Molecular-dynamics quark forces

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1. Introduction

In O(a)-improved lattice QCD [1,2], the computation of the quark forces that enter the molecular-dynamics equations is quite complicated. The steps described in this note are intended to minimize both the computational and the communication effort required for this calculation.

The notational and normalization conventions used here are the same as the ones employed in ref. [3]. In particular, the representation of the Dirac matrices specified in these notes is assumed. The SU(3) conventions are summarized in appendix A.

2. Actions and forces

HMC simulations of QCD [4] now usually involve a frequency splitting of the quark determinant. As a consequence, there are many contributions to the force that drives the molecular-dynamics evolution of the link variables $U(x,\mu)$ and their momenta $\Pi(x,\mu)$. Here the case of the twisted-mass frequency splitting proposed by Hasenbusch [5] is considered, but most formulae obtained in sect. 3 do not depend on this choice.

2.1 Molecular dynamics

As usual, the momentum field

$$\Pi(x,\mu) = \Pi(x,\mu)^a T^a \tag{2.1}$$

takes values in the Lie algebra of SU(3) (cf. appendix A). Memory space is allocated for the momenta on all links (x, μ) of the lattice, but those on the inactive links (the time-like links at time $x_0 = N_0 - 1$, for example, if open boundary conditions are chosen) are not used and set to zero in the simulation programs.

The molecular-dynamics Hamilton function

$$H(\Pi, U) = \tfrac{1}{2}(\Pi, \Pi) + S(U) \tag{2.2}$$

consist of the kinetic part

$$\tfrac{1}{2}(\Pi, \Pi) = \tfrac{1}{2} \sum_{x,\mu} \Pi(x, \mu)^a \Pi(x, \mu)^a \tag{2.3}$$

and the sum

$$S(U) = S_{\mathrm{G}}(U) + S_{\mathrm{pf}}(U) \tag{2.4}$$

of the gauge action $S_{\mathrm{G}}(U)$ and the pseudo-fermion action $S_{\mathrm{pf}}(U)$.

The molecular-dynamics evolution of the fields is determined by Hamilton's equations

$$\partial_t \Pi(x, \mu) = -T^a \partial^a_{x,\mu} S(U), \tag{2.5}$$

$$\partial_t U(x, \mu) = \Pi(x, \mu) U(x, \mu), \tag{2.6}$$

where t denotes the molecular-dynamics time and $\partial^a_{x,\mu}$ the partial derivatives with respect to the link variables $U(x, \mu)$ (see appendix A).

2.2 Factorization of the quark determinant

Let D be the massive O(a) improved lattice Dirac operator [3] and $\mu_0, \ldots, \mu_n$ a set of twisted-mass parameters such that

$$\mu_n > \mu_{n-1} > \ldots > \mu_0 \geq 0. \tag{2.7}$$

The partition function of a doublet of mass-degenerate quarks may then be factorized according to

$$\det(D^\dagger D + \mu_0^2) = \det(D^\dagger D + \mu_n^2) \prod_{k=0}^{n-1} \det \left\{ \frac{D^\dagger D + \mu_k^2}{D^\dagger D + \mu_{k+1}^2} \right\}. \tag{2.8}$$

If non-zero, the lowest twisted mass μ_0 can serve as infrared regulator [6] or it may be interpreted as a physical (twisted) mass of the quark doublet.

The pseudo-fermion action corresponding to the factorized quark determinant is given by

$$S_{\mathrm{pf}} = \sum_{k=0}^{n} S_{\mathrm{pf},k}, \tag{2.9}$$

$$S_{\mathrm{pf},k} = (\phi_k, (D^\dagger D + \mu_{k+1}^2)(D^\dagger D + \mu_k^2)^{-1}\phi_k), \quad k = 0, 1, \ldots, n-1, \tag{2.10}$$

$$S_{\mathrm{pf},n} = (\phi_n, (D^\dagger D + \mu_n^2)^{-1}\phi_n), \tag{2.11}$$

where $\phi_0, \ldots, \phi_n$ are independent pseudo-fermion fields. Introducing the fields

$$\psi_k = (D + i\mu_k\gamma_5)^{-1}\gamma_5\phi_k, \tag{2.12}$$

$$\chi_k = (D - i\mu_k\gamma_5)^{-1}\gamma_5\psi_k, \tag{2.13}$$

a little algebra shows that

$$\partial_{x,\mu}^a S_{\mathrm{pf},k} = -2\,(\mu_{k+1}^2 - \mu_k^2)\,\mathrm{Re}\,(\chi_k, \gamma_5\partial_{x,\mu}^a D\psi_k), \quad k = 0, 1, \ldots, n-1, \tag{2.14}$$

$$\partial_{x,\mu}^a S_{\mathrm{pf},n} = -2\,\mathrm{Re}\,(\chi_n, \gamma_5\partial_{x,\mu}^a D\psi_n). \tag{2.15}$$

The quark force deriving from the action $S_{\mathrm{pf},k}$ can thus be calculated by computing the fields ψ_k and χ_k, using a suitable solver for the twisted-mass Dirac equation, and subsequently the matrix element (2.14) or (2.15) (if $k = n$).

3. Explicit expressions for the quark forces

The force field

$$F^a(x, \mu) = -2\,\mathrm{Re}\,(\chi, \gamma_5\partial_{x,\mu}^a D\psi) \tag{3.1}$$

is a sum of two terms,

$$F_{\mathrm{sw}}^a(x, \mu) = -2\,\mathrm{Re}\,(\chi, \gamma_5\partial_{x,\mu}^a (D_{\mathrm{ee}} + D_{\mathrm{oo}})\psi), \tag{3.2}$$

$$F^a_{\rm hop}(x,\mu) = -2\,{\rm Re}\,(\chi,\gamma_5\partial^a_{x,\mu}(D_{\rm eo}+D_{\rm oe})\psi), \tag{3.3}$$

where $D_{\rm ee}, D_{\rm eo}, \ldots$ are the even-even, even-odd, etc., parts of the Dirac operator [3]. These two contributions are quite different and are kept apart in the following.

3.1 X-matrices

In both cases, the computation can be divided in roughly two steps, where one first sums over the Dirac indices and then over the colour indices. More precisely, the matrices computed in the first step are

$$X_{\mu\nu}(x) = i\sum_{A=1}^{4}\bigl\{(\gamma_5\sigma_{\mu\nu}\psi)_A(x)\otimes\chi_A(x)^\dagger + (\psi\leftrightarrow\chi)\bigr\}, \tag{3.4}$$

$$X_\mu(x) = \sum_{A=1}^{4}\bigl\{(\gamma_5(1-\gamma_\mu)\psi)_A(x+\hat\mu)\otimes\chi_A(x)^\dagger + (\psi\leftrightarrow\chi)\bigr\}. \tag{3.5}$$

The sums in these equations run over the Dirac index of the spinors involved and the tensor products are taken in colour space, i.e. both $X_{\mu\nu}(x)$ and $X_\mu(x)$ are 3×3 complex matrices in colour space.

With the Dirac matrices chosen as in appendix A of ref. [3], the matrices $X_{\mu\nu}$ are given by

$$X_{01}(x) = i\bigl\{M_{12}+M_{21}+M_{34}+M_{43}\bigr\}, \tag{3.6}$$

$$X_{02}(x) = i\bigl\{i(M_{12}-M_{21})+i(M_{34}-M_{43})\bigr\}, \tag{3.7}$$

$$X_{03}(x) = i\bigl\{M_{11}-M_{22}+M_{33}-M_{44}\bigr\}, \tag{3.8}$$

$$X_{23}(x) = i\bigl\{-M_{12}-M_{21}+M_{34}+M_{43}\bigr\}, \tag{3.9}$$

$$X_{31}(x) = i\bigl\{-i(M_{12}-M_{21})+i(M_{34}-M_{43})\bigr\}, \tag{3.10}$$

$$X_{12}(x) = i\bigl\{-M_{11}+M_{22}+M_{33}-M_{44}\bigr\}, \tag{3.11}$$

where

$$M_{AB} = \psi_A(x)\otimes\chi_B(x)^\dagger + \chi_A(x)\otimes\psi_B(x)^\dagger. \tag{3.12}$$

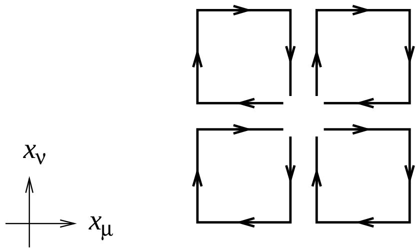

Fig. 1. Graphical representation of the products of gauge field variables contributing to the lattice field strength tensor (3.19). Each square corresponds to one of the terms in eq. (3.20).

Note that only the hermitian 6×6 matrices

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} M_{33} & M_{34} \\ M_{43} & M_{44} \end{pmatrix} \tag{3.13}$$

need to be computed to be able to evaluate eqs. (3.6)–(3.11).

In the case of the other matrices, $X_\mu(x)$, the explicit expressions are

$$\begin{aligned} X_0(x) = {} & (\psi_1 + \psi_3)(x + \hat{\mu}) \otimes (\chi_1 - \chi_3)(x)^\dagger + \\ & (\psi_2 + \psi_4)(x + \hat{\mu}) \otimes (\chi_2 - \chi_4)(x)^\dagger + (\psi \leftrightarrow \chi), \end{aligned} \tag{3.14}$$

$$\begin{aligned} X_1(x) = {} & (\psi_1 + i\psi_4)(x + \hat{\mu}) \otimes (\chi_1 - i\chi_4)(x)^\dagger + \\ & (\psi_2 + i\psi_3)(x + \hat{\mu}) \otimes (\chi_2 - i\chi_3)(x)^\dagger + (\psi \leftrightarrow \chi), \end{aligned} \tag{3.15}$$

$$\begin{aligned} X_2(x) = {} & (\psi_1 + \psi_4)(x + \hat{\mu}) \otimes (\chi_1 - \chi_4)(x)^\dagger + \\ & (\psi_2 - \psi_3)(x + \hat{\mu}) \otimes (\chi_2 + \chi_3)(x)^\dagger + (\psi \leftrightarrow \chi), \end{aligned} \tag{3.16}$$

$$\begin{aligned} X_3(x) = {} & (\psi_1 + i\psi_3)(x + \hat{\mu}) \otimes (\chi_1 - i\chi_3)(x)^\dagger + \\ & (\psi_2 - i\psi_4)(x + \hat{\mu}) \otimes (\chi_2 + i\chi_4)(x)^\dagger + (\psi \leftrightarrow \chi). \end{aligned} \tag{3.17}$$

Contrary to the tensor X-matrices (which are anti-Hermitian), these matrices are generic complex 3×3 matrices.

3.2 SW part of the force

The exact form of $D_{\rm ee}+D_{\rm oo}$ depends on whether the traditional or the exponential variant of the O(a)-improvement terms is chosen [3]. As explained in appendix B, the computation of the SW part of the force however proceeds almost identically in the two cases. In the following, the traditional form of the improvement terms is assumed, the modifications required when the exponential variant is chosen being discussed in the appendix.

The diagonal part of the Dirac operator,

$$D_{\rm ee}+D_{\rm oo}=\text{constant}+c_{\rm sw}\sum_{\mu,\nu=0}^{3}\tfrac{i}{4}\sigma_{\mu\nu}\widehat{F}_{\mu\nu}, \tag{3.18}$$

involves the field tensor

$$\widehat{F}_{\mu\nu}(x)=\tfrac{1}{8}\left\{Q_{\mu\nu}(x)-Q_{\nu\mu}(x)\right\}, \tag{3.19}$$

$$\begin{aligned}Q_{\mu\nu}(x)=\;&U(x,\mu)U(x+\hat{\mu},\nu)U(x+\hat{\nu},\mu)^{-1}U(x,\nu)^{-1}+\\&U(x,\nu)U(x-\hat{\mu}+\hat{\nu},\mu)^{-1}U(x-\hat{\mu},\nu)^{-1}U(x-\hat{\mu},\mu)+\\&U(x-\hat{\mu},\mu)^{-1}U(x-\hat{\mu}-\hat{\nu},\nu)^{-1}U(x-\hat{\mu}-\hat{\nu},\mu)U(x-\hat{\nu},\nu)+\\&U(x-\hat{\nu},\nu)^{-1}U(x-\hat{\nu},\mu)U(x+\hat{\mu}-\hat{\nu},\nu)U(x,\mu)^{-1}\end{aligned} \tag{3.20}$$

(see fig. 1). The force (3.2) is thus given by

$$F^{a}_{\rm sw}(x,\mu)=\partial^{a}_{x,\mu}S_{\rm sw}, \tag{3.21}$$

where

$$S_{\rm sw}=-\tfrac{1}{8}c_{\rm sw}\sum_{y}\sum_{\rho<\sigma}\mathrm{Re}\,\mathrm{tr}\{Q_{\rho\sigma}(y)X_{\rho\sigma}(y)\}. \tag{3.22}$$

After substituting eq. (3.20), the "action" $S_{\rm sw}$ is seen to be a sum of plaquette terms. There are four terms per plaquette, one for each point where the X matrix can be.

The SW force field may thus be computed by running through all plaquettes and adding the associated contributions to the force field. In order to write down these contributions explicitly, it is helpful to introduce some notation. Suppose the current

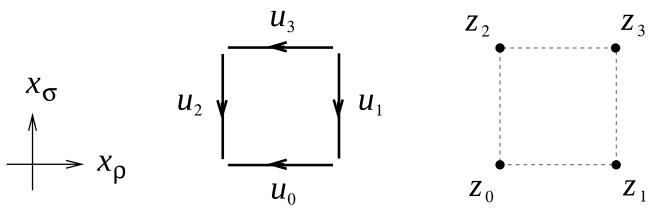

Fig. 2. Labeling of the link variables [eqs. (3.23)–(3.26)] and X-matrices [eqs. (3.27)–(3.30)] along a plaquette in the (ρ, σ)-plane.

plaquette is in the (ρ, σ)-plane at the point y. The link variables and X-matrices residing on that plaquette are

$$u_0 = U(y, \rho), \tag{3.23}$$

$$u_1 = U(y + \hat{\rho}, \sigma), \tag{3.24}$$

$$u_2 = U(y, \sigma), \tag{3.25}$$

$$u_3 = U(y + \hat{\sigma}, \rho), \tag{3.26}$$

and

$$z_0 = X_{\rho\sigma}(y), \tag{3.27}$$

$$z_1 = X_{\rho\sigma}(y + \hat{\rho}), \tag{3.28}$$

$$z_2 = X_{\rho\sigma}(y + \hat{\sigma}), \tag{3.29}$$

$$z_3 = X_{\rho\sigma}(y + \hat{\rho} + \hat{\sigma}) \tag{3.30}$$

(see fig. 2). Using these abbreviations, the contribution of the plaquette to $S_{\rm sw}$ is given by

$$-\tfrac{1}{8} c_{\rm sw} \,\mathrm{Re}\,\mathrm{tr}\{z_0 u_0 u_1 u_3^\dagger u_2^\dagger + u_0 z_1 u_1 u_3^\dagger u_2^\dagger + u_0 u_1 z_3 u_3^\dagger u_2^\dagger + u_0 u_1 u_3^\dagger z_2 u_2^\dagger\}. \tag{3.31}$$

Differentiation of this term with respect to u_0, u_1, u_2 and u_3 leads to contributions f_0, f_1, f_2 and f_3 to the force on the links $(x, \mu) = (y, \rho), (y+\hat{\rho}, \sigma), (y, \sigma)$ and $(y+\hat{\sigma}, \rho)$, respectively.

If the first product in eq. (3.31) is differentiated with respect to u_0, for example, one obtains a contribution to $T^a F^a_{\rm sw}(y, \rho)$ of the form

$$-\tfrac{1}{8} c_{\rm sw} T^a \,\mathrm{Re}\,\mathrm{tr}\{T^a u_0 u_1 u_3^\dagger u_2^\dagger z_0\} = \tfrac{1}{16} c_{\rm sw} \mathcal{P}\{u_0 u_1 u_3^\dagger u_2^\dagger z_0\}, \tag{3.32}$$

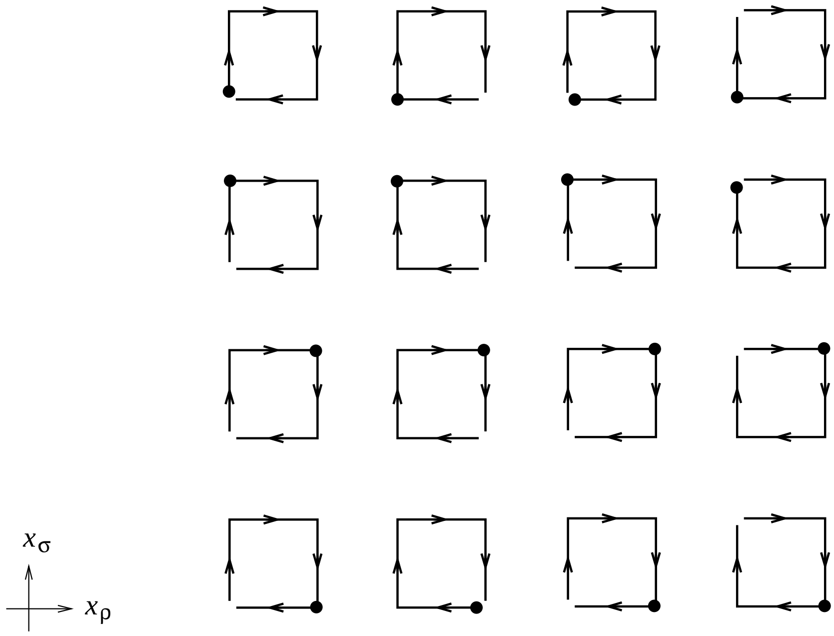

Fig. 3. Products of the link variables and X-matrices around the plaquettes in the (ρ,σ)-plane, which need to computed in order to evaluate the SW force. The products in columns 1–4 contribute to f_0, f_1, f_2 and f_3, respectively.

where

$$\mathcal{P}\{m\} = \tfrac{1}{2}(m - m^\dagger) - \tfrac{1}{6}\mathrm{tr}(m - m^\dagger) \tag{3.33}$$

projects any complex 3×3 matrix m to $\mathfrak{su}(3)$. The product on the right of eq. (3.32) is graphically represented by the top-left diagram shown in fig. 3. Similarly, one obtains 15 further terms that correspond to the other diagrams in the figure.

The associated products of 3×3 matrices may be efficiently calculated by first computing

$$w_0 = u_2^\dagger u_0, \tag{3.34}$$

$$w_1 = u_1 u_3^\dagger, \tag{3.35}$$

$$w_2 = u_2^\dagger z_0 u_0, \tag{3.36}$$

$$w_3 = z_2 w_0, \tag{3.37}$$

$$w_4 = u_1 z_3 u_3^\dagger, \tag{3.38}$$

$$w_5 = w_0 z_1. \tag{3.39}$$

After that one can calculate the $\mathfrak{su}(3)$ matrices

$$y_0 = \mathcal{P}\{w_1 w_2\}, \tag{3.40}$$

$$y_1 = \mathcal{P}\{w_2 w_1\}, \tag{3.41}$$

$$y_2 = \mathcal{P}\{w_1 w_3\}, \tag{3.42}$$

$$y_3 = \mathcal{P}\{w_3 w_1\}, \tag{3.43}$$

$$y_4 = \mathcal{P}\{w_4 w_0\}, \tag{3.44}$$

$$y_5 = \mathcal{P}\{w_0 w_4\}, \tag{3.45}$$

$$y_6 = \mathcal{P}\{w_1 w_5\}, \tag{3.46}$$

$$y_7 = \mathcal{P}\{w_5 w_1\}, \tag{3.47}$$

and finally the contributions to the force

$$f_0 = \tfrac{1}{16} c_{\rm sw} \{u_0(y_0 + y_2 + y_4)u_0^\dagger + u_2 y_7 u_2^\dagger\}, \tag{3.48}$$

$$f_1 = \tfrac{1}{16} c_{\rm sw} \{y_0 + y_2 + y_4 + y_6\}, \tag{3.49}$$

$$f_2 = -\tfrac{1}{16} c_{\rm sw} \{u_2(y_1 + y_5 + y_7)u_2^\dagger + u_0 y_2 u_0^\dagger\}, \tag{3.50}$$

$$f_3 = -\tfrac{1}{16} c_{\rm sw} \{y_1 + y_3 + y_5 + y_7\}. \tag{3.51}$$

In total these are 16 matrix products and 4 rotations in $\mathfrak{su}(3)$ per plaquette.

3.3 Hopping part of the force

A short calculation shows that

$$F^a_{\rm hop}(x,\mu) = \sum_{\mu=0}^{3} \mathrm{Re}\,\big\{\chi(x)^\dagger T^a U(x,\mu)\gamma_5(1-\gamma_\mu)\psi(x+\hat{\mu}) + (\psi \leftrightarrow \chi)\big\}. \tag{3.52}$$

Recalling the definition (3.5), this leads to the expression

$$T^a F^a_{\rm hop}(x,\mu) = -\tfrac{1}{2}\mathcal{P}\{U(x,\mu)X_\mu(x)\}. \tag{3.53}$$

The hopping part of the force is thus very much easier to evaluate than the SW part.

4. Even-odd preconditioned fermion action

If the twisted-mass terms are introduced merely for technical reasons, one has the option of adding them on the even sites of the lattice only. This choice has some advantages when even-odd preconditioning is used and is therefore made in this section.

4.1 Factorization formula

Let $1_{\rm e}$ be the projector to the subspace of quark fields that vanish on the odd sites of the lattice. Its action on any fermion field $\psi(x)$ is given by

$$1_{\rm e}\psi(x) = \begin{cases} \psi(x) & \text{if } x \text{ is even,} \\ 0 & \text{if } x \text{ is odd.} \end{cases} \tag{4.1}$$

The Dirac equation with a twisted mass on the even sites,

$$(D + i\mu\gamma_5 1_{\rm e})\psi(x) = \eta(x), \tag{4.2}$$

can be solved by solving the even-odd preconditioned system

$$(\hat{D} + i\mu\gamma_5)\psi_{\rm e} = \eta_{\rm e} - D_{\rm eo}D_{\rm oo}^{-1}\eta_{\rm o} \tag{4.3}$$

and by setting

$$\psi_{\rm o} = D_{\rm oo}^{-1}\{\eta_{\rm o} - D_{\rm oe}\psi_{\rm e}\}, \tag{4.4}$$

where $\hat{D}$ denotes the even-odd preconditioned Dirac operator [3].

With such twisted-mass terms, the factorization formula replacing eq. (2.8) reads

$$\begin{aligned} &\det\{(D^\dagger - i\mu_0\gamma_5 1_{\rm e})(D + i\mu_0\gamma_5 1_{\rm e})\} \\ &\qquad = (\det D_{\rm oo})^2 \det(\hat{D}^\dagger\hat{D} + \mu_n^2) \prod_{k=0}^{n-1} \det\left\{\frac{\hat{D}^\dagger\hat{D} + \mu_k^2}{\hat{D}^\dagger\hat{D} + \mu_{k+1}^2}\right\}. \end{aligned} \tag{4.5}$$

The formula shows that a proper frequency splitting of the quark determinant can be achieved in this way too. A notable difference with respect to the case previously discussed is, however, the presence of the "small determinant" $\det D_{\rm oo}$ on the right of eq. (4.5), which is rapidly varying with the gauge field and thus belongs to the high-frequency part of the determinant.

4.2 Pseudo-fermion actions and forces

The pseudo-fermion action corresponding to the factorized quark determinant (4.5) is given by

$$S_{\rm pf} = \sum_{k=0}^{n} \hat{S}_{{\rm pf},k}, \tag{4.6}$$

$$\hat{S}_{{\rm pf},k} = (\phi_{k,{\rm e}}, (\hat{D}^{\dagger}\hat{D} + \mu_{k+1}^2)(\hat{D}^{\dagger}\hat{D} + \mu_k^2)^{-1}\phi_{k,{\rm e}}), \quad k = 0, 1, \ldots, n-1, \tag{4.7}$$

$$\hat{S}_{{\rm pf},n} = (\phi_{n,{\rm e}}, (\hat{D}^{\dagger}\hat{D} + \mu_n^2)^{-1}\phi_{n,{\rm e}}), \tag{4.8}$$

where $\phi_{0,{\rm e}}, \ldots, \phi_{n,{\rm e}}$ are independent pseudo-fermion fields that vanish on the odd sites of the lattice. Introducing the (full lattice) fields

$$\psi_k = (D + i\mu_k\gamma_5 1_{\rm e})^{-1}\gamma_5\phi_{k,{\rm e}}, \tag{4.9}$$

$$\chi_k = (D - i\mu_k\gamma_5 1_{\rm e})^{-1}\gamma_5 1_{\rm e}\psi_k, \tag{4.10}$$

a little algebra shows that

$$\partial_{x,\mu}^a \hat{S}_{{\rm pf},k} = -2\,(\mu_{k+1}^2 - \mu_k^2)\,{\rm Re}\,(\chi_k, \gamma_5\partial_{x,\mu}^a D\psi_k), \quad k = 0, 1, \ldots, n-1, \tag{4.11}$$

$$\partial_{x,\mu}^a \hat{S}_{{\rm pf},n} = -2\,{\rm Re}\,(\chi_n, \gamma_5\partial_{x,\mu}^a D\psi_n). \tag{4.12}$$

The forces deriving from the actions $\hat{S}_{{\rm pf},k}$ can thus be computed using the generic formulae derived in sect. 3. Note that the pseudo-fermion actions

$$\hat{S}_{{\rm pf},k} = (\phi_k, \phi_k) + (\mu_{k+1}^2 - \mu_k^2)(\psi_k, 1_{\rm e}\psi_k), \quad k = 0, 1, \ldots, n-1, \tag{4.13}$$

$$\hat{S}_{{\rm pf},n} = (\psi_n, 1_{\rm e}\psi_n), \tag{4.14}$$

are easily obtained once the fields ψ_k are known.

The fields ψ_k and χ_k may alternatively be calculated through

$$\chi_{k,\mathrm{e}} = (\hat{D}^\dagger \hat{D} + \mu_k^2)^{-1} \phi_{k,\mathrm{e}}, \tag{4.15}$$

$$\chi_{k,\mathrm{o}} = -D_{\mathrm{oo}}^{-1} D_{\mathrm{oe}} \chi_{k,\mathrm{e}}, \tag{4.16}$$

$$\psi_{k,\mathrm{e}} = \gamma_5 (\hat{D} - i\mu_k \gamma_5) \chi_{k,\mathrm{e}}, \tag{4.17}$$

$$\psi_{k,\mathrm{o}} = -D_{\mathrm{oo}}^{-1} D_{\mathrm{oe}} \psi_{k,\mathrm{e}}. \tag{4.18}$$

This is the preferred scheme if the Dirac equation is to be solved with the conjugate gradient algorithm. Equations (4.9) and (4.10) may however be better suited if other solvers are used.

4.3 Force deriving from the "small determinant"

The first factor in eq. (4.5) corresponds to the action

$$S_{\mathrm{det}} = -2\,\mathrm{Tr}\ln(1_{\mathrm{e}} + D_{\mathrm{oo}}) = -2 \sum_{x\ \mathrm{odd}} \mathrm{tr}\ln M(x) \tag{4.19}$$

in the molecular-dynamics Hamilton function, where

$$M(x) = \begin{pmatrix} A_+(x) & 0 \\ 0 & A_-(x) \end{pmatrix} \tag{4.20}$$

is the matrix in spinor space representing the action of $D_{\mathrm{ee}} + D_{\mathrm{oo}}$ at the point x (see subsect. 4.2 in ref. [3]). The hermitian 6×6 blocks $A_\pm(x)$ in eq. (4.20) act on the upper and lower two Dirac components of the quark fields, respectively. They are of the form

$$A_+ = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \qquad A_- = \begin{pmatrix} A_{33} & A_{34} \\ A_{43} & A_{44} \end{pmatrix}, \tag{4.21}$$

where A_{ij} is a complex 3×3 colour matrix that acts on the j'th Dirac component of the quark spinors.

The force deriving from the action S_{det} involves the inverse of $M(x)$, which may be similarly decomposed,

$$A_+^{-1} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}, \qquad A_-^{-1} = \begin{pmatrix} B_{33} & B_{34} \\ B_{43} & B_{44} \end{pmatrix}, \tag{4.22}$$

into 3×3 colour matrices B_{ij}. As in the case of the force $F^a_{\rm sw}(x,\mu)$, it is now helpful to introduce the X-matrices

$$X_{\mu\nu}(x)=i\sum_{A=1}^{4}\{\sigma_{\mu\nu}M(x)^{-1}\}_{AA}. \tag{4.23}$$

Explicitly,

$$X_{01}(x)=i\bigl\{B_{12}+B_{21}-B_{34}-B_{43}\bigr\}, \tag{4.24}$$

$$X_{02}(x)=i\bigl\{i(B_{12}-B_{21})-i(B_{34}-B_{43})\bigr\}, \tag{4.25}$$

$$X_{03}(x)=i\bigl\{B_{11}-B_{22}-B_{33}+B_{44}\bigr\}, \tag{4.26}$$

$$X_{23}(x)=i\bigl\{-B_{12}-B_{21}-B_{34}-B_{43}\bigr\}, \tag{4.27}$$

$$X_{31}(x)=i\bigl\{-i(B_{12}-B_{21})-i(B_{34}-B_{43})\bigr\}, \tag{4.28}$$

$$X_{12}(x)=i\bigl\{-B_{11}+B_{22}-B_{33}+B_{44}\bigr\}. \tag{4.29}$$

Note that $X_{\mu\nu}(x)$ vanishes at time $x_0=0$ and $x_0=N_0-1$, since $M(x)$ is equal to the unit matrix at these points [3]. The force is then given by

$$F^a_{\rm det}(x,\mu)=\partial^a_{x,\mu}S_{\rm det}=-\tfrac{1}{4}c_{\rm sw}\sum_{y\ {\rm odd}}\sum_{\rho<\sigma}{\rm Re}\,{\rm tr}\{[\partial^a_{x,\mu}Q_{\rho\sigma}(y)]X_{\rho\sigma}(y)\}. \tag{4.30}$$

Apart from a factor 2, this formula coincides with the one obtained in sect. 3 for the force $F^a_{\rm sw}(x,\mu)$ (cf. eqs. (3.21),(3.22); the sum over y can be extended to all points by setting the X tensor field to zero on the even points).

5. Programs

The programs that compute the gauge and quark forces are contained in the directory `modules/forces`. A list of the programmed actions and forces is included in the file `README.forces` in this directory.

Appendix A

The Lie algebra $\mathfrak{su}(N)$ of SU(N) may be identified with the linear space of all anti-hermitian traceless $N \times N$ matrices. With respect to a basis T^a, $a = 1, \ldots, N^2 - 1$, of such matrices, the elements $X \in \mathfrak{su}(N)$ are given by $X = X^a T^a$ with real components X^a (repeated group indices are automatically summed over). The structure constants f^{abc} in the commutator relation

$$[T^a, T^b] = f^{abc} T^c \tag{A.1}$$

are real and totally anti-symmetric in the indices if the normalization condition

$$\mathrm{tr}\{T^a T^b\} = -\tfrac{1}{2}\delta^{ab} \tag{A.2}$$

is imposed. Moreover, $f^{acd} f^{bcd} = N\delta^{ab}$.

If $\mathcal{F}(U)$ is a differentiable function of the gauge field, its derivative with respect to the link variable $U(x, \mu)$ in the direction of the generator T^a is defined by

$$\partial^a_{x,\mu} \mathcal{F}(U) = \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{F}(U_t)\bigg|_{t=0}, \qquad U_t(y, \nu) = \begin{cases} \mathrm{e}^{tT^a} U(x, \mu) & \text{if } (y, \nu) = (x, \mu), \\ U(y, \nu) & \text{otherwise.} \end{cases} \tag{A.3}$$

In particular, in the case of a scalar function $\mathcal{F}(U)$, the combination $T^a \partial^a_{x,\mu} \mathcal{F}(U)$ is a vector field with values in $\mathfrak{su}(3)$ that transforms under the adjoint representation of the gauge group.

Appendix B*

At each point x, the diagonal $D_{\mathrm{ee}} + D_{\mathrm{oo}}$ of the Dirac operator is represented by a matrix of the form

$$\text{constant} \times \begin{pmatrix} \mathrm{e}^{A_+} & 0 \\ 0 & \mathrm{e}^{A_-} \end{pmatrix} \tag{B.1}$$

* Based in part on notes by Antonio Rago [7].

if the exponential variant of the improvement terms is chosen. The Hermitian 6×6 matrices $A_{\pm}$ in this equation represent the Pauli term

$$\frac{c_{\rm sw}}{4+m_0} \sum_{\mu,\nu=0}^{3} \tfrac{i}{4}\sigma_{\mu\nu}\widehat{F}_{\mu\nu} = \begin{pmatrix} A_+ & 0 \\ 0 & A_- \end{pmatrix} \tag{B.2}$$

as usual.

B.1 Derivative of the matrix exponentials

Let A be a 6×6 Hermitian matrix. A well-known theorem asserts that the differential of e^{A} with respect to the independent parameters of A is given by

$$\mathrm{d}\mathrm{e}^{A} = \int_0^1 \mathrm{d}t\, \mathrm{e}^{tA} \mathrm{d}A\, \mathrm{e}^{(1-t)A}. \tag{B.3}$$

Expansion of the exponentials on the right then yields the rapidly convergent series

$$\mathrm{d}\mathrm{e}^{A} = \sum_{k=0}^{N} \sum_{l=0}^{N-k} \frac{1}{(k+l+1)!} A^k \mathrm{d}A A^l + r_N(A, \mathrm{d}A) \tag{B.4}$$

for the differential, where

$$\|r_N(A,\mathrm{d}A)\| \leq \frac{\|A\|^{N+1}}{(N+1)!} \mathrm{e}^{\|A\|} \|\mathrm{d}A\|. \tag{B.5}$$

The derivatives of the exponential can thus be obtained to machine precision by truncating the series at the same value of N as the series for the exponential (cf. ref. [3]). Application of the Cayley–Hamilton theorem and the recursion that follows from it finally leads to the expression

$$\mathrm{d}\mathrm{e}^{A} = \sum_{k,l=0}^{5} C_{kl} A^k \mathrm{d}A A^l + r_N(A, \mathrm{d}A), \tag{B.6}$$

C being a real symmetric 6×6 matrix that depends on N and A.

B.2 Calculation of the force (3.2)

Insertion of eqs. (B.1),(B.2) and (B.6) in eq. (3.2) now leads to expressions for the force that coincide with the ones obtained in the case of the traditional form of the improvement terms, except for the proportionality constant and the tensor $X_{\mu\nu}$, which gets replaced by a sum of 6 tensors, constructed in the same way, with the 6 pairs of fields

$$\psi_k = \sum_{l=0}^{5} \begin{pmatrix} C_{kl}^{+} A_{+}^{l} \psi^{+} \\ C_{kl}^{-} A_{-}^{l} \psi^{-} \end{pmatrix}, \qquad \chi_k = \begin{pmatrix} A_{+}^{k} \chi^{+} \\ A_{-}^{k} \chi^{-} \end{pmatrix}, \qquad k = 0, .., 5, \tag{B.7}$$

in place of ψ and χ. In this equation, the index $\pm$ labels the upper and lower Weyl components of the Dirac spinors and the associated matrices.

B.3 Even-odd preconditioning

The exponential variant of the improvement terms does not give rise to additional complications in the case of the even-odd preconditioned fermion actions. On the contrary, since the Pauli term is traceless, the "small determinant" $\det D_{\mathrm{oo}}$ is constant and does not contribute to the force field.

References

[1] B. Sheikholeslami, R. Wohlert, *Improved continuum limit lattice action for QCD with Wilson fermions*, Nucl. Phys. B259 (1985) 572

[2] M. Lüscher, S. Sint, R. Sommer, P. Weisz, *Chiral symmetry and O(a) improvement in lattice QCD*, Nucl. Phys. B478 (1996) 365

[3] M. Lüscher, *Implementation of the lattice Dirac operator*, `doc/dirac.pdf`

[4] S. Duane, A. D. Kennedy, B. J. Pendleton, D. Roweth, *Hybrid Monte Carlo*, Phys. Lett. B195 (1987) 216

[5] M. Hasenbusch, *Speeding up the Hybrid Monte Carlo algorithm for dynamical fermions*, Phys. Lett. B519 (2001) 177

[6] M. Lüscher, F. Palombi, *Fluctuations and reweighting of the quark determinant on large lattices*, PoS (LATTICE2008) 049

[7] A. Rago, *Relevant formulas for the numerical evaluation of the exponential of a traceless Hermitian matrix*, notes (June 2018)