

# Implementation of the lattice Dirac operator<sup>\*</sup>

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## 1. Introduction

In this note, the  $O(a)$ -improved Wilson–Dirac operator that is implemented in the openQCD package is defined, with all normalization conventions and boundary conditions specified explicitly. Even-odd preconditioning and some technical issues concerning the Sheikholeslami–Wohlert term are also covered.

## 2. Definition of the lattice Dirac operator

### 2.1 Quark fields

The theory is set up on a four-dimensional hypercubic lattice of size  $N_0 \times N_1 \times N_2 \times N_3$ , where  $N_\mu$  is assumed to be even and not smaller than 4. For notational convenience, the lattice spacing is set to unity in this note. Unless stated otherwise, the Cartesian coordinates  $(x_0, x_1, x_2, x_3)$  of a lattice point  $x$  are assumed to be in the range  $0 \leq x_\mu < N_\mu$ .

Quark fields  $\psi(x)$  live on the sites  $x$  of the lattice. They have two indices, a Dirac index  $A = 1, \dots, 4$  and a colour index  $\alpha = 1, 2, 3$  on which the gauge field acts. A quark field thus has  $12N_0N_1N_2N_3$  complex components. In the openQCD package, SU(3) matrices, colour vectors and quark spinors are represented by structures that can be treated as single data items (see `include/su3.h`).

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<sup>\*</sup> Based in part on notes written in collaboration with Peter Weisz and Ulli Wolff [1] and notes by Antonio Rago [2].

Table 1. Boundary conditions supported by the openQCD programs

Type	Time extent $T$	Gauge field	Quark fields
0	$N_0 - 1$	open	SF
1	$N_0$	SF	SF
2	$N_0$	open-SF	SF
3	$N_0$	periodic	anti-periodic

Depending on the boundary conditions for the gauge field [3], Schrödinger functional (SF) or anti-periodic boundary conditions are imposed on the quark fields in the time direction (see table 1). The boundary conditions can be selected in the main programs by specifying their type (the index listed in the first column of table 1) in the input parameter file [4]. Note that the effective time extent  $T$  of the lattice (second column) depends on the boundary conditions.

With SF boundary conditions, the quark fields satisfy

$$\psi(x)|_{x_0=0} = 0 \quad (2.1)$$

and additionally

$$\psi(x)|_{x_0=N_0-1} = 0 \quad (2.2)$$

in the case of the boundary conditions of type 0. The dimension of the space of quark fields is thus reduced to  $12(N_0-1)N_1N_2N_3$  and  $12(N_0-2)N_1N_2N_3$ , respectively. All further specifications required for a complete description of the boundary conditions are deferred to the following subsections, since they concern the action of the lattice Dirac operator on the quark fields rather than the field space.

## 2.2 Wilson-Dirac operator

The (unimproved) Wilson-Dirac operator can be written in the compact form

$$D_w = \sum_{\mu=0}^3 \frac{1}{2} \{ \gamma_\mu (\nabla_\mu^* + \nabla_\mu) - \nabla_\mu^* \nabla_\mu \}, \quad (2.3)$$

where

$$\nabla_\mu \psi(x) = U(x, \mu) \psi(x + \hat{\mu}) - \psi(x), \quad (2.4)$$

$$\nabla_\mu^* \psi(x) = \psi(x) - U(x - \hat{\mu}, \mu)^{-1} \psi(x - \hat{\mu}), \quad (2.5)$$

denote the gauge-covariant forward and backward lattice derivatives in presence of the gauge field  $U(x, \mu)$ . The symbol  $\hat{\mu}$  here stands for the unit vector in direction  $\mu$  and the Dirac matrices  $\gamma_\mu$  are specified in appendix A.

More explicitly, in the time range  $0 < x_0 < N_0 - 1$ , the action of the operator on a given quark field  $\psi$  is given by

$$D_w \psi(x) = 4\psi(x) - \sum_{\mu=0}^3 \frac{1}{2} \{ U(x, \mu)(1 - \gamma_\mu)\psi(x + \hat{\mu}) + U(x - \hat{\mu}, \mu)^{-1}(1 + \gamma_\mu)\psi(x - \hat{\mu}) \}. \quad (2.6)$$

It is understood here that the field is periodically extended in the space directions,

$$\psi(x + N_k \hat{k}) = e^{i\theta_k} \psi(x), \quad k = 1, 2, 3, \quad (2.7)$$

where  $\theta_1, \theta_2, \theta_3$  are some prescribed real angles. Up to the phase factors  $e^{i\theta_k}$ , periodic boundary conditions are thus imposed in these directions. All terms in eq. (2.6) refer to the quark field at time  $x_0$  and  $x_0 \pm 1$  only and are therefore unambiguously defined when  $x_0$  is in the specified range. The action of the Dirac operator at time  $x_0 = 0$  and  $x_0 = N_0 - 1$ , on the other hand, depends on the boundary conditions and will be defined in subsection 2.5.

### 2.3 $O(a)$ -improved lattice Dirac operator

Apart from the Sheikholeslami–Wohlert (SW) term [5] and a boundary  $O(a)$  correction term, it is now convenient to include the bare mass parameter  $m_0$  in the Dirac operator (the operator thus becomes dependent on the quark flavour considered). The massive  $O(a)$ -improved Wilson–Dirac operator is then given by

$$D = D_w + \delta D_v + \delta D_b + m_0, \quad (2.8)$$

where

$$\delta D_v \psi(x) = c_{sw} \sum_{\mu, \nu=0}^3 \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu}(x) \psi(x), \quad (2.9)$$

$$\delta D_b \psi(x) = \{(c_F - 1)\delta_{x_0,1} + (c'_F - 1)\delta_{x_0, T-1}\} \psi(x). \quad (2.10)$$

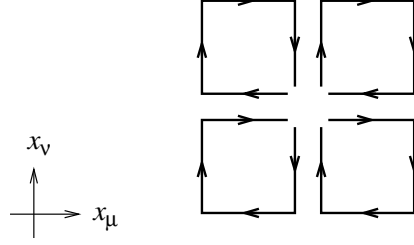


Fig. 1. Graphical representation of the products of gauge field variables contributing to the lattice field strength tensor (2.13). Each square corresponds to one of the terms in eq. (2.14).

In these equations,  $c_{\text{sw}}$ ,  $c_{\text{F}}$  and  $c'_{\text{F}}$  are improvement coefficients, the latter satisfying

$$c'_{\text{F}} = c_{\text{F}} \quad \text{for boundary conditions of type 0 and 1,} \quad (2.11)$$

$$c'_{\text{F}} = c_{\text{F}} = 1 \quad \text{for boundary conditions of type 3} \quad (2.12)$$

(and thus  $\delta D_{\text{b}} = 0$  in the case of periodic boundary conditions). For the field strength of the gauge field,

$$\widehat{F}_{\mu\nu}(x) = \frac{1}{8} \{Q_{\mu\nu}(x) - Q_{\nu\mu}(x)\}, \quad (2.13)$$

$$\begin{aligned} Q_{\mu\nu}(x) = & U(x, \mu)U(x + \hat{\mu}, \nu)U(x + \hat{\nu}, \mu)^{-1}U(x, \nu)^{-1} + \\ & U(x, \nu)U(x - \hat{\mu} + \hat{\nu}, \mu)^{-1}U(x - \hat{\mu}, \nu)^{-1}U(x - \hat{\mu}, \mu) + \\ & U(x - \hat{\mu}, \mu)^{-1}U(x - \hat{\mu} - \hat{\nu}, \nu)^{-1}U(x - \hat{\mu} - \hat{\nu}, \mu)U(x - \hat{\nu}, \nu) + \\ & U(x - \hat{\nu}, \nu)^{-1}U(x - \hat{\nu}, \mu)U(x + \hat{\mu} - \hat{\nu}, \nu)U(x, \mu)^{-1}, \end{aligned} \quad (2.14)$$

the usual symmetric lattice expression is taken (see fig. 1). The normalization conventions adopted here coincide with the ones in ref. [6]. In particular, at tree-level of perturbation theory, on-shell  $O(a)$ -improvement is achieved by setting  $c_{\text{sw}} = c_{\text{F}} = c'_{\text{F}} = 1$ .

#### 2.4 “Exponential” variant of the improvement terms

The traditional choice (2.9),(2.10) of the improvement terms is not the only possible one. In fact, any local lattice expression with the same symmetry properties and

behaviour in the classical continuum limit is, in principle, equally acceptable. One may, for example, set

$$\begin{aligned}
(\delta D_v + \delta D_b)\psi(x) &= \{4 + m_0 + (c_F - 1)\delta_{x_0,1} + (c'_F - 1)\delta_{x_0,T-1}\} \\
&\times \exp\left\{\frac{c_{sw}}{4 + m_0} \sum_{\mu,\nu=0}^3 \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu}(x)\right\} \psi(x) - (4 + m_0)\psi(x),
\end{aligned} \tag{2.15}$$

a choice that will be referred to as the exponential variant of the improvement terms.

### 2.5 Action of the Dirac operator at $x_0 = 0$ and $x_0 = N_0 - 1$

For all types of boundary conditions and at all times  $x_0$  in the range  $0 < x_0 < N_0 - 1$ , the action of the Dirac operator  $D$  on a given quark field  $\psi(x)$  is given by eqs. (2.6)–(2.15). In the specified range of time, all terms in these formulae are completely well defined and need no further explanation.

At time  $x_0 = 0$  and  $x_0 = N_0 - 1$ , the action of the Dirac operator depends on the type of boundary conditions:

*Type 0.* Here one simply sets

$$D\psi(x)|_{x_0=0} = D\psi(x)|_{x_0=N_0-1} = 0. \tag{2.16}$$

This rule is in fact implied by the requirement that the Dirac operator must be a linear operator in the space of quark fields satisfying eqs. (2.1) and (2.2).

*Type 1 and 2.* Consistency with the condition (2.1) requires again that

$$D\psi(x)|_{x_0=0} = 0, \tag{2.17}$$

but at  $x_0 = N_0 - 1$  one may choose the action of the Dirac operator to be given by the same equations as in the bulk of the lattice together with the prescription

$$\psi(x + \hat{0})|_{x_0=N_0-1} = 0, \tag{2.18}$$

which imposes Schrödinger functional boundary conditions at time  $N_0$ .

*Type 3.* In this case, the action of the Dirac operator is again given by eqs. (2.6)–(2.15), at all times in the range  $0 \leq x_0 \leq N_0 - 1$ , where

$$\psi(x)|_{x_0=-1} = -\psi(x)|_{x_0=N_0-1}, \quad \psi(x)|_{x_0=N_0} = -\psi(x)|_{x_0=0}, \tag{2.19}$$

is to be inserted in eq. (2.6) for the otherwise undefined components of the quark field at time  $-1$  and  $N_0$ .

In all cases, the field tensor and the Pauli term are only required at the interior points of the lattice. Both are unambiguously defined through eqs. (2.9),(2.13) and (2.14), at all these points, once the boundary conditions for the gauge field are taken into account. With the rules stated above, the definition of the lattice Dirac operator  $D$  is thus complete.

### 2.6 Block Dirac operators

Some of the solvers for the Dirac equation included in the openQCD package make use of a domain-decomposition (SAP) preconditioner. The domains are taken to be hypercubic blocks of lattice points. On each block  $\Lambda$ , the block Dirac operator  $D_\Lambda$  is defined by

$$D_\Lambda = P_\Lambda D P_\Lambda, \quad (2.20)$$

where

$$P_\Lambda \psi(x) = \begin{cases} \psi(x) & \text{if } x \in \Lambda, \\ 0 & \text{otherwise,} \end{cases} \quad (2.21)$$

projects any quark field  $\psi$  to the block.

The projection (2.20) amounts to imposing Dirichlet boundary conditions on the block boundaries. In addition, the quark fields on the blocks must satisfy the constraints (2.1),(2.2), if these are part of the boundary conditions on the global lattice.

## 3. Even-odd preconditioning

The discussion in the following applies to both the global and block Dirac operators, but for simplicity only the global Dirac operator is considered.

A lattice point  $x$  is classified as even or odd depending on whether the sum of its coordinates,  $x_0 + x_1 + x_2 + x_3$ , is even or odd. Any quark field  $\psi$  may be split into two parts,

$$\psi = \psi_e + \psi_o, \quad (3.1)$$

where  $\psi_e$  is supported on the even sites and  $\psi_o$  on the odd sites. If the lattice points are labeled such that the even ones come first, the Dirac operator assumes the block form

$$D = \begin{pmatrix} D_{ee} & D_{eo} \\ D_{oe} & D_{oo} \end{pmatrix}. \quad (3.2)$$

The operators  $D_{eo}$  and  $D_{oe}$  are the sums of the hopping terms in eq. (2.6) from the odd to the even and the even to the odd points, respectively, while

$$D_{ee} + D_{oo} = M_0 + c_{sw} \sum_{\mu, \nu=0}^3 \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu}, \quad (3.3)$$

$$M_0 \psi(x) = \{4 + m_0 + (c_F - 1)\delta_{x_0,1} + (c'_F - 1)\delta_{x_0,T-1}\} \psi(x), \quad (3.4)$$

in the case of the traditional choice of the improvement terms and

$$D_{ee} + D_{oo} = M_0 \exp \left\{ \frac{c_{sw}}{4 + m_0} \sum_{\mu, \nu=0}^3 \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu} \right\} \quad (3.5)$$

if the exponential variant is chosen.

In the following, it is taken for granted that the diagonal part  $D_{ee} + D_{oo}$  of the Dirac operator is safely invertible. For any given source field  $\eta$ , the Dirac equation  $D\psi = \eta$  can then be solved by first solving

$$\hat{D}\psi_e = \eta_e - D_{eo}D_{oo}^{-1}\eta_o, \quad (3.6)$$

for  $\psi_e$ , where

$$\hat{D} = D_{ee} - D_{eo}D_{oo}^{-1}D_{oe} \quad (3.7)$$

denotes the even-odd preconditioned Dirac operator. After that the odd field component is obtained through

$$\psi_o = D_{oo}^{-1} \{ \eta_o - D_{oe}\psi_e \}. \quad (3.8)$$

Note that  $\hat{D}$  is a linear operator acting on quark fields defined on the sublattice of all even points.

Even-odd preconditioning goes along with the factorization

$$\det D = \det D_{\text{oo}} \det \hat{D} \quad (3.9)$$

of the quark determinant. An important detail to keep in mind is the fact that, by definition,  $D_{\text{oe}}\psi(x)$  vanishes at time 0 and  $N_0 - 1$  if the boundary conditions require  $D\psi(x)$  to vanish there. The operator product on the right of eq. (3.6) then involves the inverse of  $D_{\text{oo}}$  on the odd sites  $x$  at all other times only, and for the same reason, the determinant  $\det D_{\text{oo}}$  is a product of determinants, one for each odd point in this range of time.

Since the Pauli term in the exponent in eq. (3.5) is traceless, the factor  $\det D_{\text{oo}}$  is independent of the gauge field, and can therefore just as well be dropped, if the exponential variant of the improvement terms is chosen.

#### 4. Computation of $D_{\text{ee}}$ and $D_{\text{oo}}$

The computation of the Pauli term tends to be slow, because there are quite many products and sums of SU(3) matrices that must be evaluated. Taking the inverse of  $D_{\text{oo}}$ , as is required for even-odd preconditioning, and the evaluation of the exponential in eq. (3.5), if the exponential variant of the improvement terms is chosen, are further numerically costly operations. The diagonal parts of the Dirac operator are therefore computed separately and stored in an array before the operator is applied.

##### 4.1 Computation of the Pauli term

In the representation of the Dirac matrices specified in appendix A, the Pauli term

$$\sum_{\mu,\nu=0}^3 \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu} = \sum_{k=1}^3 \frac{i}{16} \begin{pmatrix} \sigma_k (\mathcal{E}_k - \mathcal{B}_k) & 0 \\ 0 & -\sigma_k (\mathcal{E}_k + \mathcal{B}_k) \end{pmatrix} \quad (4.1)$$

has a block diagonal form. A factor 8 was included here in the definition

$$\mathcal{E}_k = 8\hat{F}_{0k}, \quad \mathcal{B}_k = \sum_{l,j=1}^3 4\epsilon_{klj} \hat{F}_{lj}, \quad (4.2)$$

of the electric and magnetic components of the field strength. They are then simply equal to  $Q_{\mu\nu} - Q_{\mu\nu}^\dagger$  for some  $\mu$  and  $\nu$ .



The computation of the matrix  $Q_{\mu\nu}(x)$  at fixed  $x, \mu, \nu$  requires 12 multiplications of SU(3) matrices. A straightforward code for the SW term will therefore perform 72 multiplications per point. One can do better by running through all plaquettes in the (0, 1)-plane, then those in the (0, 2)-plane, and so on. On each plaquette there are four ordered products of link variables to be added to the matrices  $(Q_{\mu\nu} - Q_{\mu\nu}^\dagger)(y)$  at the corners  $y$  of the plaquette. This requires 8 matrix multiplications per plaquette and thus a total of 48 multiplications per lattice point.

#### 4.2 Storage format

From eq. (4.1) one infers that the application of  $D_{ee} + D_{oo}$  to a given spinor field amounts to multiplying the spinors at each point  $x$  by a matrix of the block-diagonal form

$$\begin{pmatrix} A_+(x) & 0 \\ 0 & A_-(x) \end{pmatrix}, \quad (4.3)$$

where  $A_\pm(x)$  are Hermitian  $6 \times 6$  matrices. Such matrices may be represented by arrays  $u_0, \dots, u_{35}$  of 36 real numbers according to

$$\begin{pmatrix} u_0 & u_6 + iu_7 & u_8 + iu_9 & u_{10} + iu_{11} & u_{12} + iu_{13} & u_{14} + iu_{15} \\ . & u_1 & u_{16} + iu_{17} & u_{18} + iu_{19} & u_{20} + iu_{21} & u_{22} + iu_{23} \\ . & . & u_2 & u_{24} + iu_{25} & u_{26} + iu_{27} & u_{28} + iu_{29} \\ . & . & . & u_3 & u_{30} + iu_{31} & u_{32} + iu_{33} \\ . & . & . & . & u_4 & u_{34} + iu_{35} \\ . & . & . & . & . & u_5 \end{pmatrix}. \quad (4.4)$$

In openQCD the matrices  $A_\pm(x)$  are stored in this way, using the data types `pauli` and `pauli_double` for the single- and double-precision versions of  $D_{ee} + D_{oo}$ . The program that computes the matrices writes them to the elements of an array, first the matrices  $A_\pm(x)$  at all even points  $x$  and then those at the odd points. At the boundaries of the lattice (if any), the matrices are set to unity (cf. subsect. 2.5).

The field tensor  $\hat{F}_{\mu\nu}(x)$  is saved in a separate array of type `u3_alg_double` and is reused when the matrices  $A_\pm(x)$  must be recomputed for a given gauge field, as is the case, for example, if the theory includes quarks with different masses  $m_0$ .

#### 4.3 Exponential of the Pauli term

If the exponential variant of the improvement terms is chosen, the exponential (3.5) of the Pauli term must be computed. This amounts to exponentiating two traceless

$6 \times 6$  Hermitian matrices at each point  $x$ , a computation that can be efficiently performed using the Cayley-Hamilton theorem.

The theorem asserts that any matrix  $A$  satisfies its own characteristic equation. Specifically, if  $A$  is a traceless  $6 \times 6$  Hermitian matrix, the equation

$$A^6 = \sum_{k=0}^4 p_k A^k \quad (4.5)$$

holds, with real coefficients  $p_k$  given by

$$p_0 = \frac{1}{6} \text{tr} \{A^6\} - \frac{1}{8} \text{tr} \{A^4\} \text{tr} \{A^2\} - \frac{1}{18} \text{tr} \{A^3\}^2 + \frac{1}{48} \text{tr} \{A^2\}^3, \quad (4.6)$$

$$p_1 = \frac{1}{5} \text{tr} \{A^5\} - \frac{1}{6} \text{tr} \{A^3\} \text{tr} \{A^2\}, \quad (4.7)$$

$$p_2 = \frac{1}{4} \text{tr} \{A^4\} - \frac{1}{8} \text{tr} \{A^2\}^2, \quad (4.8)$$

$$p_3 = \frac{1}{3} \text{tr} \{A^3\}, \quad (4.9)$$

$$p_4 = \frac{1}{2} \text{tr} \{A^2\}. \quad (4.10)$$

An arbitrary polynomial

$$\sum_{k=0}^N c_k A^k \quad (4.11)$$

in  $A$  of degree  $N \geq 6$  can therefore be reduced to a polynomial

$$\sum_{k=0}^5 q_k A^k \quad (4.12)$$

of degree 5 with  $A$ -dependent coefficients  $q_k$ , which may be calculated through a simple recursion<sup>†</sup>.

The matrices  $A$  in the exponent in eq. (3.5) satisfy

$$\|A\| \leq 6\kappa c_{\text{sw}}, \quad \kappa = (8 + 2m_0)^{-1}. \quad (4.13)$$

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<sup>†</sup> The computational strategy followed here is the same as the one described in the notes [7] for the exponentiation of elements of the Lie algebra of  $\text{SU}(3)$ .

In practice the eigenvalues of these matrices thus have magnitude less than 2 or so. The Taylor series

$$e^A = \sum_{k=0}^N \frac{A^k}{k!} + r_N(A) \quad (4.14)$$

consequently converges rapidly, with a remainder bounded by

$$\|r_N(A)\| \leq \frac{\|A\|^{N+1}}{(N+1)!} e^{\|A\|}. \quad (4.15)$$

Using the Cayley-Hamilton theorem, as described above, the exponential of the Pauli term can in this way easily be obtained to machine precision.

## 5. Inversion of $D_{\text{ee}}$ and $D_{\text{oo}}$

As explained in sect. 3, even-odd preconditioning requires the inversion of the diagonal part  $D_{\text{oo}}$  of the Dirac operator on the odd sites of the lattice. This amounts to computing the inverse of a large number of  $6 \times 6$  matrices. Householder triangularization with subsequent inversion by back-substitution is a numerically safe and reasonably fast method that can be applied here (see refs. [8,9], for example). The precise form of the algorithm that is implemented in the openQCD package is discussed in this section.

The fact that  $D_{\text{oo}}$  may turn out to be ill-conditioned is a possible source of difficulty. Catastrophically large rounding errors are then practically unavoidable when the matrices are inverted (see appendix B). The program that performs the inversion returns with a non-zero error code in this case, which is propagated to the top level of the simulation program.

If the exponential variant of the improvement terms is chosen, the matrices are always well-conditioned. Moreover, the inverse of  $D_{\text{oo}}$  may also be directly computed simply by changing the sign of the Pauli term in eq. (3.5) before it is exponentiated.

### 5.1 Householder triangularization

In the following, the inversion of a general complex  $n \times n$  matrix  $A$  is considered. The Householder algorithm transforms the matrix to upper triangular form by applying

a series of reflections of the type

$$R = 1 - 2 \frac{u \otimes u^\dagger}{\|u\|^2}, \quad (5.1)$$

where  $u$  is some non-zero complex vector in  $n$  dimensions. One needs  $n-1$  reflections to completely triangularize  $A$ , i.e. the triangular matrix  $T$  that one constructs is given by

$$T = R_{n-1} R_{n-2} \dots R_1 A. \quad (5.2)$$

The basic idea is to choose the reflections  $R_k$  recursively in such a way that the matrix

$$R_{j-1} R_{j-2} \dots R_1 A \quad (5.3)$$

has no non-zero entries below the diagonal in the first  $j-1$  columns.

Suppose we have achieved this for all  $j \leq k$  and let us denote the  $k$ 'th column vector of the matrix  $R_{k-1} \dots R_1 A$  by  $v$ . We then take  $R_k$  to be of the form (5.1) with

$$u_l = \begin{cases} 0 & \text{if } l < k, \\ v_k - y_k & \text{if } l = k, \\ v_l & \text{if } l > k, \end{cases} \quad (5.4)$$

where  $y_k$  is given by

$$y_k = -\frac{v_k}{|v_k|} r, \quad r^2 = \sum_{j=k}^n |v_j|^2, \quad r \geq 0. \quad (5.5)$$

It is easy to check that the first  $k-1$  columns of  $R_{k-1} \dots R_1 A$  are left intact when this matrix is multiplied with  $R_k$ , while the  $k$ 'th column vector becomes

$$(v_1, \dots, v_{k-1}, y_k, 0, \dots, 0). \quad (5.6)$$

If we continue in this way up to  $k = n-1$ , the final matrix (5.2) will hence be upper triangular with diagonal elements  $y_1, \dots, y_{n-1}, -y_n$ .

Evidently the algorithm breaks down if  $u$  vanishes for some  $k$ . Noting

$$\frac{1}{2} \|u\|^2 = r^2 + r|v_k|, \quad (5.7)$$

it follows that this happens if and only if  $A$  is singular. During the execution of the program one can easily check that  $r$  is positive and take the appropriate action if it vanishes.

Another potentially unstable situation occurs when  $v_k = 0$ . It turns out, however, that this does not present a fundamental difficulty. If  $v_k$  is so small that  $|v_k| + r = r$  to machine precision, we simply set  $y_k = -r$ . The reflection  $R_k$ , defined through eqs. (5.1),(5.4), then transforms the column vector  $v$  to the vector (5.6) up to rounding errors. Equation (5.7) remains true in the same sense, i.e. to machine precision. The choice  $y_k = -r$  is hence completely satisfactory in this case.

### 5.2 Inversion of $T$

We now describe the computation of the inverse  $S$  of the triangular matrix  $T$ , assuming that none of the diagonal elements of  $T$  vanish. It can be shown that  $S$  is also upper triangular, i.e. the matrix elements  $t_{ij}$  and  $s_{ij}$  of  $T$  and  $S$  are equal to zero for all  $i > j$ .

The linear equations from which  $S$  is to be determined are

$$\sum_{j=i}^k t_{ij} s_{jk} = \delta_{ik}. \quad (5.8)$$

Choosing  $i = k$  one immediately concludes that

$$s_{ii} = 1/t_{ii}. \quad (5.9)$$

For  $i < k$  the equations can then be written in the form

$$s_{ik} = -s_{ii} \sum_{j=i+1}^k t_{ij} s_{jk}. \quad (5.10)$$

They can be solved recursively, first setting  $k = n$ , then  $k = n - 1$  and so on, while for each  $k$  one starts with  $i = k - 1$  and continues to  $i = 1$ . It is not difficult to see that the element  $t_{ik}$  may be overwritten by  $s_{ik}$  in this process, since  $t_{ik}$  is not needed at the later stages of the recursion. In other words, the inversion can be achieved in place without a second array.

### 5.3 Final steps

Using the orthogonality of the Householder reflections, it is trivial to show that

$$A^{-1} = SR_{n-1}R_{n-2} \dots R_1. \quad (5.11)$$

The computation can thus be completed by evaluating the product on the right-hand side of this equation recursively.

## 6. Programs

The programs that compute the field tensor (2.13),(2.14) and the diagonal part  $D_{ee} + D_{oo}$  of the Dirac operator are contained in the directories `modules/tcharge` and `modules/sw_term`, respectively. Whether the traditional or the exponential variant of the improvement terms is used depends on what is specified in the parameter data base [4].

The programs for the Dirac operator are in the directory `modules/dirac`. There are programs implementing the action of  $D$  and  $\hat{D}$  on quark fields on the full lattice and on blocks of lattice points. Most programs admit a further mass parameter  $\mu$  and add the twisted-mass term  $i\mu\gamma_5$  to the Dirac operator. Moreover, it is possible to restrict the twisted-mass term to the even sites of the lattice by setting a flag (see `modules/flags/lat_parms.c`).

Anti-periodic boundary conditions in time for the quark fields are implemented by changing the sign of the link variables  $U(x, 0)$  at time  $x_0 = N_0 - 1$  before calling any programs for the Dirac operator. Similarly, the phases in eq. (2.7) are taken into account by phase-shifting the spatial link variables according to

$$U(x, k) \rightarrow e^{i\theta_k/N_k} U(x, k), \quad k = 1, 2, 3. \quad (6.1)$$

The correctness of this formulation can be shown by applying a  $U(1)$  gauge transformation. In the simulation programs, where only the (gauge-invariant) quark determinant enters, the transformation has no effect, but when observables are evaluated one must be careful to make consistent use of the calculated quark propagators.

The functions that change the  $U(1)$  phase of the link variables are `set_ud_phase()` and `unset_ud_phase()` in the module `uflds/uflds.c`. When gauge configurations are written to disk, all link variables are guaranteed to have the phase-change undone and thus have determinant 1 within rounding errors. Measurement programs based on openQCD modules should therefore call `set_ud_phase()` immediately after importing a field configuration from disk in order to ensure that the boundary conditions are correctly implemented (see `main/ms1.c` for example).

## Appendix A

It is advantageous to work with a chiral representation of the Dirac matrices, where

$$\gamma_\mu = \begin{pmatrix} 0 & e_\mu \\ (e_\mu)^\dagger & 0 \end{pmatrix}. \quad (\text{A.1})$$

A possible choice for the  $2 \times 2$  matrices  $e_\mu$  is

$$e_0 = -1, \quad e_k = -i\sigma_k \quad (\text{A.2})$$

( $k = 1, 2, 3$ , and  $\sigma_k$  are the Pauli matrices). It is then easy to check that

$$(\gamma_\mu)^\dagger = \gamma_\mu, \quad \{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}. \quad (\text{A.3})$$

Furthermore, if we define  $\gamma_5 = \gamma_0\gamma_1\gamma_2\gamma_3$ , we have

$$\gamma_5 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (\text{A.4})$$

In particular,  $(\gamma_5)^\dagger = \gamma_5$  and  $(\gamma_5)^2 = 1$ . The hermitian matrices

$$\sigma_{\mu\nu} = \frac{i}{2} [\gamma_\mu, \gamma_\nu] \quad (\text{A.5})$$

that appear in the SW term are explicitly given by

$$\sigma_{0k} = \begin{pmatrix} \sigma_k & 0 \\ 0 & -\sigma_k \end{pmatrix}, \quad \sigma_{ij} = -\epsilon_{ijk} \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}, \quad (\text{A.6})$$

where  $\epsilon_{ijk}$  is the totally anti-symmetric tensor with  $\epsilon_{123} = 1$ .

The hopping terms in the Wilson–Dirac operator involve the projected spinors

$$\phi = (1 - s\gamma_\mu)\psi, \quad s = \pm 1. \quad (\text{A.7})$$

In the programs that implement the operator, these terms are hand-programmed, following the lines

$$s = +1, \quad \mu = 0 :$$

$$\phi_1 = \psi_1 + \psi_3$$

$$\begin{aligned}
\phi_2 &= \psi_2 + \psi_4 \\
\phi_3 &= \phi_1 \\
\phi_4 &= \phi_2
\end{aligned} \tag{A.8}$$

$$\begin{aligned}
s &= -1, \quad \mu = 0 : \\
\phi_1 &= \psi_1 - \psi_3 \\
\phi_2 &= \psi_2 - \psi_4 \\
\phi_3 &= -\phi_1 \\
\phi_4 &= -\phi_2
\end{aligned} \tag{A.9}$$

$$\begin{aligned}
s &= +1, \quad \mu = 1 : \\
\phi_1 &= \psi_1 + i\psi_4 \\
\phi_2 &= \psi_2 + i\psi_3 \\
\phi_3 &= -i\phi_2 \\
\phi_4 &= -i\phi_1
\end{aligned} \tag{A.10}$$

$$\begin{aligned}
s &= -1, \quad \mu = 1 : \\
\phi_1 &= \psi_1 - i\psi_4 \\
\phi_2 &= \psi_2 - i\psi_3 \\
\phi_3 &= i\phi_2 \\
\phi_4 &= i\phi_1
\end{aligned} \tag{A.11}$$

$$\begin{aligned}
s &= +1, \quad \mu = 2 : \\
\phi_1 &= \psi_1 + \psi_4 \\
\phi_2 &= \psi_2 - \psi_3 \\
\phi_3 &= -\phi_2 \\
\phi_4 &= \phi_1
\end{aligned} \tag{A.12}$$

$$s = -1, \quad \mu = 2 :$$



$$\begin{aligned}
\phi_1 &= \psi_1 - \psi_4 \\
\phi_2 &= \psi_2 + \psi_3 \\
\phi_3 &= \phi_2 \\
\phi_4 &= -\phi_1
\end{aligned} \tag{A.13}$$

$$\begin{aligned}
s &= +1, \quad \mu = 3 : \\
\phi_1 &= \psi_1 + i\psi_3 \\
\phi_2 &= \psi_2 - i\psi_4 \\
\phi_3 &= -i\phi_1 \\
\phi_4 &= i\phi_2
\end{aligned} \tag{A.14}$$

$$\begin{aligned}
s &= -1, \quad \mu = 3 : \\
\phi_1 &= \psi_1 - i\psi_3 \\
\phi_2 &= \psi_2 + i\psi_4 \\
\phi_3 &= i\phi_1 \\
\phi_4 &= -i\phi_2
\end{aligned} \tag{A.15}$$

## Appendix B

In this appendix, the numerical stability of the matrix inversion algorithm described in sect. 5 is discussed. For the matrices of interest the inversion requires a relatively small number of arithmetic operations and the accumulation of rounding errors is hence not expected to produce an instability. The algorithm is in any case known to be well behaved in this respect [8,9].

A problem may however arise if the matrix is ill-conditioned. Any initial numerical uncertainty in the matrix may lead to large changes in the calculated inverse in this case. The result that one obtains is only meaningful up to such variations.

### B.1 Condition number

Let  $A$  be any complex invertible  $n \times n$  matrix. In the following the norm  $\|v\|$  of an  $n$ -component complex vector  $v$  is defined through

$$\|v\|^2 = \sum_{k=1}^n |v_k|^2. \quad (\text{B.1})$$

The associated norm of  $A$  and its condition number are then given by

$$\|A\| = \sup_{\|v\|=1} \|Av\|, \quad (\text{B.2})$$

$$k(A) = \|A\| \|A^{-1}\|. \quad (\text{B.3})$$

In terms of the eigenvalues

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n \quad (\text{B.4})$$

of the hermitean matrix  $A^\dagger A$  we have

$$k(A) = \sqrt{\lambda_1/\lambda_n}. \quad (\text{B.5})$$

In particular, matrices with condition numbers near 1 are close to being unitary up to an overall normalization factor. When the condition number is large the matrix is said to be ill-conditioned.

If  $A$  is hermitean its eigenvalues  $\mu_1, \dots, \mu_n$  may be ordered such that  $\mu_k^2 = \lambda_k$  and the condition number  $k(A)$  is then equal to  $|\mu_1/\mu_n|$ . It should be emphasized, however, that the eigenvalues of  $A$  are in general not directly related to its condition number. If we take

$$A = \begin{pmatrix} 1 & z \\ 0 & 1 \end{pmatrix}, \quad (\text{B.6})$$

for example, the eigenvalues of  $A$  are both equal to 1, while

$$k(A) = \rho + \sqrt{\rho^2 - 1}, \quad \rho = 1 + \frac{1}{2}|z|^2, \quad (\text{B.7})$$

depends on  $z$  and can be made arbitrarily large.

### B.2 Stability of the linear system $Av = b$

We now consider the perturbed linear system

$$(A + \epsilon B)v = b, \quad (\text{B.8})$$

where  $\epsilon$  is a small parameter and  $\|B\| \leq \|A\|$ . The perturbation  $\epsilon B$  may be regarded as a model for the numerical uncertainty in  $A$  which may have incurred during its computation. We are then interested in the sensitivity of the solution vector  $v$  on the perturbation. Neglecting higher orders in  $\epsilon$ , we have

$$v = (1 - \epsilon A^{-1}B)A^{-1}b, \quad (\text{B.9})$$

and the relative deviation of the perturbed from the unperturbed solution is hence bounded by

$$\frac{\|v - A^{-1}b\|}{\|A^{-1}b\|} \leq \epsilon k(A). \quad (\text{B.10})$$

This suggests that the numerical error on the solution vector may be amplified by a factor  $k(A)$  relative to the error on the matrix  $A$ .

In any given case the actual error may be significantly smaller, but the bound (B.10) is not unrealistic in general. For illustration we again consider the matrix (B.6) and take

$$B = \begin{pmatrix} 0 & 0 \\ z^* & 0 \end{pmatrix}, \quad b = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (\text{B.11})$$

One easily checks that  $\|B\| \leq \|A\|$  and a short calculation then yields

$$\frac{\|v - A^{-1}b\|}{\|A^{-1}b\|} = \epsilon |z| \sqrt{1 + |z|^2} \quad (\text{B.12})$$

up to terms of order  $\epsilon^2$ . For large  $|z|$  (large condition numbers in other words) the inequality (B.10) is hence saturated.

We thus conclude that there can be large significance losses when calculating the inverse of an ill-conditioned matrix. In particular, the inversion algorithm described in sect. 5 may not be safe in such cases.

### B.3 Estimating condition numbers

An exact calculation of the condition number  $k(A)$  requires the computation of the extremal eigenvalues of  $A^\dagger A$ . This may be rather time-consuming and a faster method to estimate  $k(A)$  is clearly needed.

To this end we introduce the Frobenius norm

$$\|A\|_{\text{F}}^2 = \sum_{i,j=1}^n |a_{ij}|^2, \quad (\text{B.13})$$

where  $a_{ij}$  are the matrix elements of  $A$ . Noting

$$\|A\|_{\text{F}}^2 = \text{tr} \{A^\dagger A\} = \sum_{k=1}^n \lambda_k, \quad (\text{B.14})$$

it is immediately clear that

$$\|A\| \leq \|A\|_{\text{F}},$$

and an upper bound on the condition number  $k(A)$  is hence given by

$$k(A) \leq k_{\text{F}}(A) = \|A\|_{\text{F}} \|A^{-1}\|_{\text{F}}. \quad (\text{B.15})$$

With some additional work one may also establish the inequality

$$k_{\text{F}}(A) \leq \frac{1}{2}n [k(A) + 1/k(A)], \quad (\text{B.16})$$

which shows that  $k_{\text{F}}(A)$  overestimates  $k(A)$  by at most a factor  $\frac{1}{2}n$  if  $k(A)$  is large (which is the case of interest).

### B.4 Stability criterion

In the program that computes the inverse of  $D_{\text{oo}}$ , the inversion is considered to be safe if the  $6 \times 6$  matrices  $A = A_{\pm}(x)$  satisfy the bound

$$k_{\text{F}}(A) \leq k_{\text{max}} = 100. \quad (\text{B.17})$$

Significance losses of more than 2 decimal places are then excluded and the inverted matrices are obtained with an estimated numerical precision of at least 14 decimal places (assuming standard 64 bit floating-point arithmetic). The program returns 1 if the bound is violated and 0 otherwise.

A last point to be mentioned here is that the diagonal elements of the triangular matrix  $T$  are bounded from below through

$$|t_{ii}| \geq \|A\|_{\text{F}}/k_{\text{max}} \quad (\text{B.18})$$

if (B.17) holds. In particular, the Householder triangularization is guaranteed to be numerically safe. Equation (B.18) is obtained straightforwardly by inserting

$$\|A^{-1}\|_{\text{F}} = \|S\|_{\text{F}} \geq |s_{ii}| \quad (\text{B.19})$$

in the definition of  $k_{\text{F}}(A)$  and using eq. (5.9).

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