Charm and strange quark in openQCD simulations

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1. Introduction

The inclusion of the charm and the strange quark in lattice QCD simulations is not completely trivial. In the openQCD package, a version of the RHMC algorithm [1,2] is used for these quarks. The factorization of the quark determinant, the associated pseudo-fermion actions and the computation of the forces deriving from them are briefly described in this note along with further implementation details.

2. Quark determinant

The discussion in this section roughly follows the lines of sect. 6.2.6 of ref. [3], which should be consulted for further explanations. Since the charm and the strange quark are treated in the same way, it suffices to consider the latter.

2.1 Factorization of the strange-quark determinant

Let D be the massive $\mathrm{O}(a)$-improved Wilson–Dirac operator with bare mass parameter m_0 set to the bare mass of the strange quark (see ref. [4] for the exact definition of D). The RHMC algorithm implemented in the openQCD package makes use of even-odd preconditioning and thus starts from the decomposition

$$\det D = \det(1_{\mathrm{e}} + D_{\mathrm{oo}}) \det \hat{D} \tag{2.1}$$

of the strange-quark determinant. In this equation, $\hat{D}$ denotes the even-odd preconditioned Dirac operator, 1_{e} the projector to the subspace of quark fields that vanish

on the odd sites of the lattice and D_{oo} the odd-odd part of the Dirac operator. As explained in sect. 4 of ref. [5], the first factor in eq. (2.1) can be directly included in the molecular-dynamics Hamilton function.

The other factor is then further decomposed according to

$$\det \hat{D} = W \det R^{-1}, \tag{2.2}$$

where the operator R is a suitable rational approximation to $(\hat{D}^{\dagger}\hat{D})^{-1/2}$ while the residual factor,

$$W = \det(\hat{D}R), \tag{2.3}$$

is treated as a reweighting factor.

2.2 Zolotarev rational approximation

The Zolotarev rational function

$$R_{n,\epsilon}(y) = A \frac{(y+a_1)(y+a_3)\ldots(y+a_{2n-1})}{(y+a_2)(y+a_4)\ldots(y+a_{2n})} \tag{2.4}$$

of degree $[n,n]$ approximates $1/\sqrt{y}$ in the range $\epsilon \leq y \leq 1$ with the smallest possible relative deviation

$$\delta = \max_{\epsilon \leq y \leq 1} |1 - \sqrt{y}R_{n,\epsilon}(y)|. \tag{2.5}$$

Somewhat surprisingly, the coefficients $a_1,\ldots,a_{2n}$ of this optimal rational function, the proportionality constant A and the approximation error δ can be determined analytically (see ref. [6]; the results derived there are reproduced in appendix A).

Since the strange quark has a fairly large mass, the eigenvalues of the operator

$$(\hat{D}^{\dagger}\hat{D})^{1/2} = |\gamma_5\hat{D}| \tag{2.6}$$

are expected to be separated from zero by a solid spectral gap. Once the simulation has thermalized, a spectral range $[r_a, r_b]$, $r_a > 0$, can thus be found, which, with probability practically equal to 1, contains all eigenvalues.

In the openQCD package, the operator R in eqs. (2.2),(2.3) is taken to be

$$R = r_b^{-1} R_{n,\epsilon}(r_b^{-2}\hat{D}^{\dagger}\hat{D}), \qquad \epsilon = (r_a/r_b)^2. \tag{2.7}$$

With this choice, the norm bound

$$\| 1 - |\gamma_5 \hat{D}| R \| \leq \delta \tag{2.8}$$

holds when the spectrum of $|\gamma_5 \hat{D}|$ is contained in the range $[r_a, r_b]$, i.e. with high probability in a representative ensemble of gauge fields.

2.3 Further factorizations

The Zolotarev rational function (2.4) may be broken up into two or more factors of the form

$$P_{k,l} = \prod_{j=k}^{l} \frac{y + a_{2j-1}}{y + a_{2j}}. \tag{2.9}$$

If $n = 12$, for example, a possible factorization is

$$R_{n,\epsilon} = A P_{1,5} P_{6,9} P_{10,12}. \tag{2.10}$$

Substituting $y = r_b^{-2} \hat{D}^\dagger \hat{D}$ as before, the associated decomposition

$$\det R^{-1} = \text{constant} \times \det\{P_{1,5}^{-1}\} \det\{P_{6,9}^{-1}\} \det\{P_{10,12}^{-1}\} \tag{2.11}$$

of the second factor in eq. (2.2) effectively achieves a frequency splitting of the quark determinant, because the coefficients $a_1, \ldots, a_{2n}$ are monotonically decreasing,

$$a_1 > a_2 > \ldots > a_{2n} > 0, \tag{2.12}$$

and range over the whole spectral interval from 1 down to ϵ.

3. Pseudo-fermion action and strange-quark force

In the following, $P_{k,l}$ denotes the product (2.9) with y replaced by $r_b^{-2} \hat{D}^\dagger \hat{D}$. Explicitly, the product is given by

$$P_{k,l} = \prod_{j=k}^{l} \frac{\hat{D}^\dagger \hat{D} + \nu_j^2}{\hat{D}^\dagger \hat{D} + \mu_j^2}, \tag{3.1}$$

where the parameters

$$\mu_k = r_b(a_{2k})^{1/2}, \qquad \nu_k = r_b(a_{2k-1})^{1/2}, \qquad k = 1, 2, \ldots, n, \qquad (3.2)$$

will be referred to as "twisted masses".

3.1 Actions and fields

Since the operators $P_{k,l}$ are hermitian and strictly positive, the determinants appearing in a decomposition such as (2.12) can be taken into account in the simulations by including the pseudo-fermion actions

$$S_{\mathrm{pf},k,l} = (\phi_{k,l,\mathrm{e}}, P_{k,l}\phi_{k,l,\mathrm{e}}) \qquad (3.3)$$

in the molecular-dynamics Hamilton function. The fields $\phi_{k,l,\mathrm{e}}$ in this expression are independent pseudo-fermion fields that live on the even sites of the lattice.

Apart from the fact that the product (3.1) may have more than one factor, the pseudo-fermion actions (3.3) are very similar to the actions discussed in sect. 4 of ref. [5]. The partial fraction decomposition

$$P_{k,l} = 1 + \sum_{j=k}^{l} \frac{\rho_{\mu,j}}{\hat{D}^\dagger \hat{D} + \mu_j^2}, \qquad (3.4)$$

$$\rho_{\mu,j} = (\nu_j^2 - \mu_j^2) \prod_{m=k, m\neq j}^{l} \frac{\nu_m^2 - \mu_j^2}{\mu_m^2 - \mu_j^2}, \qquad (3.5)$$

actually shows that the actions (3.3) are sums of the actions previously considered.

3.2 Forces

The force

$$F_{k,l}^a(x, \mu) = \partial_{x,\mu}^a S_{\mathrm{pf},k,l} \qquad (3.6)$$

can therefore be computed following the lines of ref. [5]. In the course of this calculation, the fields

$$\chi_{j,\mathrm{e}} = (\hat{D}^\dagger \hat{D} + \mu_j^2)^{-1} \phi_{k,l,\mathrm{e}} \qquad (3.7)$$

must be computed, which requires the normal even-odd preconditioned Dirac equation to be solved for $j = k, \ldots, l$ and thus possibly many times.

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Since the source field $\phi_{k,l,\mathrm{e}}$ is the same for all j, the multi-shift conjugate gradient algorithm [7,8] can be used for the simultaneous solution of the equations. This works well as long as the masses $\mu_k, \ldots, \mu_l$ are not too small. Highly optimized single-shift solvers may otherwise prove to be more efficient. The openQCD package includes several solvers and one can choose the solver to be used for each factor $P_{k,l}$ separately.

3.3 Pseudo-fermion field generation

At the beginning of the molecular-dynamics trajectories, the pseudo-fermion fields must be chosen randomly with the proper distribution. A moment of thought shows that this is achieved by setting

$$\phi_{k,l,\mathrm{e}} = A_{k,l} \eta_{k,l,\mathrm{e}}, \qquad A_{k,l} = \prod_{j=k}^{l} \frac{\gamma_5 \hat{D} + i\mu_j}{\gamma_5 \hat{D} + i\nu_j}, \tag{3.8}$$

where $\eta_{k,l,\mathrm{e}}$ is a random field on the even sites of the lattice with normal distribution. Since

$$A_{k,l} = 1 + i \sum_{j=k}^{l} \frac{\rho_{\nu,j}}{\gamma_5 \hat{D} + i\nu_j}, \qquad \rho_{\nu,j} = (\mu_j - \nu_j) \prod_{m=k,m\neq j}^{l} \frac{\mu_m - \nu_j}{\nu_m - \nu_j}, \tag{3.9}$$

the application of $A_{k,l}$ to the source field $\eta_{k,l,\mathrm{e}}$ amounts to solving the Dirac equation $l-k+1$ times. Again the multi-shift CG solver can be used here for the simultaneous solution of these equations, but in the case of the few smallest masses ν_j the use of a highly efficient single-shift solver may be preferable.

4. Stochastic estimation of the reweighting factor W

The hermiticity properties of the lattice Dirac operator guarantee that the reweighting factor (2.3) is real, but the factor may, in principle, change sign from one gauge-field configuration to the next. Sign changes are however practically excluded when the quark mass is set to values as large as the physical strange-quark mass (see ref. [3] for a more extensive discussion of the issue). In the following, the reweighting factor is therefore assumed to be positive.

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4.1 Stochastic estimator

Let $\eta_{j,\mathrm{e}}(x)$, $j = 1, \ldots, N$, be a set of independent random quark fields on the even lattice sites with normal distribution. As in the case of the light-quark reweighting factors discussed in ref. [9], a stochastic estimator for W is given by

$$W_N = \frac{1}{N} \sum_{j=1}^{N} \exp\{-(\eta_{j,\mathrm{e}}, [(1 + Z)^{-1/2} - 1]\eta_{j,\mathrm{e}})\}, \tag{4.1}$$

where

$$Z = \hat{D}^\dagger \hat{D} R^2 - 1. \tag{4.2}$$

Recalling the bound (2.8), the inequality

$$\|Z\| \leq \delta(2 + \delta) \tag{4.3}$$

is easily established, and since the approximation error δ is, in practice, much smaller than 1, the inverse square root of $1 + Z$ in eq. (4.1) is well defined.

4.2 Power series expansion

Actually, the series

$$(1 + Z)^{-1/2} = 1 - \tfrac{1}{2}Z + \tfrac{3}{8}Z^2 - \tfrac{5}{16}Z^3 + \tfrac{35}{128}Z^4 - \ldots \tag{4.4}$$

is rapidly convergent in the operator norm. The exponents in eq. (4.1) can therefore be computed by evaluating the first few terms in the expansion

$$(\eta_{j,\mathrm{e}}, [(1 + Z)^{-1/2} - 1]\eta_{j,\mathrm{e}}) = -\tfrac{1}{2}(\eta_{j,\mathrm{e}}, Z\eta_{j,\mathrm{e}}) + \tfrac{3}{8}(\eta_{j,\mathrm{e}}, Z^2\eta_{j,\mathrm{e}}) - \ldots \tag{4.5}$$

It is possible to estimate the size of these terms by noting that $\|\eta_{j,\mathrm{e}}\|^2$ is very nearly equal to 12 times the number N_e of even lattice points. Taking the bound (4.3) into account, the matrix element $(\eta_{j,\mathrm{e}}, Z^p\eta_{j,\mathrm{e}})$ is thus expected to be less than $12N_\mathrm{e}(2\delta)^p$.

4.3 Statistical fluctuations

The statistical fluctuations of the exponents in eq. (4.1) derive from those of the gauge field and those of the random sources $\eta_{j,\mathrm{e}}$. For a given gauge field, the variance of the exponents is equal to

$$\mathrm{Tr}\{[(1 + Z)^{-1/2} - 1]^2\} = \tfrac{1}{4}\mathrm{Tr}\{Z^2\} - \tfrac{3}{8}\mathrm{Tr}\{Z^3\} + \ldots \tag{4.6}$$

Since the traces $\mathrm{Tr}\{Z^p\}$ are at most $12N_e(2\delta)^p$, these fluctuations are guaranteed to be small if, say, $12N_e\delta^2 \leq 10^{-4}$. One can then just as well set $N = 1$ in eq. (4.1), i.e. a sufficiently accurate stochastic estimate of W is obtained in this case with a single random source.

When the stronger constraint $12N_e\delta \leq 0.01$ is satisfied, the reweighting factor deviates from 1 by at most 1%. Larger approximation errors can however be tolerated in practice as long as the fluctuations of W remain small.

5. Parameter tuning

When a new simulation is started, the required approximation error δ and the appropriate spectral range $[r_a, r_b]$ may not be known. Reasonable initial choices of δ are such that $12N_e\delta^2 \simeq 10^{-4}$, while for the spectral range one may take $[am_q, 6.0]$, for example, where m_q is an estimate of the bare current quark mass of the quark considered.

In the course of the thermalization phase, the parameters will then need to be adjusted by calculating the reweighting factor W, following the lines of sect. 4, and the true spectral range of $|\gamma_5\hat{D}|$ for a subset of the generated gauge field configurations. The openQCD package includes two main programs, `main/ms1.c` and `main/ms2.c`, that can be used for this purpose.

The computer time required for the simulation increases with the degree of the Zolotarev rational function. A compromise thus needs to be found, where the number of poles is as small as possible while the fluctuations of the reweighting factor remain tolerable. Compromises should however not be made in the case of the spectral range, since the correctness of the simulation may otherwise be difficult to guarantee. Adding a safety margin of 10% to the low end and 3% to the upper end of the measured spectral range is therefore recommended.

Appendix A

The analytic expressions for the coefficients of the rational function (2.4) that minimizes the approximation error (2.5) involve the Jacobi elliptic functions $\mathrm{sn}(u, k)$,

$\mathrm{cn}(u, k)$ and the complete elliptic integral $K(k)$ (see ref. [10], for example, for the definition of these functions). Explicitly, they are given by

$$a_r = \frac{\mathrm{cn}^2(rv, k)}{\mathrm{sn}^2(rv, k)}, \quad r = 1, 2, \ldots, 2n, \tag{A.1}$$

where

$$k = \sqrt{1 - \epsilon}, \qquad v = \frac{K(k)}{2n + 1}. \tag{A.2}$$

The formulae for the amplitude A and the error δ,

$$A = \frac{2}{1 + \sqrt{1 - d^2}} \frac{c_1 c_3 \ldots c_{2n-1}}{c_2 c_4 \ldots c_{2n}}, \tag{A.3}$$

$$\delta = \frac{d^2}{\left(1 + \sqrt{1 - d^2}\right)^2}, \tag{A.4}$$

involve the coefficients

$$c_r = \mathrm{sn}^2(rv, k), \quad r = 1, 2, \ldots, 2n, \tag{A.5}$$

$$d = k^{2n+1} \left(c_1 c_3 \ldots c_{2n-1}\right)^2. \tag{A.6}$$

All these expressions are free of singularities and can be programmed using well-known methods for the numerical evaluation of the Jacobi elliptic functions.

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