Gauge actions in openQCD simulations

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1. Introduction

The gauge actions supported in the openQCD package include the Wilson plaquette action, the tree-level Symanzik-improved action and other closely related actions. In this note, the actions and the boundary conditions for the gauge field are defined and the computation of the associated molecular-dynamics forces is briefly discussed. The notation and the normalization conventions are the same as in refs. [1,2,6].

2. Definition

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 supported gauge actions are of the form

$$S_{\mathrm{G}} = \frac{1}{g_0^2} \sum_{k=0}^{1} c_k \sum_{\mathcal{C} \in \mathcal{S}_k} w_k(\mathcal{C}) \operatorname{tr}\{1 - U(\mathcal{C})\}, \tag{2.1}$$

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 sect. 3).

In order to ensure the correct normalization of the bare coupling g_0, the coefficients c_k must be such that
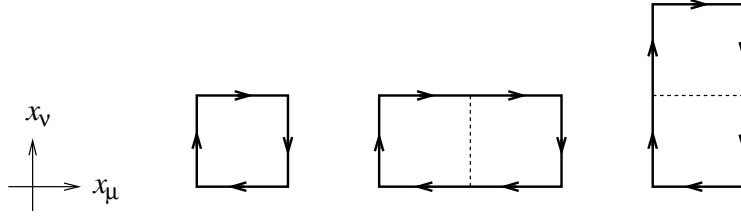
$$c_0 + 8c_1 = 1. \tag{2.2}$$

Fig. 1.   Plaquette and planar double-plaquette loops in a (μ, ν)–plane of the lattice. The sums in eq. (2.1) run over all these loops, where loops differing by their orientation are considered to be different.

Moreover, the constraint $c_0 > 0$ is imposed as otherwise there may be fields with lowest action which are not locally pure gauge configurations [3].

In the case of the Wilson plaquette action,

$$c_0 = 1, \quad c_1 = 0, \tag{2.3}$$

while the tree-level Symanzik improved action is obtained by setting [4]

$$c_0 = \tfrac{5}{3}, \quad c_1 = -\tfrac{1}{12}. \tag{2.4}$$

Another choice of the coefficients,

$$c_0 = 3.648, \quad c_1 = -0.331, \tag{2.5}$$

was proposed by Iwasaki on the basis of a renormalization-group analysis of the pure gauge theory [5]. In the openQCD main programs, the coefficient c_0 is an adjustable parameter so that one is free to choose any one of these popular actions.

3. Boundary conditions

The openQCD programs support various types of boundary conditions in the time direction. In the spatial directions, periodic boundary conditions are imposed as usual. Independently of the boundary conditions, the lattice always includes the points x with Cartesian coordinates

$$x = (x_0, x_1, x_2, x_3) = a(n_0, n_1, n_2, n_3),$$

$$n_\mu \in \mathbb{Z}, \qquad 0 \le n_\mu < N_\mu, \tag{3.1}$$

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where a denotes the lattice spacing and the lattice sizes $N_\mu \geq 4$, $\mu = 0, \ldots, 3$, are even integers. Another time-slice of points is added to the lattice at time $x_0 = aN_0$ in the case of Schrödinger functional (SF) and open-SF boundary conditions.

The *active* link variables are those integrated over in the QCD functional integral. In general, there are further link variables, the *static* ones, on which the gauge action depends but which are set to some fixed values.

3.1 Open boundary conditions

There are no static link variables in this case and the active link variables reside on the links, where both endpoints are contained in the lattice (3.1) (modulo spatial translations by multiples of the lattice sizes aN_1, aN_2, aN_3). The sum in eq. (2.1) then extends over all loops $\mathcal{C}$ that are fully contained in the lattice, i.e. which pass through only such links.

With open boundary conditions, the lattice has two boundaries, one at time 0 and the other at time $T = a(N_0 - 1)$. The weight factors $w_k(\mathcal{C})$ in eq. (2.1) are equal to 1 except for the space-like loops $\mathcal{C}$ at these times, where

$$w_k(\mathcal{C}) = \tfrac{1}{2} c_\mathrm{G}. \tag{3.2}$$

As previously discussed in ref. [1], the coefficient c_G is required for $\mathrm{O}(a)$ improvement of correlation functions involving local fields close to or at the boundaries of the lattice. In particular, setting $c_\mathrm{G} = 1$ ensures on-shell improvement at tree-level of perturbation theory.

3.2 SF boundary conditions

As already mentioned, the lattice includes an additional time-slice at time $x_0 = aN_0$ when SF boundary conditions are chosen. The time extent T of the lattice is thus $T = aN_0$ in this case, but the spatial link variables on the boundaries at time 0 and T are static and taken to be of the form [6]

$$U(x, k) = \begin{cases} \exp\{aC_k\} & \text{if } x_0 = 0, \\ \exp\{aC_k'\} & \text{if } x_0 = T, \end{cases} \tag{3.3}$$

$$C_k = \frac{i}{aN_k} \begin{pmatrix} \phi_1 & 0 & 0 \\ 0 & \phi_2 & 0 \\ 0 & 0 & \phi_3 \end{pmatrix}, \qquad C_k' = \frac{i}{aN_k} \begin{pmatrix} \phi_1' & 0 & 0 \\ 0 & \phi_2' & 0 \\ 0 & 0 & \phi_3' \end{pmatrix}, \tag{3.4}$$
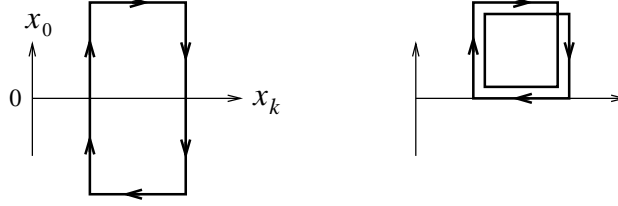
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Fig. 2. At the boundaries of the lattice where SF boundary conditions are imposed, the double-plaquette loops $\mathcal{C}$ that cross the boundary are included in the gauge action (2.1), with weight $w_1(\mathcal{C}) = 1/2$ and $U(\mathcal{C})$ set to the product of the link variables around the loop shown on the right, which winds twice around the inner plaquette.

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

$$\sum_{j=1}^{3} \phi_j = \sum_{j=1}^{3} \phi'_j = 0, \tag{3.5}$$

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

With SF boundary conditions, the active link variables reside on the links that have both endpoints in the time range $0 \leq x_0 \leq T$, at most one of them being at time 0 or T. 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 [7]. In the openQCD programs, another possible choice of the action is implemented, which combines the advantages of choice A and B (see appendix A for further explanations).

The sets of loops $\mathcal{C}$ summed over in the gauge action eq. (2.1) includes all loops that are fully contained in the range $0 \leq x_0 \leq T$ 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 (3.3),(3.4), 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 left unspecified. For the plaquette loops, the weights are then

$$w_0(\mathcal{C}) = \begin{cases} c_{\mathrm{G}} & \text{if } \mathcal{C} \text{ has exactly one link on a boundary,} \\ 1 & \text{otherwise,} \end{cases} \tag{3.6}$$

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

$$w_1(\mathcal{C}) = \begin{cases} \frac{1}{2} & \text{if } \mathcal{C} \text{ crosses a boundary as in fig. 2,} \\ 1 & \text{otherwise.} \end{cases} \tag{3.7}$$

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Tree-level O(a)-improvement is then again guaranteed if $c_{\mathrm{G}} = 1$, but at higher orders of perturbation theory O(a)-improvement probably requires the coefficient c_{G} to be different from the one required for improvement of the theory with open boundary conditions.

3.3 Open-SF boundary conditions

The openQCD programs also support open boundary conditions at time 0 together with SF boundary conditions at time $T = aN_0$. Lattices with these boundary conditions have the same size as the lattices with SF boundary conditions at both time 0 and T. The only static link variables are

$$
U(x,k)|_{x_0=T} = \exp\{aC'_k\}, \qquad C'_k = \frac{i}{aN_k} \begin{pmatrix} \phi'_1 & 0 & 0 \\ 0 & \phi'_2 & 0 \\ 0 & 0 & \phi'_3 \end{pmatrix}, \tag{3.8}
$$

in this case, while all link variables at time 0 are active.

When open-SF boundary conditions are chosen, the weights $w_k(\mathcal{C})$ are given by eq. (3.2) for loops in the vicinity of the boundary at $x_0 = 0$ and by eqs. (3.6),(3.7), with c_{G} replaced by c'_{G}, for loops near $x_0 = T$. In the bulk of the lattice, all weights are set to 1 as usual. The adjustable parameters describing open-SF boundary conditions are thus the angles ϕ'_j and the improvement coefficients c_{G} and c'_{G}.

3.4 Periodic boundary conditions

In this case, the lattice coincides with the set (3.1) of points. Since the points at time $x_0 = a(N_0 - 1)$ are considered to be neighbours of the points at $x_0 = 0$, the time extent T of the lattice is aN_0. With these boundary conditions, the lattice has no boundaries, all link variables are active and the weights $w_k(\mathcal{C})$ are all equal to 1.

3.5 Remarks

Except for open boundary conditions, where $T = a(N_0 - 1)$, the time extent T of the lattice is always equal to aN_0. Open boundary conditions are special in this respect for purely technical reasons related to the chosen data structures and parallelization strategies.

In practice, lattices with open boundary conditions are of interest for studies of the theory on large lattices. A difference in the time extent of the lattice by plus or minus one lattice spacing is quite irrelevant in this case. Having $T = aN_0$ is however an advantage for step-scaling, using SF or open-SF boundary conditions, since the multiplication of the lattice sizes N_μ by a common scale factor then preserves the
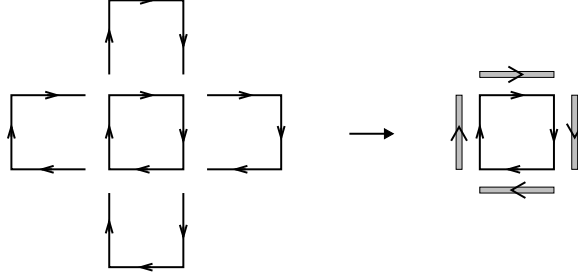
Fig. 3. In total, there are ten oriented plaquette and planar double-plaquette loops that pass through all corners of a given plaquette. The computation of the force (4.1) along the edges of the plaquette deriving from these loops can be simplified by first calculating the staples shown in this figure and saving them in a temporary array (fat links on the right).

ratios of the physical lattice sizes T and aN_k exactly and not only up to terms of order a.

The boundary conditions imposed on the quark fields depend on the ones chosen for the gauge field. They are described in all detail in the notes `doc/dirac.pdf`. The boundary conditions and the associated action parameters to be used in a simulation must be specified in the input parameter files (see `doc/parms.pdf`).

4. Computation of the gauge force

There are probably many good ways to calculate the force field

$$F^a(x, \mu) = \partial^a_{x,\mu} S_{\mathrm{G}}. \tag{4.1}$$

The method described in the following proceeds from one plaquette to the next and accumulates the contributions to the force components at the edges of the plaquette which derive from the loops that pass through all corners of the plaquette (see fig. 3).

By reversing the orientation of a given loop $\mathcal{C}$ one obtains a different loop $\mathcal{C}'$. The contribution to the gauge action of such a pair of loops is

$$s(\mathcal{C}) = \frac{2}{g_0^2} c_k w_k(\mathcal{C}) \operatorname{Re} \operatorname{tr}\{1 - U(\mathcal{C})\}, \tag{4.2}$$

where $k = 0$ or 1 depending on whether $\mathcal{C}$ is a plaquette or double-plaquette loop. Now if $\mathcal{C}$ passes through the link (x, μ) from $x + a\hat{\mu}$ to x, the dependence of the action (3.2) on the link variable $U(x, \mu)$ is made explicit by

$$s(\mathcal{C}) = -\frac{2}{g_0^2} c_k w_k(\mathcal{C}) \operatorname{Re} \operatorname{tr}\{U(x, \mu)V(x, \mu; \mathcal{C})\} + \text{constant}, \tag{4.3}$$

$V(x, \mu; \mathcal{C})$ being the product of the other link variables on the loop. Similarly, if the loop passes through the link in the opposite direction, the action may be written in the form

$$s(\mathcal{C}) = -\frac{2}{g_0^2} c_k w_k(\mathcal{C}) \operatorname{Re} \operatorname{tr}\{V(x, \mu; \mathcal{C})U(x, \mu)^{-1}\} + \text{constant}. \tag{4.4}$$

The contribution $f(x, \mu)$ of these terms to the total force $F(x, \mu) = F(x, \mu)^a T^a$ is

$$f(x, \mu) = +\frac{1}{g_0^2} c_k w_k(\mathcal{C}) \mathcal{P}\{U(\mathcal{C})\}, \tag{4.5}$$

$$f(x, \mu) = -\frac{1}{g_0^2} c_k w_k(\mathcal{C}) \mathcal{P}\{U(\mathcal{C})\}, \tag{4.6}$$

respectively, where $U(\mathcal{C})$ is the product of the link variables around $\mathcal{C}$ starting and ending at x, while

$$\mathcal{P}\{M\} = \tfrac{1}{2}(M - M^\dagger) - \tfrac{1}{6}\operatorname{tr}(M - M^\dagger) \tag{4.7}$$

projects any 3×3 matrix M to the Lie algebra of SU(3).

The computation of the force field may thus proceed in the following steps:

(1) Run through all unoriented plaquettes of the lattice. At a given plaquette, choose one of the two possible orientations.

(2) Consider the plaquette and double-plaquette loops that pass through all corners of the current plaquette and that have the chosen orientation. Compute the staples (fat links) shown in fig. 3.

(3) Compute the plaquette loops plotted in fig. 4 and add or subtract the associated force contribution to the force field according to eqs. (4.5),(4.6).

In step (3), the number of SU(3) multiplications can be significantly reduced by factoring common products.
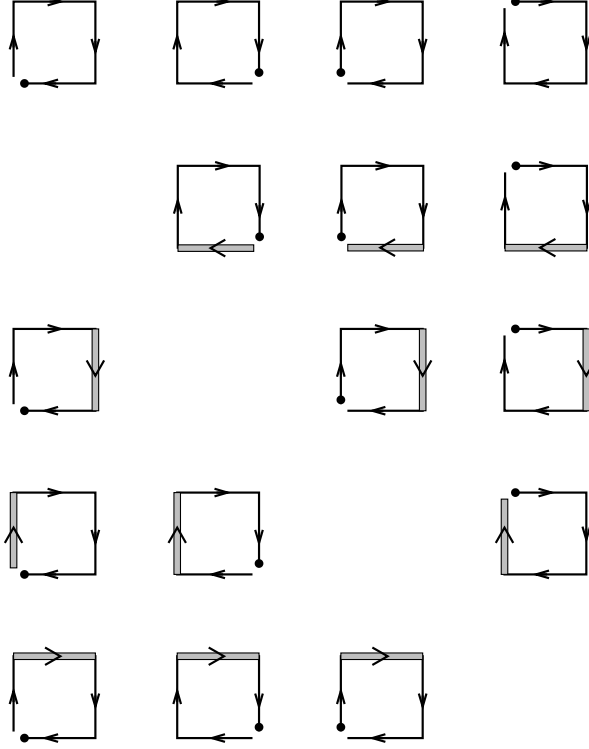
Fig. 4. Products $U(\mathcal{C})$ of link variables that contribute to the force field at the edges of the current plaquette. The dot indicates which edge is concerned and also coincides with the point x in eqs. (4.5),(4.6). The contributions from the loops on the first row must be multiplied by $\pm g_0^{-2} c_0 w_0(\mathcal{C})$ and those from all other loops by $\pm g_0^{-2} c_1 w_1(\mathcal{C})$.

5. Communication requirements

In the openQCD simulation programs, the local lattices (the parts of the full lattice on which a given MPI process operates) do not contain all the link variables required for the computations described in the previous section.

A double-counting of plaquettes can be avoided by locally running through all (x, μ, ν)–plaquettes, where x is in the local lattice and $\mu, \nu = 0, \ldots, 3$, $\mu < \nu$. The link variables on the edges of these plaquettes, which are not part of the local gauge field, must then first be copied from the neighbouring processes (see fig. 5). After that it is still not possible to compute all staples locally, but the missing ones can be calculated on the neighbouring lattices and be communicated to the local process
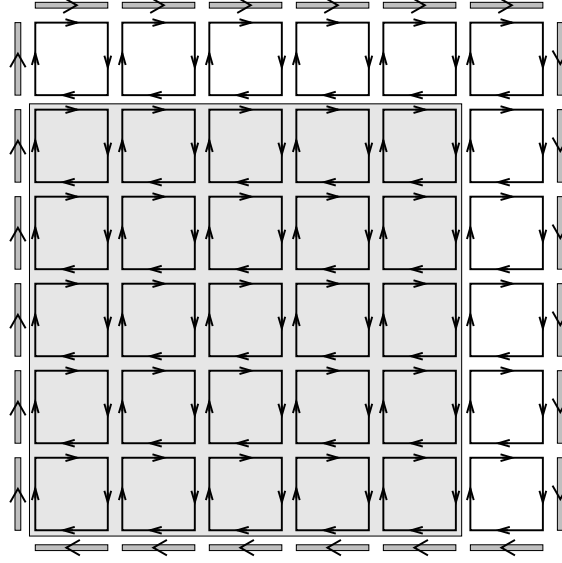
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Fig. 5. Plaquettes in a two-dimensional plane of a 6^4 local lattice. The plaquettes that are fully contained in the local lattice are those in the grey square. Half of the link variables on the edges of the other plaquettes must be fetched from the neighbouring MPI processes. The staples (fat links) at the exterior boundary of the set of plaquettes shown in the figure must be copied from the neighbouring lattices too.

(fat links in fig. 5). It is advantageous to store the copied staples in a buffer before the calculation of the force starts.

Appendix A

When SF boundary conditions are imposed, there is no obviously preferred form of the gauge action near the boundaries of the lattice. The choices A and B proposed in ref. [7] were guided by the requirements of simplicity, O(a)-improvement and ease of use in perturbation theory. For reasons to become clear below, choice A or choice B were recommended depending on whether the boundary values C_k and C'_k vanish or not.

The action defined in subsect. 3.2 includes the required O(a) boundary counterterms and has a number of attractive features:

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

(2) The classical background field

$$U(x, \mu) = \exp\{aB_\mu(x)\},$$

$$B_0(x) = 0, \quad B_k(x) = \{(T - x_0)C_k + x_0 C'_k\}/T, \tag{A.1}$$

is an exact solution of the lattice field equations that are obtained from the action with $c_\mathrm{G} = 1$ by varying the active link variables.

(3) To leading order of perturbation theory, and if $C_k = C'_k = 0$, the action assumes a simple diagonal form in the natural momentum-space representation

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

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

$$p_0 \in \left\{ \frac{\pi n}{T} \;\Big|\; n = 0, 1, \ldots, T - 1 \right\}, \qquad p_k \in \left\{ \frac{2\pi n}{L} \;\Big|\; n = 0, 1, \ldots, L - 1 \right\}, \tag{A.4}$$

of the gauge potential. For simplicity, the lattice spacing was set to unity in these equations and the three lattice sizes $N_k = L$ were taken to be the same. 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 $1/2$. A somewhat lengthy calculation then shows that the action

$$S_\mathrm{G} = \frac{1}{TL^3} {\sum_p}' \sum_{\mu,\nu} \tilde{A}_\mu(p)^* \Delta_{\mu\nu}(p) \tilde{A}_\nu(p) + \mathrm{O}(g_0), \tag{A.5}$$

$$\Delta_{\mu\nu}(p) = \delta_{\mu\nu}\hat{p}^2 - \hat{p}_\mu\hat{p}_\nu - c_1 \left\{ \delta_{\mu\nu} \left[\hat{p}^4 + \tfrac{1}{2}\hat{p}^2 \left(\hat{p}_\mu^2 + \hat{p}_\nu^2 \right) \right] - \hat{p}_\mu^3\hat{p}_\nu - \hat{p}_\mu\hat{p}_\nu^3 \right\}, \tag{A.6}$$

$$\hat{p}_\mu = 2\sin(p_\mu/2), \quad \hat{p}^2 = \sum_\mu \hat{p}_\mu^2, \quad \hat{p}^4 = \sum_\mu \hat{p}_\mu^4, \tag{A.7}$$

is indeed diagonal in Fourier space.

The actions A and B considered in ref. [7] both have property (1), but property (2) is shared only by B and property (3) only by A. For studies of the Schrödinger functional with non-zero boundary values, choice B therefore became the preferred one.

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