IMPLEMENTATION OF $C^\ast$ BOUNDARY CONDITIONS IN THE
HYBRID MONTE CARLO ALGORITHM

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In the study of QCD dynamics, $C^\ast$ boundary conditions are physically relevant in certain cases. In this paper we study the implementation of these boundary conditions in the lattice formulation of full QCD with staggered fermions. In particular, we show that the usual even-odd partition trick to avoid the redoubling of the fermion matrix is still valid in this case. We give an explicit implementation of these boundary conditions for the Hybrid Monte Carlo algorithm.

1. Introduction

Lattice QCD simulations are usually performed with periodic boundary conditions (BC). However, other type of BC may be important in certain cases. For example, a comparison between systems with different BC can be used to understand finite size-effects in lattice QCD. Some years ago$^1$ $C$-periodic BC were studied as an alternative to periodic conditions. Then they were considered with the general idea of studying the spontaneous symmetry breaking aspects of the QCD dynamics in a simple way.$^2$ In that work an analysis was done in the continuum, and it was shown that in pure gauge theory these BC break the $Z(3)$ symmetry explicitey, which has important consequences for the high-temperature deconfinement phase transition. These conditions are also useful in numerical lattice simulations of this transition. When quarks are present, $C$-periodic BC break both chiral and flavour symmetries.

These boundary conditions are also especially important when topological properties are relevant in the system under consideration. This is the case of the lattice studies of confinement through monopole condensation. Recently the role of monopoles in connection with colour confinement has been evidenced in SU(2) and SU(3) gluodynamics,$^3$ for which a disorder parameter based on the magnetic U(1) symmetry has been constructed and studied by Monte Carlo techniques. The disorder parameter is the vacuum expectation value ($\langle vev \rangle$) of a disorder operator, which is an operator that creates a magnetic monopole in the gauge configuration.
The definition of this disorder operator requires $C$-periodic BC in the time direction. For the pure gauge case, this means that the links at time $t + N_t$, where $N_t$ is the temporal extension of the lattice, are the complex conjugate of the links at time $t$. The effect on the simulation algorithm is a simple redefinition of the staples containing links that pierce the temporal boundary. The natural extension of the procedure used for the pure gauge case to full QCD requires the implementation of $C$-periodic BC in the presence of fermions. In particular, we will be concerned with the case of staggered fermions. $C$-periodic BC modify the fermionic matrix, and many proofs of properties used for the setup of standard simulation algorithms no longer hold.

$C$-periodic BC in the continuum are defined by the action of the charge conjugation operator $C$ on the fields.

We will call $C^\dagger$ this symmetry of the lattice action:

$$C^\dagger U_{i,\mu} = U_{i,\mu}^*, \quad C^\dagger \psi_i = \epsilon_i \bar{\psi}_i^T, \quad C^\dagger \bar{\psi}_i = -\psi_i^T \epsilon_i,$$

(1.2)

where $\epsilon_i = (-1)^{x_i + y_i + z_i + t_i}$, $(x_i, y_i, z_i, t_i)$ being the lattice coordinates of point $i$, the “T” represents the transpose operation, and we will use $\psi^* \equiv \bar{\psi}^T$. Translation invariance implies that a BC must correspond to a symmetry of the action. $C^\dagger$-BC are defined as the boundary conditions corresponding to the symmetry (1.2):

$$\Phi_{i+N} = C^\dagger \Phi_i,$$

(1.3)

where $\Phi$ is a field, $U_{\mu}$ or $\psi$, and $N$ is the number of lattice points in the direction in which we use this boundary condition.

In the chiral limit the lattice action has a $U(1)_E \otimes U(1)_O$ chiral symmetry of independent rotations on $(x + y + z + t)$-even and -odd lattice points. $C^\dagger$-BC break explicitly this symmetry to $U(1)_{E=O}$. Baryon number $U(1)_{E=O}$ is also broken explicitly down to $Z(2)_{E=O}$.2

In this paper we will have in mind the physical problem mentioned above: computation of the vev of a monopole creation operator in lattice QCD. This means that we will consider imposing $C^\dagger$-BC in the time direction, and periodic BC in the spatial directions. However this is just to fix the notation in what follows; the
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$C^*$ conditions could in fact be assumed in any direction. The purpose of the paper is to show the theoretical framework to be used in a lattice simulation with these BC (section 2) and how usual algorithms\(^5\) need to be modified (section 3). Our conclusions are summarized in section 4.

2. Mathematical description

Let us consider the partition function of lattice QCD with staggered fermions

$$Z = \int (DU)(D\bar{\psi}D\tilde{\psi}) e^{-S_g-S_f},$$

(2.1)

where $S_g(U)$ is the Wilson action for the pure gauge sector, and $S_f$ is given by Eq. (1.1). The fermionic variables can be integrated out to give

$$Z = \int (DU) e^{-S_g(U)} \det M(U),$$

(2.2)

where\(^*\)

$$M(U)_{i,j} = m\delta_{i,j} + \frac{1}{2} \left( U_{i,\mu} \delta_{i,j-\mu} - U^\dagger_{i+\mu,\mu} \delta_{i,j+\mu} \right),$$

(2.3)

is the fermionic matrix, and periodic BC are assumed. Using this matrix notation, we can write

$$S_f = \bar{\psi}M\psi = \frac{1}{2} \left[ (\bar{\psi}M\psi) + (\bar{\psi}M\psi)^T \right],$$

(2.4)

since $S_f$ is a number. We can use the new variable $\Psi$ defined as the column vector formed by $\psi$ and $\psi^*$, so that the fermionic integral is

$$\int (D\psi)(D\bar{\psi}) e^{-S_f} = \int (D\Psi) e^{-\frac{1}{2} \Psi^T A \Psi} = \text{Pf}(A),$$

(2.5)

$$\Psi^T A \Psi \equiv \left( \begin{array}{c} \psi^T \\ \bar{\psi}^* \end{array} \right) A \left( \begin{array}{c} \psi \\ \bar{\psi}^* \end{array} \right),$$

(2.6)

with

$$A = \left( \begin{array}{cc} 0 & -M^T \\ M & 0 \end{array} \right),$$

(2.7)

and we have introduced the Pfaffian of the matrix $A$, Pf($A$). It is well known that\(^6\)

$$\text{Pf}^2(A) = \det A.$$  

(2.8)

Now let us consider $C^*$-BC in the time direction. Then, following Eqs. (1.2) and (1.3), $\psi_N = \epsilon_0 \psi_0^*$, and $\bar{\psi}_N = -\epsilon_0 \bar{\psi}_0^*$, where we have written in the subscript

\(^*\)We have absorbed the staggered phases by a redefinition of the link matrices $U$.\n
the temporal coordinate and omitted the spatial coordinates. Now Eq. (2.4) gives, for the terms connecting the slices \( N_t - 1 \) and \( N_t \),
\[
\frac{1}{2} \left( \bar{\psi}_{N_t-1} U_{N_t-1,t} \psi_0^* + \psi_0^T U_{N_t-1,t}^\dagger \psi_{N_t-1} \right) \epsilon_0
\]
\[
- \frac{1}{2} \left( \bar{\psi}_0 U_{N_t-1,t}^\dagger \psi_{N_t-1} + \psi_{N_t-1}^T U_{N_t-1,t}^* \psi_0 \right) \epsilon_0 .
\]

(2.9)

In this way the matrix \( A \) of Eq. (2.7) is substituted by
\[
A = \begin{pmatrix} B & -\tilde{M}^T \\ \tilde{M} & -B^* \end{pmatrix} ,
\]

(2.10)

where \( B \) satisfies the properties:
\[
B^\dagger = -B^* \quad B = -B^T
\]

(2.11)

and \( \tilde{M} \) is the fermionic matrix Eq. (2.3) apart from the terms connecting the slices \( N_t - 1 \) and \( N_t \), which have gone to the matrices \( B \) and \( -B^* \).

Eq. (2.5) is still valid and we are interested in calculating \( \text{Pf}(A) \).

### 2.1. Pseudofermionic variables

The usual approach\(^7\) to the simulation of theories with dynamical fermions is to rewrite the determinant of the fermionic matrix in Eq. (2.2) using that
\[
\det(M^\dagger M) \propto \int \mathcal{D}\phi^\dagger \mathcal{D}\phi \exp \left[ -\phi^\dagger (M^\dagger M)^{-1} \phi \right] ,
\]

(2.12)

where \( \phi \) is a complex bosonic field with the same quantum numbers as the Grassmann field. One introduces the matrix \((M^\dagger M)^{-1}\), instead of \(M^{-1}\), so that the pseudofermionic fields can be generated using a simple heatbath method. Since \( \det M \) is a real number, \( \det(M^\dagger M) = (\det M)^2 \). So, actually, this corresponds to a double number of flavours with respect to the original theory. However, the matrix \( M^\dagger M \) has two important properties: it has no matrix elements connecting even and odd lattice sites, and the determinants of its submatrices on the even and odd sites are equal.\(^8\) Therefore one can avoid the redoubling of flavours by defining the pseudofermionic field only on even lattice sites.

A remarkable difference between the partition function with periodic BC and the partition function with \( C^\ast \)-BC is that in the latter case the determinant of \( M \), Eq. (2.2), has to be replaced by the Pfaffian of \( A \), i.e. \( \pm \sqrt{\det A} \). Because of the square root, the usual trick of introducing pseudofermionic fields and rewriting this factor as the integral over these fields can only be applied if the number of continuum fermion flavours is such that the square root cancels. Moreover, in order to have a positive-definite integration measure, we need that the sign in front of this factor be +. Both conditions are satisfied if the number of continuum flavours is a
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multiple of eight. This generates a further unavoidable redoubling. Until Sect. 3.2, we will be concerned with the numerical simulation of $\det A$, which is equivalent to simulating a double number of fermion flavours in the continuum limit (eight instead of four). In Sect. 3.2 we will discuss how to deal with the usual case of four staggered fermion flavours.

Since the case of a system with eight fermion flavours in the continuum limit and $C^\star$-BC and the case of a system with four fermion flavours in the continuum limit and periodic BC are similar, we would like to follow in the former case the standard procedure to obtain the determinant of the matrix $(2.10)$. First, in the Appendix A it is shown that $\det A$ is a real number. So we can also in this case use the matrix $A^\dagger A$ to introduce the pseudofermionic field, which will have now twice the number of components as in the usual case. Second, we will now see that the matrix $A^\dagger A$ does not connect even and odd lattice sites.

Using the form of the fermionic matrix (2.3) and the definitions of $B$ and $\tilde{M}$ given by Eqs. (2.9) and (2.10), we can split the blocks of the matrix $A$ in even and odd lattice sites:

$$A = \begin{pmatrix}
0 & \frac{1}{2} B_{eo} & -m & -\frac{1}{2} D^\dagger_{eo} \\
\frac{1}{2} B_{oe} & 0 & -\frac{1}{2} D^\dagger_{eo} & -m \\
m & \frac{1}{2} D_{eo} & 0 & -\frac{1}{2} B^*_{eo} \\
\frac{1}{2} D_{oe} & m & -\frac{1}{2} B^*_{oe} & 0
\end{pmatrix}. \quad (2.13)$$

From Eqs. (2.3) and (2.11) it is easy to see that

$$D^\dagger_{oe} = -D_{eo}, \quad D^\dagger_{oe} = -D^*_{eo} \quad (2.14)$$

$$B^\dagger_{oe} = -B^*_{eo}, \quad B^\dagger_{oe} = -B_{eo}. \quad (2.15)$$

In the expression (2.13), the new blocks divide the matrix in rows and columns identified by the pairs $[0,e]$, $[0,o]$, $[1,e]$ and $[1,o]$, where the number indicates the blocks defined in Eq. (2.10) and the letter the even/odd subblock. Reorganizing the rows and columns to $[0,e]$, $[1,e]$, $[0,o]$ and $[1,o]$ (the determinant does not change), we rewrite the matrix $A$ in the following form:

$$A = \begin{pmatrix}
\mu \\
\frac{1}{2} A_{eo} \\
\mu
\end{pmatrix}, \quad (2.16)$$

where

$$\mu = \begin{pmatrix}
0 & -m \\
m & 0
\end{pmatrix}, \quad (2.17)$$

$$A_{eo} = \begin{pmatrix}
B_{eo} & D^*_{eo} \\
D_{eo} & -B^*_{eo}
\end{pmatrix}, \quad (2.18)$$

and $A_{oe}$ has the same form as $A_{eo}$ with the exchange $e \leftrightarrow o$. Eqs. (2.14) and (2.15) give

$$A^\dagger_{oe} = -A^*_{eo}. \quad (2.19)$$
From Eqs. (2.3) and (2.9) we obtain the explicit form of the matrices \( D_{eo} \) and \( B_{eo} \):

\[
(D_{eo})_{j,k} = \sum_\mu (U_{j,\mu} \delta_{k,j} + U_{j-\mu,\mu}^\dagger \delta_{k,j} - \mu U_{j,\mu}^\dagger - \mu U_{j-\mu,\mu}) ,
\]

(2.20)

where \( j \) is an even site and the link between \( j \) and \( k \) does not connect the \( t = N_t - 1 \) and \( t = 0 \) time slices (otherwise \( (D_{eo})_{j,k} = 0 \)), and

\[
(B_{eo})_{j,k} = \begin{cases}
U_{j,t}^* & j = N_t - 1, k = 0 \\
U_{k,t}^\dagger & j = 0, k = N_t - 1 \\
0 & \text{in every other case}
\end{cases}
\]

(2.21)

where \( j = N_t - 1 \) or \( j = 0 \) means that the temporal coordinate of site \( j \) is \( N_t - 1 \) or zero, respectively. When \( j \) is an odd site, \( (D_{oe})_{j,k} \) has the same expression as Eq. (2.20), and

\[
(B_{oe})_{j,k} = \begin{cases}
-U_{j,t}^* & j = N_t - 1, k = 0 \\
-U_{k,t}^\dagger & j = 0, k = N_t - 1 \\
0 & \text{in every other case}
\end{cases}
\]

(2.22)

These expressions completely determine every element of the matrices \( A_{eo} \) and \( A_{oe} \).

We now compute

\[
A^\dagger A = \begin{pmatrix}
-\mu^2 + \frac{1}{4} A_{oe}^\dagger A_{oe} & -\frac{1}{2} (\mu A_{eo} - A_{oe}^\dagger \mu) \\
\frac{1}{2} (A_{oe}^\dagger \mu - \mu A_{oe}) & -\mu^2 - \frac{1}{4} A_{oe}^\dagger A_{oe}
\end{pmatrix} .
\]

(2.23)

But using the properties (2.14) and (2.15) it is direct to see that the blocks out of the diagonal in Eq. (2.23) are zero. Then, using Eq. (2.19),

\[
A^\dagger A = \begin{pmatrix}
-\mu^2 - \frac{1}{4} A_{oe}^\dagger A_{oe} & 0 \\
0 & -\mu^2 - \frac{1}{4} A_{oe}^\dagger A_{oe}
\end{pmatrix} .
\]

(2.24)

and, as a result, we see that the matrix \( A^\dagger A \) connects only lattice points of the same parity.

In order to use the same trick to avoid the flavour doubling produced by the introduction of \( A^\dagger A \), that is, to define the pseudofermionic field on even sites only, we need to show that, also in this case, the determinant of the even and odd parts in the matrix (2.24) are equal. This is done in the following subsection.

2.2. Reducing the number of flavours: even-odd partitioning

Let us write \( K \equiv A^\dagger A \). Then we have

\[
K = \begin{pmatrix}
m^2 I_2 - \frac{1}{4} A_{oe}^\dagger A_{oe} & 0 \\
0 & m^2 I_2 - \frac{1}{4} A_{oe}^\dagger A_{oe}
\end{pmatrix} = \begin{pmatrix}
K_e & 0 \\
0 & K_o
\end{pmatrix} ,
\]

(2.25)

where \( I_2 \) is the \( 2 \times 2 \) identity matrix. We need to show that \( \det K_e = \det K_o \). The strategy will be to show that both \( \det K_e \) and \( \det K_o \) are equal to \( \det A \). To this
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aim, let us consider the matrix $A$ written in the e–o partitioned form, Eq. (2.16),

$$ A = \begin{pmatrix} \mu & 1/2 A_{eo} \\ 1/2 A_{eo} & \mu \end{pmatrix}, \quad (2.26) $$

where

$$ \mu = \begin{pmatrix} 0 & -m \\ m & 0 \end{pmatrix}, \quad (2.27) $$

$$ A_{eo} = \begin{pmatrix} B_{eo} & D_{eo}^* \\ D_{eo} & -B_{eo}^* \end{pmatrix}, \quad (2.28) $$

and

$$ A_{oe} = \begin{pmatrix} B_{oe} & D_{oe}^* \\ D_{oe} & -B_{oe}^* \end{pmatrix}. \quad (2.29) $$

We will make use of a general property of the determinant of a square $2N \times 2N$ block matrix,

$$ \det \begin{pmatrix} X & Y \\ W & Z \end{pmatrix} = \det(X) \det(Z - WX^{-1}Y), \quad (2.30) $$

where $X, Y, W, Z$ are $N \times N$ square matrices and $X$ is invertible. Applying this equality to the computation of $\det A$, we obtain

$$ \det A = \det(\mu) \det \left( \mu - 1/4 A_{oe} \mu^{-1} A_{eo} \right) = \det \left( \mu^2 - 1/4 \mu A_{oe} \mu^{-1} A_{eo} \right). \quad (2.31) $$

Using the explicit form of $\mu$ and $A_{oe}$ it is easily shown that

$$ \mu A_{oe} = -A_{oe}^* \mu. \quad (2.32) $$

Inserting this equality in Eq. (2.31), it follows that

$$ \det A = \det \left( \mu^2 + 1/4 A_{oe}^* A_{eo} \right) = \det K_o, \quad (2.33) $$

where the last equality is implied by the fact that $N$ is an even number.

We can compute again $\det A$ using the same procedure after exchanging even and odd variables in $A$. Using a property analogous to that in Eq. (2.32), namely $\mu A_{eo} = -A_{eo}^* \mu$, it is then easily shown that

$$ \det A = \det \left( \mu^2 + 1/4 A_{eo}^* A_{oe} \right) = \det K_e, \quad (2.34) $$

This is a proof that $\det K_e = \det K_o$.

We have shown that $\det K_e \det K_o = (\det A)^2$. On the other hand it is also true that $\det K_e \det K_o = \det(A^\dagger A) = \det A^\dagger \det A$, therefore we have also obtained a proof that $\det A = \det A^\dagger$ alternative to that given in Appendix A. Moreover, we have that

$$ \det A = \det K_e = \det \left( m^2 I_2 + 1/4 A_{oe}^\dagger A_{eo} \right) > 0, \quad (2.35) $$
since both \( m^2 I_2 \) and \( A^{\dagger}_{\mu e} A_{\kappa e} \) are positive definite matrices. Therefore \( \det A \) is a positive number.

We notice that this method can be easily applied also to the standard case, thus providing a proof alternative to those presented in Ref. 8. This is shown in detail in Appendix B.

3. Hybrid Monte Carlo Implementation

We will show now how the standard Hybrid Monte Carlo (HMC) algorithm\(^5\) needs to be modified to incorporate \( C^*\)-BC. In this algorithm one introduces fictitious momenta, conjugate variables of the links, as dynamical variables, and makes fields evolve with a mixed dynamics, in which deterministic and stochastic steps are alternated in a prescribed way. In the deterministic part of the algorithm, the system follows the equations of motion derived from the Hamiltonian of the \((4+1)\)-dimensional system. These equations give the evolution of the fields in the fictitious time \( \tau \). The equation of motion for the matrix \( U_{j,\mu} \) is

\[
\dot{U}_{j,\mu} = i H_{j,\mu} U_{j,\mu},
\]

where the conjugate momentum \( H_{j,\mu} \) is a traceless Hermitian matrix, and \( \dot{U} \) is the derivative of \( U \) with respect to \( \tau \). The equations of motion for the momenta \( H \) are obtained by imposing that the Hamiltonian be constant. The integration of these equations of motion is carried out numerically after discretization of \( \tau \). Usually the temporal step is of order \( 10^{-2} \)–\( 10^{-3} \) and the configuration space is sampled with a total length of the trajectory of order 1. The stochastic part of the algorithm consists in the generation of new momenta and new pseudofermionic variables according to their probability distributions at the beginning of each trajectory. Moreover, at the end of each trajectory a Metropolis accept-reject step is performed, which makes the algorithm exact.

3.1. HMC algorithm with \( C^* \) boundary conditions

Once introduced the pseudofermionic fields, defined only on even sites, and the auxiliary momenta fields, the partition function of the system is

\[
Z = \int (DU D\phi^\dagger D\phi DH) e^{-\mathcal{H}},
\]

with

\[
\mathcal{H} = \frac{1}{2} \sum_{j,\mu} \text{tr}H_{j,\mu}^2 + S_g + \phi^\dagger (A^\dagger A)^{-1} \phi.
\]
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\[ \hat{H}_f = -\sum_{j,\mu} \phi_j (A_j^\dagger A_j)^{-1} \phi_j \left[ \frac{\partial A_j^\dagger}{\partial U_j^\mu} H_{j,\mu} U_{j,\mu} A_j + \frac{\partial A_j^\dagger}{\partial U_j^\mu} \bar{U}_{j,\mu} \bar{H}_{j,\mu} \bar{A}_j + \right. \\
\left. \frac{A_j^\dagger}{\partial U_j^\mu} H_{j,\mu} U_{j,\mu} A_j + \frac{A_j^\dagger}{\partial U_j^\mu} \bar{U}_{j,\mu} \bar{H}_{j,\mu} \bar{A}_j - \frac{A_j^\dagger}{\partial U_j^\mu} H_{j,\mu} \bar{U}_{j,\mu} \bar{A}_j - \frac{A_j^\dagger}{\partial U_j^\mu} \bar{U}_{j,\mu} \bar{H}_{j,\mu} A_j - \right. \\
\left. \frac{U_j^\dagger H_{j,\mu}}{\partial U_j^\mu} A_j - \frac{A_j^\dagger H_{j,\mu}^T}{\partial U_j^\mu} \bar{A}_j - \frac{A_j^\dagger}{\partial U_j^\mu} H_{j,\mu} \bar{U}_{j,\mu} \bar{A}_j - \frac{A_j^\dagger}{\partial U_j^\mu} \bar{U}_{j,\mu} \bar{H}_{j,\mu} \bar{A}_j \right] \\
\times (A_j^\dagger A_j)^{-1} \phi_j, \quad (3.4) \]

where we have made use of Eq. (3.1) and the fact that \( H \) is Hermitian. We have also used that \( A \) is linear in \( U, U^T, U^* \) and \( U^\dagger \), and then the partial derivatives in the previous expression commute with \( H \) and \( U \).

It is convenient to introduce the operator

\[ P_{ij} = X_i X_j^\dagger, \quad (3.5) \]

where

\[ X = (A^\dagger A)^{-1} \phi. \quad (3.6) \]

It is easily seen that \( P \) is Hermitian:

\[ (P^\dagger)_{ij} = (P_{ji})^\dagger = X_i X_j^\dagger = P_{ij}, \quad (3.7) \]

and, being \( \phi \) defined only on even sites, \( P_{ij} \) is taken to be zero unless \( i \) and \( j \) are both even sites. On the other hand, we have that

\[ \left( \frac{\partial A^\dagger}{\partial U} \right)^\dagger = \frac{\partial A}{\partial U^\dagger} \quad \left( \frac{\partial A}{\partial U} \right)^\dagger = \frac{\partial A^\dagger}{\partial U^\dagger} \]

\[ \left( \frac{\partial A^\dagger}{\partial U^T} \right)^\dagger = \frac{\partial A}{\partial U^*} \quad \left( \frac{\partial A}{\partial U^T} \right)^\dagger = \frac{\partial A^\dagger}{\partial U^*} \quad (3.8) \]

and then we can write

\[ \mathcal{H}_f = -\sum_{j,\mu} \text{tr} \left[ i H_{j,\mu} \left( U_{j,\mu} A \frac{\partial A^\dagger}{\partial U_{j,\mu}} + U_{j,\mu} P A^\dagger \frac{\partial A}{\partial U_{j,\mu}} \right) + \right. \\
\left. i H_{j,\mu}^T \left( A \frac{\partial A^\dagger}{\partial U_{j,\mu}^T} U_{j,\mu}^T + P A^\dagger \frac{\partial A}{\partial U_{j,\mu}^T} U_{j,\mu}^T \right) + \text{H.c.} \right], \quad (3.9) \]

where H.c. means the Hermitian conjugate and we have used the cyclic property of the trace operation.
The trace in Eq. (3.9) is taken over both color and site indices. Taking this into account and using the cyclic property again, we have

\[ \mathcal{H}_f = - \sum_{j,\mu} \mathrm{tr} \left( H_{j,\mu} \left\{ i \left[ U_{j,\mu} \left( AP \frac{\partial A^\dagger}{\partial U_{j,\mu}} \right) + U_{j,\mu} \left( PA^\dagger \frac{\partial A}{\partial U_{j,\mu}} \right) \right] + \right. \right. \]

\[ \left. \left. U_{j,\mu} \left( AP \frac{\partial A^\dagger}{\partial U_{j,\mu}^T} \right)^T + U_{j,\mu} \left( PA^\dagger \frac{\partial A}{\partial U_{j,\mu}^T} \right)^T \right\} \right) + \text{H.c.} \right) \].

(3.10)

The following step is to calculate the derivatives appearing in Eq. (3.10). From Eqs. (2.16) and (2.19), we have that

\[ A^\dagger = -A^* \].

(3.11)

We write again \( A \) and \( A^\dagger \) in terms of subblocks, identifying the rows and columns with the pairs \([0, e], [1, e], [0, o] \) and \([1, o] \):

\[ A = \begin{pmatrix} 0 & -m & \frac{1}{2} B_{\text{eo}} & \frac{1}{2} D_{\text{eo}}^* \\ \frac{1}{2} B_{\text{eo}} & 0 & \frac{1}{2} D_{\text{eo}} & -\frac{1}{2} B_{\text{eo}}^* \\ \frac{1}{2} D_{\text{eo}} & -\frac{1}{2} B_{\text{eo}}^* & m & 0 \end{pmatrix} \],

(3.12)

\[ A^\dagger = \begin{pmatrix} 0 & m & -\frac{1}{2} B_{\text{eo}}^* & -\frac{1}{2} D_{\text{eo}} \\ -m & 0 & -\frac{1}{2} D_{\text{eo}}^* & \frac{1}{2} B_{\text{eo}} \\ -\frac{1}{2} B_{\text{eo}} & \frac{1}{2} D_{\text{eo}}^* & 0 & m \\ -\frac{1}{2} D_{\text{eo}}^* & -\frac{1}{2} B_{\text{eo}} & -m & 0 \end{pmatrix} \].

(3.13)

Once written everything in terms of \( B \) and \( D \) we can easily see where \( U \) and \( U^T \) appear, from Eqs. (2.20)–(2.22), and compute the derivatives. The result is given in Table 1.

Now it is easy to calculate the different terms in Eq. (3.10). Let us do, as an example, the first one. The trace over lattice site indices affects only the expressions between parentheses. From Table 1, we see that, for \( j \) even, and \( j \neq N_t - 1 \) or \( \mu \neq t \), the first one gives

\[ \mathrm{tr} \left( AP \frac{\partial A^\dagger}{\partial U_{j,\mu}} \right) = A_{k_2, k_1} X_k X_k^\dagger \left( \frac{\partial A^\dagger}{\partial U_{j,\mu}} \right)_{k_1, k_2} = -\frac{1}{2} A_{[1, o] j + \mu, k} X_k X_k^\dagger_{[0, o] j} = \]

\[ \left( -\frac{1}{4} (D_{\text{eo}})_{j + \mu, k} X_k^0 + \frac{1}{4} (B_{\text{eo}}^*)_{j + \mu, k} X_k^1 \right) (X_k^\dagger)^0_j = \]

\[ -\frac{1}{4} ((A_{\text{eo}})_{j + \mu, k} X_k) (X_k^\dagger)^0_j = -\frac{1}{4} (A_{\text{eo}} X_k^\dagger)^0_{j + \mu} (X_k^\dagger)^0_j, \]

(3.14)

where we have used Eqs. (3.12) and (2.18), and called \( X_k^0 \) the first three components of the vector \( X_k \), and \( X_k^1 \) the second three components. Notice that there is not a mass term because it is diagonal, which would imply that \( k = j + \mu \), that is, \( k \).
Implementacions of $C^*$ boundary conditions in the Hybrid Monte Carlo algorithm

Table 1. Value of the derivatives appearing in Eq. (3.10). $\mu = t$ indicates the time direction, in which we are imposing the $C^*$-BC.

|                      | $j$ even | $j$ odd |
|----------------------|----------|---------|
| ($\partial A^\dagger_{J_{\mu}} / \partial U_{\mu}$)$_{\alpha,\beta}$ | $j \neq N_t - 1$ or $\mu \neq t$ | $\frac{1}{2} \delta_{\alpha,1} [e,j] \delta_{\beta,0} [o,j+\mu] + \frac{1}{2} \delta_{\alpha,0} [e,j] \delta_{\beta,1} [o,j+\mu]$ |
|                      | $j = N_t - 1$ and $\mu = t$ | $-\frac{1}{2} \delta_{\alpha,1} [e,j] \delta_{\beta,1} [o,j+\mu] - \frac{1}{2} \delta_{\alpha,0} [e,j] \delta_{\beta,0} [o,j+\mu]$ |
| ($\partial A^\dagger_{J_{\mu}} / \partial U_{\mu}$)$_{\alpha,\beta}$ | $j \neq N_t - 1$ or $\mu \neq t$ | $-\frac{1}{2} \delta_{\alpha,0} [o,j] \delta_{\beta,1} [o,j+\mu] - \frac{1}{2} \delta_{\alpha,1} [o,j] \delta_{\beta,0} [o,j+\mu]$ |
|                      | $j = N_t - 1$ and $\mu = t$ | $-\frac{1}{2} \delta_{\alpha,0} [o,j] \delta_{\beta,0} [o,j+\mu] + \frac{1}{2} \delta_{\alpha,1} [o,j] \delta_{\beta,1} [o,j+\mu]$ |
| ($\partial A^\dagger_{J_{\mu}} / \partial U_{\mu}$)$_{\alpha,\beta}$ | $j \neq N_t - 1$ or $\mu \neq t$ | $- \frac{1}{2} \delta_{\alpha,1} [o,j+\mu] \delta_{\beta,1} [e,j] - \frac{1}{2} \delta_{\alpha,0} [o,j+\mu] \delta_{\beta,0} [e,j]$ |
|                      | $j = N_t - 1$ and $\mu = t$ | $\frac{1}{2} \delta_{\alpha,1} [o,j+\mu] \delta_{\beta,1} [e,j] + \frac{1}{2} \delta_{\alpha,0} [o,j+\mu] \delta_{\beta,0} [e,j]$ |
| ($\partial A^\dagger_{J_{\mu}} / \partial U_{\mu}$)$_{\alpha,\beta}$ | $j \neq N_t - 1$ or $\mu \neq t$ | $\frac{1}{2} \delta_{\alpha,1} [o,j] \delta_{\beta,0} [o,j+\mu] + \frac{1}{2} \delta_{\alpha,0} [o,j] \delta_{\beta,1} [o,j+\mu]$ |
|                      | $j = N_t - 1$ and $\mu = t$ | $-\frac{1}{2} \delta_{\alpha,1} [o,j] \delta_{\beta,1} [o,j+\mu] - \frac{1}{2} \delta_{\alpha,0} [o,j] \delta_{\beta,0} [o,j+\mu]$ |

would be odd, and then $X_k = 0$. For $j$ even and $j = N_t - 1$, $\mu = t$, an analogous calculation gives

$$\text{tr} \left( AP \partial A^\dagger_{J_{\mu}} \right) = -\frac{1}{4} (A_{\text{oc}} X)^0_{j+\mu} (X^\dagger)^0_j.$$  \hfill (3.15)

This term does not contribute when $j$ is odd, because in this case $(X^\dagger)^0_j$ is zero ($X$ is defined on even sites only).

Computing every other contribution in Eq. (3.10), the final result can be written

$$\mathcal{H}_f = -\sum_{j,\mu} \text{tr} \left\{ H_{j,\mu} \left( i F_{j,\mu} - i F^\dagger_{j,\mu} \right) \right\},$$  \hfill (3.16)

where $F_{j,\mu}$ takes a different form depending on $j$ and $\mu$.

For $j$ even and $(j, \mu) \neq (N_t - 1, t)$,

$$F_{j,\mu} = U_{j,\mu} \left( -\frac{1}{4} (A_{\text{oc}} X)^0_{j+\mu} (X^\dagger)^0_j = \left( \frac{1}{4} X^\dagger_A \left( (A_{\text{oc}} X)^\dagger_{j+\mu} \right) \right)^0_j \right); \hfill (3.17)$$

for $j$ even and $(j, \mu) = (N_t - 1, t)$,

$$F_{j,\mu} = U_{j,\mu} \left( -\frac{1}{4} (A_{\text{oc}} X)^0_{j+\mu} (X^\dagger)^0_j = \left( \frac{1}{4} X^\dagger_A \left( (A_{\text{oc}} X)^\dagger_{j+\mu} \right) \right)^0_j \right); \hfill (3.18)$$

for $j$ odd and $(j, \mu) \neq (N_t - 1, t)$,

$$F_{j,\mu} = U_{j,\mu} \left( \frac{1}{4} X^0_{j+\mu} \left( (A_{\text{oc}} X)^\dagger \right) + \left( \frac{1}{4} (A_{\text{oc}} X)^0_{j+\mu} \right)^0_1 \right); \hfill (3.19)$$
for \( j \) odd and \((j, \mu) = (N_t - 1, t)\),

\[
F_{j,\mu} = U_{j,\mu} \left( \frac{1}{4} X_j^1 ((A_{oe}X)^\dagger)_j - \frac{1}{4} (A_{oe}X)_j^0 (X^\dagger)_j^0 \right)^T .
\]  (3.20)

Since we determined completely the elements of the matrices \( A_{oe} \) and \( A_{oe} \) in section 2.1, these expressions allow us to obtain \( F_{j,\mu} \) as a function of the links \( U \) for every \( j \) and \( \mu \).

Coming back to Eq. (3.3), the condition \( \dot{H} = 0 \) gives

\[
\dot{H} = 0 = \sum_{j,\mu} \text{tr} \left( \dot{H}_{j,\mu} H_{j,\mu} + \frac{\beta}{6} (iH_{j,\mu} V_{j,\mu} + \text{H.c.}) - (iH_{j,\mu} F_{j,\mu} + \text{H.c.}) \right),
\]  (3.21)

where \( V_{j,\mu} \) is the sum of staples, or products of the other three matrices in the plaquettes containing \( U_{j,\mu} \), and arises from the differentiation of the Wilson action \( S_g \). Of course, the staples at the border of the lattice contain links defined by the boundary conditions (\( C^* \) or periodic, depending on the direction). The final solution for \( \dot{H}_{j,\mu} \) is

\[
i\dot{H}_{j,\mu} = \left[ \frac{\beta}{3} U_{j,\mu} V_{j,\mu} - 2F_{j,\mu} \right]_{\text{TA}},
\]  (3.22)

where the subscript TA indicates the traceless anti-Hermitian part of the matrix:

\[
Q_{\text{TA}} = \frac{1}{2}(Q - Q^\dagger) - \frac{1}{6} \text{tr}(Q - Q^\dagger) .
\]  (3.23)

3.2. Reducing the number of flavours: the Hybrid algorithm

Because of Eq. (2.8), the HMC algorithm that we have just described simulates eight fermion flavours in the continuum. In order to come back to four flavours, we note that

\[
\text{Pf}(A) = \pm (\det A)^{1/2}
\]  (3.24)

(we saw in Eq. (2.35) that \( \det A \) is a positive number).

One can simulate \( (\det A)^{1/2} \) by reverting to an approximate algorithm. A suitable choice is the \( R \) algorithm,\(^5\) in which discretization errors in the molecular dynamics part are of \( \mathcal{O}(\Delta \tau^2) \).

On a lattice closed with \( C^*\text{-BC} \), the full QCD action in the presence of \( N_f \) families of degenerate continuum fermions can be written as follows:

\[
Z = \int (DU) [\det(A^\dagger A)^e]^{N_f/8} e^{-S_g(U)} = \int (DU) e^{-S_g(U) + \frac{N_f}{8} \text{tr} \log(A^\dagger A)^e} ,
\]  (3.25)

where \( (A^\dagger A)^e \) is the restriction of \( A^\dagger A \) to the even lattice sites.

Since the implementation of the \( R \) algorithm in the present case reduces to simple adaptation of a standard technique to the system described by the equation
of motion obtained in the previous subsection, we do not elaborate further on this point. However, we still have the “sign problem” of Eq. (3.24). The sign of the Pfaffian can be included by reweighting the expectation values according to

\[ \langle O \rangle = \langle O \cdot \text{signPf}(A) \rangle_+ / \langle \text{signPf}(A) \rangle_+ , \]  

(3.26)

where \( \langle \cdots \rangle_+ \) means that the expectation values have been obtained simulating \( + (\det A)^{1/2} \). One then needs to monitorize the sign of the Pfaffian depending on the gauge configurations. Some techniques to do that are explained in Ref. 9.

4. Conclusions

\( C^* \) boundary conditions are interesting to study some spontaneous symmetry breaking aspects of QCD. They are relevant when one analyses confinement through monopole condensation. We have shown in this work how these boundary conditions can be implemented to carry out a lattice simulation of full QCD with staggered fermions. We have proved that the common even-odd trick used to avoid the fermion redoubling produced by the introduction of the pseudofermionic field can be applied also to this case. However, there is an additional redoubling which forces to work with a minimum number of eight flavours with the usual Hybrid Monte Carlo algorithm, which we have adapted to this case. An alternative to avoid that is to consider a non-exact algorithm, which can be applied to any number of flavours.

These algorithms have been implemented and are presently running on an APE Quadrics machine to explore monopole condensation in full QCD.

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Appendix A

We will show that $\det A$ is a real number, or, equivalently, that $A^\dagger = \det A$. This property is required in order that one can use the matrix $A^\dagger A$ to introduce the pseudofermionic field.

Let us consider $A$ in the form

$$A = \begin{pmatrix} B & -m - D^T \\ m + D & B^\dagger \end{pmatrix},$$

(A.1)

where $D_{i,j} = \tilde{M}_{i,j} - m\delta_{i,j}$.

Using the general property of the determinant of a square block matrix reported in Eq. (2.30) and exchanging the two rows of blocks of $A$ we can rewrite

$$\det A = \det \begin{pmatrix} m + D & B^\dagger \\ B & -m - D^T \end{pmatrix} = \det(m + D) \det(-m - D^T - B(D + m)^{-1}B^\dagger).$$

(A.2)

Remembering that $D^\dagger = -D$, we can write $A^\dagger$ in the form

$$A^\dagger = \begin{pmatrix} B^\dagger & m - D \\ -m + D^T & B \end{pmatrix},$$

(A.3)

so that, exchanging the two columns of blocks in $A^\dagger$ and using again Eq. (2.30), we can write

$$\det A^\dagger = \det \begin{pmatrix} m - D & B^\dagger \\ B & -m + D^T \end{pmatrix} = \det(m - D) \det(-m + D^T - B(-D + m)^{-1}B^\dagger).$$

(A.4)

After extracting a factor $(-1)^N m^{2N} = m^{2N}$ from both $\det A$ and $\det A^\dagger$ and defining $\alpha = 1/m$, we can write

$$\det A = m^{2N} \det(1 + \alpha D) \det(1 + \alpha D^T + \alpha^2 B(1 + \alpha D)^{-1}B^\dagger)$$

$$\det A^\dagger = m^{2N} \det(1 - \alpha D) \det(1 - \alpha D^T + \alpha^2 B(1 - \alpha D)^{-1}B^\dagger)$$

(A.5)

It clearly appears from Eq. (A.5) that $\det A^\dagger$ is obtained from $\det A$ by changing the sign of $\alpha$. Therefore, in order to show that $\det A = \det A^\dagger$, it is sufficient to show that $\det A$ is an even function of $\alpha$.

\footnote{This corresponds to an even number of row exchanges, since $A$ has dimension $2N$ and $N$, being the dimension of the fermion matrix with periodic boundary conditions, is always an even number. Therefore $\det A$ does not change under this operation.}
Implementacion of C* boundary conditions in the Hybrid Monte Carlo algorithm

Let us consider $\det(1 + \alpha D)$ at first. We can expand the determinant as follows:

$$\det(1 + \alpha D) = \exp \left( \text{tr} \ln(1 + \alpha D) \right) = \exp \left( -\text{tr} \sum_{k=1}^{\infty} \frac{(-1)^k}{k} (\alpha D)^k \right).$$  \hspace{1cm} (A.6)

It is easy to see that the trace of the product of an odd number of $D$ matrices is zero. Indeed $D$ only connects nearest neighbour lattice sites, so it is not possible to connect a site to itself using the product of an odd number of $D$ matrices. Therefore only even powers of $\alpha$ appear in the expansion in Eq. (A.6) and $\det(1 + \alpha D)$ is an even function of $\alpha$.

Let us consider now $\det(1 + \alpha D^T + \alpha^2 B (1 + \alpha D)^{-1} B^\dagger)$, which we rewrite as $\det(1 + P(\alpha))$, where

$$P(\alpha) = \alpha D^T + \alpha^2 B \left( \sum_{k=0}^{\infty} (-1)^k \alpha^k D^k \right) B^\dagger. \hspace{1cm} (A.7)$$

We notice that the matrix $P(\alpha)$ is expressed as series expansion in $\alpha$, where the coefficient of the $k$-th term is a homogeneous polynomial of degree $k$ in the matrices $B, B^\dagger, D$ and $D^T$. Therefore, expanding again the determinant as

$$\det(1 + P(\alpha)) = \exp \left( \text{tr} \ln(1 + P(\alpha)) \right) = \exp \left( -\text{tr} \sum_{k=1}^{\infty} \frac{(-1)^k}{k} P(\alpha)^k \right),$$  \hspace{1cm} (A.8)

we see that $\det(1 + P(\alpha))$ can be expanded as a power series in $\alpha$ and that the coefficient of the $k$-th term is the trace of a homogeneous polynomial of degree $k$ in the matrices $B, B^\dagger, D$ and $D^T$: since these matrices only connect nearest neighbour sites, the trace is zero for $k$ odd. Therefore also in this case the determinant is an even function of $\alpha$.

We conclude that $\det A$, being the product of even functions of $\alpha$, is also an even function of $\alpha$, and therefore, from Eq. (A.5), $\det A = \det A^\dagger$.

Appendix B

We will give here a proof, alternative to that presented in Ref. 8, of the equality of the determinants of the submatrices on even and odd sites of $M^\dagger M$ in the case with standard boundary conditions.

In the standard case the fermion matrix $M$, defined in Eq. (2.3), has the following form

$$M = \left( \begin{array}{cc} m & \frac{1}{2} D_{eo} \\ \frac{1}{2} D_{oe} & m \end{array} \right),$$  \hspace{1cm} (B.1)
and it is easily shown that $D_{eo}^\dagger = -D_{oe}$. Using this last property it follows that

$$M^\dagger M = \begin{pmatrix} m^2 - \frac{1}{4}D_{eo}D_{oe} & 0 \\ 0 & m^2 - \frac{1}{4}D_{oe}D_{eo} \end{pmatrix}.$$  \hspace{1cm} (B.2)

Using the decomposition of the determinant given in Eq. (2.30), it is easy to show that

$$\det M = \det \left( m^2 - \frac{1}{4}D_{eo}D_{oe} \right).$$ \hspace{1cm} (B.3)

On the other hand, if we exchange even and odd variables in $M$ before applying Eq. (2.30), we obtain

$$\det M = \det \left( m^2 - \frac{1}{4}D_{eo}D_{oe} \right),$$ \hspace{1cm} (B.4)

and therefore

$$\det \left( m^2 - \frac{1}{4}D_{eo}D_{eo} \right) = \det \left( m^2 - \frac{1}{4}D_{oe}D_{oe} \right).$$ \hspace{1cm} (B.5)