Schrödinger functional boundary conditions in the `openQCD` code

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Abstract

Notes on the introduction of Schrödinger functional boundary conditions into the `openQCD` code.

1 Definitions

Schrödinger functional boundary conditions for the gauge link variables are defined by (notation slightly different from Ref. [1])

$$U(x,k)|_{x_0=0} = \exp\{aC_k\} , \qquad C_k = \frac{i}{L}\mathrm{diag}(\phi_1, \phi_2, \phi_3) \tag{1}$$

$$U(x,k)|_{x_0=T} = \exp\{aC'_k\} , \qquad C'_k = \frac{i}{L}\mathrm{diag}(\phi'_1, \phi'_2, \phi'_3), \tag{2}$$

where we have assumed periodic spatial boundary conditions. The $\{\phi_i\}$ and $\{\phi'_i\}$ assume various values and therefore must be left as input parameters, subject to the constraint

$$\sum_{i=1}^{3} \phi_i = \sum_{i=1}^{3} \phi'_i = 0 \tag{3}$$

to ensure that the boundary fields are elements of the group.

For the quark fields we have

$$P_-\psi(x)|_{x_0=0} = P_+\psi(x)|_{x_0=T} = 0 \tag{4}$$

$$\psi(x + L\hat{k}) = e^{i\theta_k}\psi(x), \quad \bar{\psi}(x + L\hat{k}) = \bar{\psi}(x)e^{-i\theta_k}, \tag{5}$$

where $P_\pm = \frac{1}{2}(1 \pm \gamma_0)$. Typically, various values of the $\{\theta_k\}$ are also used. However, due to the periodic spatial boundary conditions implemented in the current version of the `openQCD` code, we shall restrict ourselves to the case $\theta_k = 0$ for the time being.

Sums over loops in the gauge action are restricted to those loops whose corners are in the time interval $[0, T]$. However, some clarification about the relation of the temporal and spatial extents of the lattice is needed. In order to facilitate parallelization, typically an even number (perhaps even a power of two) of sites in both the spatial and temporal directions is used. These extents are requested by specifying the local lattice sizes

via `L0,..,L3` and the number of processors in each direction via `NPROC0,..,NPROC3` such that the total number of sites in each direction is $(\texttt{N0=L0*NPROC0}),..,(\texttt{N3=L3*NPROC3})$.

As discussed above, the values of the temporal links at $t = (\texttt{N0} - 1)a$ are set to zero. The boundary conditions from Eq. 1 and Eq. 4 are then imposed at $t = 0$ and $t = (\texttt{N0} - 1)a$ so that the temporal and spatial extents of the lattice are

$$T = (\texttt{N0} - 1)a, \qquad L_1 = (\texttt{N1})a, \qquad ... \tag{6}$$

Because of Eq. 6, care must be taken in choosing lattices for a continuum limit extrapolation at fixed T/L.

2 Improvement

Apart from bulk improvement terms, additional boundary improvement terms must be added to the action to ensure that correlation functions near the boundary are $\mathrm{O}(a)$-improved. Recall that our gauge action is defined as [2]

$$S_G = \frac{1}{g_0^2} \sum_{k=0}^{1} c_k \sum_{\mathcal{C} \in \mathcal{S}_k} w_k(\mathcal{C}) \mathrm{tr}\{1 - U(\mathcal{C})\}, \tag{7}$$

where $\mathcal{S}_0$ and $\mathcal{S}_1$ are the sets of oriented plaquette and double-plaquette loops (respectively) and $U(\mathcal{C})$ is the product of links around loop $\mathcal{C}$.

Boundary improvement for this action has been examined in Ref. [3]. For the weights $w_k(\mathcal{C})$ we shall use Choice B of Ref. [3], where

$$w_0(\mathcal{C}) = \begin{cases} \frac{1}{2}, & \text{all links in } \mathcal{C} \text{ are on a boundary} \\ c_G, & \mathcal{C} \text{ has exactly one link on a boundary} \\ 1, & \text{otherwise} \end{cases} \tag{8}$$

$$w_1(\mathcal{C}) = \begin{cases} \frac{1}{2}, & \text{all links in } \mathcal{C} \text{ are on a boundary} \\ \frac{3}{2}, & \mathcal{C} \text{ has exactly two links on a boundary} \\ 1, & \text{otherwise.} \end{cases}$$

This choice enables the lattice background field to be expressed analytically. Note that loops that are entirely on the boundaries simply add an irrelevant constant to the action. Also, it should be noted that the choice $c_G = 1$ implements boundary improvement at tree level, regardless of the c_k.

In the fermion sector, the single boundary improvement term required for the Schrödinger functional has the same form as the one for open boundary conditions so the required improvement coefficient (c_F) has the same meaning. Therefore, as with open boundary conditions, two boundary improvement coefficients must be specified, c_F and c_G.

3 Implementation

The main program for performing a Schrödinger functional simulation is `main/qcd2.c`, which takes `main/qcd2.in` as input. More details can be found in `main/README.qcd2`. The input file `main/qcd2.in` is very similar to `main/qcd1.in`, differing only by an additional input parameter group

```
[Boundary values]
phi 0.0 0.0
phi' 0.0 0.0
```

where `phi` and `phi'` are read as arrays of type `double` and length two. In both cases the two elements are taken as the first two diagonal elements of C_k and C_k' from Eq. 1 while the third element is obtained from the condition in Eq. 3.

As discussed above, the fermionic boundary improvement coefficient, which is given by `cF` in the `[Lattice parameters]` input parameter group, has the same meaning in both SF and open boundary conditions. However, the gauge improvement coefficient (`cG`) has a different meaning in SF and open boundary conditions. In the `qcd2` executable, this coefficient is defined as in Eq. 8.

References

[1] M. Luscher, R. Narayanan, P. Weisz, and U. Wolff, Nucl.Phys. **B384**, 168 (1992), hep-lat/9207009.

[2] file `doc/gauge_action.pdf`.

[3] S. Aoki, R. Frezzotti, and P. Weisz, Nucl.Phys. **B540**, 501 (1999), hep-lat/9808007.