R_{\mu\nu}(p) = \hat{p}_\mu^2 D_{\nu\nu}(p) + \hat{p}_\nu^2 D_{\mu\mu}(p) - 2\hat{p}_\mu \hat{p}_\nu D_{\mu\nu}(p), \quad (8.13)$$

for the normalization factors.

In the case of open-SF boundary conditions,

$$F_{0k}(t,x) = -\frac{2}{TL^3} \sum_p \mathrm{e}^{-t\hat{p}^2} \sin(p_0 x_0 + \tfrac{1}{2}p_0) \mathrm{e}^{i\boldsymbol{px} + \frac{i}{2}p_k} \big(\hat{p}_0 \tilde{A}_k(p) - \hat{p}_k \tilde{A}_0(p)\big), \quad (8.14)$$

$$F_{kl}(t,x) = \frac{2i}{TL^3} \sum_p \mathrm{e}^{-t\hat{p}^2} \cos(p_0 x_0) \mathrm{e}^{i\boldsymbol{px} + \frac{i}{2}(p_k + p_l)} \big(\hat{p}_k \tilde{A}_l(p) - \hat{p}_l \tilde{A}_k(p)\big), \quad (8.15)$$

and for the normalization factors, the expressions

$$k_{\mathrm{ps}}^{-1} = \frac{N^2-1}{TL^3} \sum_p \left\{ t^2 \mathrm{e}^{-2t\hat{p}^2} \right\}_{\sqrt{8t}=cL} \cos(p_0 x_0)^2 \sum_{l>j=1}^{3} R_{lj}(p), \quad (8.16)$$

$$k_{\rm pt}^{-1}=\frac{N^2-1}{TL^3}\sum_p\left\{t^2{\rm e}^{-2t\hat{p}^2}\right\}_{\sqrt{8t}=cL}$$
$$\times\tfrac{1}{2}\left\{\sin(p_0x_0+\tfrac{1}{2}p_0)^2+\sin(p_0x_0-\tfrac{1}{2}p_0)^2\right\}\sum_{l=1}^{3}R_{l0}(p), \qquad (8.17)$$

are then obtained.

Appendix A

Some sample results for the normalization factors are shown in tables 1–4. In all cases considered

$$T=L, \quad x_0=T/2, \quad c=0.3, \qquad (A.1)$$

and the action is chosen to be the Wilson plaquette action (thus $c_1=0$). In the tables, $k_{\rm c}$ and $k_{\rm p}$ denote the normalization factors

$$k_{\rm c}=\left\{k_{\rm cs}^{-1}+k_{\rm ct}^{-1}\right\}^{-1}, \qquad k_{\rm p}^{-1}=\left\{k_{\rm ps}^{-1}+k_{\rm pt}^{-1}\right\}^{-1}, \qquad (A.2)$$

of the couplings defined with the clover and plaquette definitions of the full Yang-Mills action density.

References

[1] M. Lüscher, *Properties and uses of the Wilson flow in lattice QCD*, JHEP 1008 (2010) 071 [E: *ibid.* 03 (2014) 092].

[2] M. Lüscher, P. Weisz, *Perturbative analysis of the gradient flow in non-Abelian gauge theories*, JHEP 1102 (2011) 051.

[3] M. Lüscher, P. Weisz, U. Wolff, *A numerical method to compute the running coupling in asymptotically free theories*, Nucl. Phys. B359 (1991) 221.

[4] Z. Fodor, K. Holland, J. Kuti, D. Nogradi, C. H. Wong, *The Yang–Mills gradient flow in finite volume*, JHEP 1211 (2012) 007; *The gradient flow running coupling scheme*, PoS (Lattice 2012) 050.

Table 1. Values of $k_{\mathrm{c}}, k_{\mathrm{cs}}, k_{\mathrm{ct}}$ (Wilson action, SF bc)

L	k_{c}	k_{cs}	k_{ct}	$1/k_{\mathrm{c}}$	$1/k_{\mathrm{cs}}$	$1/k_{\mathrm{ct}}$
8	62.63179	126.80459	123.75958	0.015966332	0.007886150	0.008080183
12	59.76292	120.86541	118.21564	0.016732783	0.008273666	0.008459117
16	58.86940	119.01310	116.49148	0.016986755	0.008402436	0.008584319
24	58.26019	117.74943	115.31671	0.017164380	0.008492610	0.008671770
32	58.05230	117.31806	114.91597	0.017225847	0.008523837	0.008702011
48	57.90543	117.01327	114.63291	0.017269537	0.008546039	0.008723498

Table 2. Values of $k_{\mathrm{c}}, k_{\mathrm{cs}}, k_{\mathrm{ct}}$ (Wilson action, open-SF bc)

L	k_{c}	k_{cs}	k_{ct}	$1/k_{\mathrm{c}}$	$1/k_{\mathrm{cs}}$	$1/k_{\mathrm{ct}}$
8	56.47240	125.26966	102.82791	0.017707765	0.007982779	0.009724986
12	54.20452	119.53041	99.18101	0.018448647	0.008366072	0.010082575
16	53.49427	117.74292	98.03430	0.018693591	0.008493079	0.010200512
24	53.00905	116.52421	97.24983	0.018864702	0.008581908	0.010282794
32	52.84330	116.10833	96.98167	0.018923874	0.008612646	0.010311227
48	52.72616	115.81453	96.79208	0.018965919	0.008634495	0.010331424

[5] P. Fritzsch, A. Ramos, *The gradient flow coupling in the Schrödinger functional*, JHEP 1310 (2013) 008; *Studying the gradient flow coupling in the Schrödinger functional*, PoS (Lattice 2013) 319.

[6] A. Ramos, *The gradient flow in a twisted box*, PoS (Lattice 2013) 053.

[7] M. Lüscher, Stefan Schaefer, *Lattice QCD without topology barriers*, JHEP 1107 (2011) 036.

[8] P. Fritzsch, A. Ramos, F. Stollenwerk, *Critical slowing down and the gradient flow coupling in the Schrödinger functional*, PoS Lattice2013 (2014) 461.

[9] M. Lüscher, P. Weisz, *On-shell improved lattice gauge theories*, Commun. Math. Phys. 97 (1985) 59 [E: *ibid.* 98 (1985) 433].

[10] M. Lüscher, R. Narayanan, P. Weisz, U. Wolff, *The Schrödinger functional — a renormalizable probe for non-Abelian gauge theories*, Nucl. Phys. B384 (1992) 168.

Table 3. Values of $k_{\rm p}, k_{\rm ps}, k_{\rm pt}$ (Wilson action, SF bc)

L	$k_{\rm p}$	$k_{\rm ps}$	$k_{\rm pt}$	$1/k_{\rm p}$	$1/k_{\rm ps}$	$1/k_{\rm pt}$
8	45.34635	91.53343	89.86726	0.022052493	0.010924970	0.011127523
12	52.77780	106.60610	104.52559	0.018947361	0.009380326	0.009567035
16	55.03284	111.18038	108.97309	0.018170970	0.008994392	0.009176577
24	56.57998	114.31891	112.02427	0.017674096	0.008747459	0.008926637
32	57.11174	115.39767	113.07294	0.017509535	0.008665686	0.008843849
48	57.48881	116.16262	113.81655	0.017394690	0.008608621	0.008786068

Table 4. Values of $k_{\rm p}, k_{\rm ps}, k_{\rm pt}$ (Wilson action, open-SF bc)

L	$k_{\rm p}$	$k_{\rm ps}$	$k_{\rm pt}$	$1/k_{\rm p}$	$1/k_{\rm ps}$	$1/k_{\rm pt}$
8	41.95890	90.56246	78.18155	0.023832844	0.011042103	0.012790741
12	48.35863	105.48026	89.29861	0.020678830	0.009480447	0.011198383
16	50.28593	110.02139	92.61716	0.019886277	0.009089142	0.010797136
24	51.60468	113.14123	94.88049	0.019378086	0.008838511	0.010539575
32	52.05729	114.21432	95.65592	0.019209606	0.008755470	0.010454136
48	52.37803	114.97549	96.20502	0.019091974	0.008697506	0.010394468

[11] S. Aoki, R. Frezzotti, P. Weisz, *Computation of the improvement coefficient $c_{\rm sw}$ to 1-loop with improved gluon actions*, Nucl. Phys. B540 (1999) 501.

[12] M. Lüscher, *Gauge actions in openQCD simulations*, notes March 2012 (revised November 2013).

[13] M. Lüscher, *Selected topics in lattice field theory*, Lectures given at Les Houches (1988), in: Fields, strings and critical phenomena, ed. E. Brézin and J. Zinn-Justin (North-Holland, Amsterdam, 1989).

[14] M. Lüscher, S. Schaefer, *Lattice QCD with open boundary conditions and twisted-mass reweighting*, Comput. Phys. Commun. 184 (2013) 519.