RHMC algorithm in `openQ*D`

Agostino Patella, RC* collaboration October 2017

with excerpts from: M. Lüscher, *Charm and strange quark in openQCD simulations*, Feb 2012, `doc/openQCD-1.6/rhmc.pdf`

Contents

1 Introduction

Let D be the Dirac operator for some choice of parameters. Each degenerate quark multiplet contributes to the gauge-field probability distribution with a factor of the type

$$|\det D|^{2\alpha} = \det(D^\dagger D)^\alpha \ , \tag{1}$$

where α is a positive number. Three values of α are useful in typical simulations with the openQ*D code.

- $\alpha = 1$: for the up/down doublet in isosymmetric simulations with periodic boundary conditions in space.
- $\alpha = 1/2$: for the strange and charm quarks in isosymmetric simulations with periodic boundary conditions in space; for the up/down doublet in isosymmetric simulations with C* boundary conditions in space.
- $\alpha = 1/4$: for all quarks in simulations with isospin-breaking correction (QCD+QED) with C* boundary conditions in space.

In the case $\alpha = 1$ the HMC algorithm can be used, in the other two cases the RHMC algorithm must be used.

2 Quark determinant

The RHMC algorithm implemented in the openQ*D code makes use of even-odd preconditioning, i.e. of the decomposition

$$\det D = \det(\mathbf{1}_\mathrm{e} + D_\mathrm{oo}) \det \hat{D} \ , \tag{2}$$

where the notation of ref. [1] is followed. In short, D is the Dirac operator, D_oo is the odd-odd part of the Dirac operator, $\hat{D}$ is the even-odd preconditioned Dirac operator, and $\mathbf{1}_\mathrm{e}$ is the projector over the space of spinor fields with support on the even sites.

The first determinant in the r.h.s. of eq. (2) is referred to as *small determinant*. The D_{oo} matrix is diagonal in coordinate space, i.e.

$$D_{\text{oo}}(x,y) = (\mathbf{1}_{\text{o}})_{xy} M(x) \ , \tag{3}$$

where $M(x)$ is a matrix in spin and color space, and $\mathbf{1}_{\text{o}}$ is the projector over the space of spinor fields with support on the odd sites. It turns out that $M(x)$ is positive if the gauge field tensors are close enough to zero (i.e. close enough to the continuum limit). Therefore one can write

$$\ln \det(\mathbf{1}_{\text{e}} + D_{\text{oo}}) = \sum_{x \text{ odd}} \ln \det M(x) = -S_{\text{sdet}} \ . \tag{4}$$

It is worth to stress that the determinant in $\det M(x)$ is taken in spin and color space only, therefore the action S_{sdet} and the associated forces can be calculated exactly. Details on the implementation of the small-determinant action and force are given in ref. [2].

A generic power of the determinant of D can be represented as

$$|\det D|^{2\alpha} = e^{-2\alpha S_{\text{sdet}}} \det(\hat{D}^\dagger \hat{D})^\alpha \ . \tag{5}$$

The non-integer power of $\hat{D}^\dagger \hat{D}$ is dealt with by means of a rational approximation. Also, in order to suppress configurations with exceptionally small eigenvalues of $\hat{D}$, the `openQ*D` code allows for twisted-mass preconditioning. In practice this means that a fictitious twisted-mass parameter $\hat{\mu}$ is introduced, and a rational approximation R for $(\hat{D}^\dagger \hat{D} + \hat{\mu}^2)^{-\alpha}$ is considered. The quark determinant in eq. (5) can be written as

$$|\det D|^{2\alpha} = W \ e^{-2\alpha S_{\text{sdet}}} \ \det R^{-1} \ , \tag{6}$$

$$W = \det[(\hat{D}^\dagger \hat{D})^\alpha R] \ , \tag{7}$$

$$R \simeq (\hat{D}^\dagger \hat{D} + \hat{\mu}^2)^{-\alpha} \ . \tag{8}$$

The `openQ*D` code simulates the probability distribution *without* W which has to be separately calculated and included as a reweighting factor.

3 Rational approximation

It is convenient to introduce the hermitian operator $\hat{Q} = \gamma_5 \hat{D}$, in terms of which $\hat{D}^\dagger \hat{D} = \hat{Q}^2$. Let us assume that the spectrum of $|\hat{Q}|$ is contained in the interval $[r_a, r_b]$, and let us choose an integer n. A rational function of order $[n,n]$ in q^2 has the form

$$\rho(q^2) = A \prod_{j=1}^{n} \frac{q^2 + \nu_j^2}{q^2 + \mu_j^2} \ . \tag{9}$$

Without loss of generality one can assume

$$\nu_1 > \nu_2 > \cdots > \nu_n \ , \qquad \mu_1 > \mu_2 > \cdots > \mu_n \ . \tag{10}$$

Let us choose $\rho(q^2)$ to be the optimal rational approximation of order $[n,n]$ of the function $(q^2 + \hat{\mu}^2)^{-\alpha}$ in the domain $q \in [r_a, r_b]$, i.e. the rational function of the form (9) which minimizes the uniform relative error

$$\delta = \max_{q \in [r_a, r_b]} |1 - (q^2 + \hat{\mu}^2)^{\alpha} \rho(q^2)| \ . \tag{11}$$

The optimal rational approximation can be calculated with the `MinMax` code (in the `minmax` directory of the `openQ*D` code) which implements the minmax approximation algorithm in multiple precision. As explained in ref. [3], the output of the `MinMax` code can be cut and paste in an input file for the `openQ*D` code.

If $\rho(q^2)$ is the desired optimal rational approximation, the operator R which appears in eq. (6) is defined simply as

$$R = \rho(\hat{Q}^2) = \rho(\hat{D}^\dagger \hat{D}) = A \prod_{j=1}^{n} \frac{\hat{D}^\dagger \hat{D} + \nu_j^2}{\hat{D}^\dagger \hat{D} + \mu_j^2} \ . \tag{12}$$

Eq. (11) implies the following norm bound

$$\| 1 - (\hat{D}^\dagger \hat{D} + \hat{\mu}^2)^{\alpha} R \| \leq \delta \ . \tag{13}$$

4 Frequency splitting and pseudofermion action

The rational approximation constructed in section 3 can be broken up in factors of the form

$$P_{k,l} = \prod_{j=k}^{l} \frac{\hat{D}^\dagger \hat{D} + \nu_j^2}{\hat{D}^\dagger \hat{D} + \mu_j^2} \ . \tag{14}$$

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

$$R = AP_{1,5}P_{6,9}P_{10,12} \ . \tag{15}$$

The contribution of R to the quark determinant is

$$\det R^{-1} = \text{constant} \times \det P_{1,5}^{-1} \ \det P_{6,9}^{-1} \ \det P_{10,12}^{-1} \ . \tag{16}$$

In practice this decomposition achieves a frequency splitting similar to the Hasenbusch decomposition for the HMC algorithm.

Each $P_{k,l}^{-1}$ determinant is simulated as usual by adding a pseudofermion action of the form

$$S_{\mathrm{pf},k,l} = (\phi_{\mathrm{e}}^{k,l}, P_{k,l}\phi_{\mathrm{e}}^{k,l}) \ , \tag{17}$$

where the fields $\phi_{\mathrm{e}}^{k,l}$ are independent pseudofermions that live on the even sites of the lattice. By using a partial fraction decomposition

$$P_{k,l} = 1 + \sum_{j=k}^{l} \frac{\sigma_j}{\hat{D}^\dagger \hat{D} + \mu_j^2} \ , \tag{18}$$

$$\sigma_j = (\nu_j^2 - \mu_j^2) \prod_{\substack{m=l,\ldots,k \\ m\neq j}} \frac{\nu_m^2 - \mu_j^2}{\mu_m^2 - \mu_j^2} \ , \tag{19}$$

the pseudofermion action in eq. (17) is cast into a sum of terms formally identical to the action of an HMC with twisted mass

$$\begin{aligned} S_{\mathrm{pf},k,l} &= (\phi_{\mathrm{e}}^{k,l}, \phi_{\mathrm{e}}^{k,l}) + \sum_{j=k}^{l} \sigma_j \ (\phi_{\mathrm{e}}^{k,l}, (\hat{D}^\dagger \hat{D} + \mu_j^2)^{-1} \phi_{\mathrm{e}}^{k,l}) = \\ &= \|\phi_{\mathrm{e}}^{k,l}\|^2 + \sum_{j=k}^{l} \sigma_j \ \|(\hat{D} + i\gamma_5\mu_j)^{-1}\gamma_5\phi_{\mathrm{e}}^{k,l}\|^2 = \\ &= \|\phi_{\mathrm{e}}^{k,l}\|^2 + \sum_{j=k}^{l} \sigma_j \ \|\mathbf{1}_e(D + i\gamma_5\mu_j\mathbf{1}_e)^{-1}\gamma_5\phi_{\mathrm{e}}^{k,l}\|^2 \ , \end{aligned} \tag{20}$$

where the following identities has been used

$$\hat{D}^\dagger \hat{D} + \mu_j^2 = \gamma_5(\hat{D} + i\gamma_5\mu_j)(\hat{D} + i\gamma_5\mu_j)^\dagger\gamma_5 \ , \tag{21}$$

$$(\hat{D} + i\gamma_5\mu_j^2)^{-1} = \mathbf{1}_e(D + i\gamma_5\mu_j^2\mathbf{1}_e)^{-1}\mathbf{1}_e \ . \tag{22}$$

5 Molecular dynamics

No C* boundary conditions are assumed in this section. If C* boundary conditions are used, the molecular-dynamics Hamiltonian and equations need to be modified because of the orbifold construction as explained in [4]. However the expressions of the molecular-dynamics forces are the same with or without C* boundary conditions.

The momentum fields associated to the SU(3) and U(1) gauge fields are denoted by $\Pi(x,\mu)$ and $\pi(x,\mu)$ respectively. The momentum $\Pi(x,\mu)$ lives in the Lie algebra of SU(3),

$$\Pi(x,\mu) = \Pi^a(x,\mu) T^a \ , \tag{23}$$

where $\Pi^a(x,\mu)$ are taken to be real. The momentum field $\pi(x,\mu)$ is taken to be real, like the gauge field $A(x,\mu)$. The molecular-dynamics Hamiltonian is

$$H = \frac{1}{2} \sum_{x,\mu} \left\{ [\pi(x,\mu)]^2 + \sum_a [\Pi^a(x,\mu)]^2 \right\} + S(U,A) \ , \tag{24}$$

where the total action is the sum of the gauge actions, terms of the type in eq. (20), and the effective action for the small determinant given in eq. (4).

The evolution equations generated by the Hamiltonian (24)

$$\partial_t U(x,\mu) = \Pi(x,\mu) U(x,\mu) \ , \qquad \partial_t \Pi(x,\mu) = F(x,\mu) \ , \tag{25a}$$

$$\partial_t A(x,\mu) = \pi(x,\mu) \ , \qquad \partial_t \pi(x,\mu) = f(x,\mu) \ , \tag{25b}$$

where the forces are defined as

$$F(x,\mu) = -\partial_{U(x,\mu)} S(U,A) \ , \tag{26a}$$

$$f(x,\mu) = -\partial_{A(x,\mu)} S(U,A) \ . \tag{26b}$$

The forces can be split in different contributions, accordingly to the action splitting. The gauge action and forces are discussed in [5, 6].

5.1 Forces

The forces associated to the pseudofermion action in eq. (20) has the following form

$$F^a_{k,l}(x,\mu) = -\partial^a_{U(x,\mu)} S_{\mathrm{pf},k,l} = 2\sum_{j=k}^{l} \sigma_j \ \mathrm{Re}(\chi^{k,l}_j, \gamma_5 \partial^a_{U(x,\mu)} D\, \psi^{k,l}_j) \ , \tag{27}$$

$$f^a_{k,l}(x,\mu) = -\partial_{A(x,\mu)} S_{\mathrm{pf},k,l} = 2\sum_{j=k}^{l} \sigma_j \ \mathrm{Re}(\chi^{k,l}_j, \gamma_5 \partial_{A(x,\mu)} D\, \psi^{k,l}_j) \ , \tag{28}$$

with the definitions

$$\psi^{k,l}_j = (D + i\gamma_5\mu_j \mathbf{1}_e)^{-1}\gamma_5 \phi^{k,l}_{\mathrm{e}} \ , \tag{29}$$

$$\chi^{k,l}_j = (D - i\gamma_5\mu_j \mathbf{1}_e)^{-1}\gamma_5 \mathbf{1}_e \psi^{k,l}_j \ . \tag{30}$$

The calculation of the fields $\psi^{k,l}$ and $\chi^{k,l}$ requires the Dirac equation to be solved $2(l-k+1)$ times. If the physical and twisted mass are small enough, it may be convenient to use highly optimized single-shift solvers. Otherwise the previous equations can be recast into the following scheme

$$\chi^{k,l}_{j,\mathrm{e}} = (\hat{D}^\dagger \hat{D} + \mu_j^2)^{-1} \psi^{k,l} \ , \tag{31}$$

$$\chi^{k,l}_{j,\mathrm{o}} = -D^{-1}_{\mathrm{oo}} D_{\mathrm{oe}} \chi^{k,l}_{j,\mathrm{e}} \ , \tag{32}$$

$$\psi^{k,l}_{j,\mathrm{e}} = \gamma_5(\hat{D} - i\gamma_5\mu_j)\chi^{k,l}_{j,\mathrm{e}} \ , \tag{33}$$

$$\psi^{k,l}_{j,\mathrm{o}} = -D^{-1}_{\mathrm{oo}} D_{\mathrm{oe}} \psi^{k,l}_{j,\mathrm{e}} \ . \tag{34}$$

In this case the $\chi^{k,l}_{j,\mathrm{e}}$ fields can be calculated by means of a multi-shift conjugate gradient solver (while the other fields do not require to solve the Dirac equation).

In the following the j,k,l indices will be suppressed, and so the σ_j prefactor. Each force can be split in the sum of two terms. The SU(3) and U(1) hopping forces

$$\begin{aligned} F^a_{\mathrm{hop}}(x,\mu) &= 2\,\mathrm{Re}(\chi, \gamma_5 \partial^a_{U(x,\mu)} (D_{\mathrm{eo}} + D_{\mathrm{oe}})\, \psi) = \\ &= \mathrm{Re}\,\mathrm{tr}_{\mathrm{color}} \{ e^{i\hat{q}A(x,\mu)} T^a U(x,\mu) X_\mu(x) \} \ , \end{aligned} \tag{35}$$

$$\begin{aligned} f_{\mathrm{hop}}(x,\mu) &= 2\,\mathrm{Re}(\chi, \gamma_5 \partial_{A(x,\mu)} (D_{\mathrm{eo}} + D_{\mathrm{oe}})\, \psi) = \\ &= \hat{q}\,\mathrm{Re}\,\mathrm{tr}_{\mathrm{color}} \{ i e^{i\hat{q}A(x,\mu)} U(x,\mu) X_\mu(x) \} \ , \end{aligned} \tag{36}$$

are written in terms of the vector field

$$X_\mu(x) = \mathrm{tr}_{\mathrm{spin}}\left\{\gamma_5(1-\gamma_\mu)\psi(x+\hat{\mu})\chi(x)^\dagger + \gamma_5(1-\gamma_\mu)\chi(x+\hat{\mu})\psi(x)^\dagger\right\} . \tag{37}$$

The SU(3) and U(1) Sheikholeslami–Wohlert (SW) forces

$$\begin{aligned} F^a_{\mathrm{sw}}(x,\mu) &= 2\,\mathrm{Re}(\chi, \gamma_5 \partial^a_{U(x,\mu)}(D_{\mathrm{ee}} + D_{\mathrm{oo}})\,\psi) = \\ &= \frac{c_{\mathrm{sw}}^{\mathrm{SU(3)}}}{4} \sum_{y\nu\rho} \mathrm{Re}\,\mathrm{tr}_{\mathrm{color}}\left\{X_{\nu\rho}(y)\partial^a_{U(x,\mu)}\widehat{F}_{\nu\rho}(y)\right\} , \end{aligned} \tag{38}$$

$$\begin{aligned} f_{\mathrm{sw}}(x,\mu) &= 2\,\mathrm{Re}(\chi, \gamma_5 \partial_{A(x,\mu)}(D_{\mathrm{ee}} + D_{\mathrm{oo}})\,\psi) = \\ &= \frac{q\, c_{\mathrm{sw}}^{\mathrm{U(1)}}}{4} \sum_{y\nu\rho} \mathrm{Re}\,\mathrm{tr}_{\mathrm{color}}\left\{X_{\nu\rho}(y)\partial_{A(x,\mu)}\widehat{A}_{\nu\rho}(y)\right\} , \end{aligned} \tag{39}$$

are written in terms of the tensor field

$$X_{\mu\nu}(x) = i\mathrm{tr}_{\mathrm{spin}}\left\{\gamma_5\sigma_{\mu\nu}\psi(x)\chi(x)^\dagger + \gamma_5\sigma_{\mu\nu}\chi(x)\psi(x)^\dagger\right\} . \tag{40}$$

The exact formula for the derivative of the SU(3) field tensor $\widehat{F}_{\nu\rho}$ with respect to the gauge field can be found in [2]. The derivative of the U(1) field tensor $\widehat{A}_{\nu\rho}$ with respect to the gauge field is a trivial generalization.

The forces associated to the small-determinant action (4) are

$$\begin{aligned} F^a_{\mathrm{sdet}}(x,\mu) &= -\partial^a_{U(x,\mu)} S_{\mathrm{sdet}} = \sum_{y\ \mathrm{odd}} \mathrm{tr}\left\{M(y)^{-1}\partial^a_{U(x,\mu)}M(y)\right\} = \\ &= \frac{ic^{\mathrm{SU(3)}}}{4} \sum_{y\ \mathrm{odd}} \sum_{\nu\rho} \mathrm{tr}\left\{M(y)^{-1}\sigma_{\nu\rho}\partial^a_{U(x,\mu)}\widehat{F}_{\nu\rho}(y)\right\} , \end{aligned} \tag{41}$$

$$\begin{aligned} f_{\mathrm{sdet}}(x,\mu) &= -\partial_{A(x,\mu)} S_{\mathrm{sdet}} = \sum_{y\ \mathrm{odd}} \mathrm{tr}\left\{M(y)^{-1}\partial_{A(x,\mu)}M(y)\right\} = \\ &= \frac{iq\, c^{\mathrm{U(1)}}}{4} \sum_{y\ \mathrm{odd}} \sum_{\nu\rho} \mathrm{tr}\left\{M(y)^{-1}\sigma_{\nu\rho}\partial_{A(x,\mu)}\widehat{A}_{\nu\rho}(y)\right\} . \end{aligned} \tag{42}$$

5.2 Pseudofermion field generation

At the beginning of the molecular-dynamics trajectories, the pseudo-fermion fields must be chosen randomly with the proper distribution. In order to do so, one can use the identities

$$P_{k,l} = \prod_{j=k}^{l} \frac{\hat{Q}^2 + \nu_j^2}{\hat{Q}^2 + \mu_j^2} = \prod_{j=k}^{l} \frac{(\hat{Q} - i\nu_j)(\hat{Q} + i\nu_j)}{(\hat{Q} - i\mu_j)(\hat{Q} + i\mu_j)} = (A_{k,l}^{-1})^\dagger A_{k,l}^{-1} \ , \tag{43}$$

$$A_{k,l} = \prod_{j=k}^{l} \frac{\hat{Q} + i\mu_j}{\hat{Q} + i\nu_j} \ , \tag{44}$$

$$S_{\mathrm{pf},k,l} = \| A_{k,l}^{-1} \phi_{\mathrm{e}}^{k,l} \|^2 \ . \tag{45}$$

Therefore the correct distribution for the pseudofermion fields is obtained by generating the fields $\eta_{\mathrm{e}}^{k,l}$ randomly with normal distribution and by setting

$$\phi_{\mathrm{e}}^{k,l} = A_{k,l} \eta_{\mathrm{e}}^{k,l} \ . \tag{46}$$

In practice one uses a partial fraction decomposition

$$A_{k,l} = 1 + i \sum_{j=k}^{l} \frac{\tau_j}{\hat{Q} + i\nu_j} \ , \tag{47}$$

$$\tau_j = (\mu_j^2 - \nu_j^2) \prod_{\substack{m=l,\ldots,k \\ m \neq j}} \frac{\mu_m - \nu_j}{\nu_m - \nu_j} \ . \tag{48}$$

The application of $A_{k,l}$ to the source field $\eta_{\mathrm{e}}^{k,l}$ amounts to solving the Dirac equation $l-k+1$ times. 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.

6 Reweighting factors

Let $\tilde{R}$ and R be the optimal rational approximations of order $[n,n]$ for $(\hat{D}^\dagger \hat{D})^{-\alpha}$ and $(\hat{D}^\dagger \hat{D} + \hat{\mu}^2)^{-\alpha}$ respectively. It is assumed that the relative errors of the two rational approximations are not greater than δ in the common spectral range $[r_a, r_b]$.

The reweighting factor W defined in eq. (7) is decomposed in two factors which are calculated separately, i.e.

$$W = W_{\rm rat} W_{\rm rtm} \ , \tag{49}$$

$$W_{\rm rat} = \det[(\hat{D}^\dagger \hat{D})^\alpha \tilde{R}] \ , \tag{50}$$

$$W_{\rm rtm} = \det[\tilde{R}^{-1} R] \ . \tag{51}$$

6.1 Reweighting factor W_{rat}

In the calculation of the reweighting factor $W_{\rm rat}$ in eq. (50), it is assumed that the exponent α is a positive rational number of the form

$$\alpha = \frac{u}{v} \ , \tag{52}$$

where u and v are natural numbers. The reweighting factor can be represented as

$$W_{\rm rat} = \det[\hat{Q}^{2u} \tilde{R}^v]^{\frac{1}{v}} = \det(1+Z)^{\frac{1}{v}} \ , \tag{53}$$

where the operator Z is defined as

$$Z = \hat{Q}^{2u} \tilde{R}^v - 1 \ . \tag{54}$$

The determinant in eq. (53) is estimated stochastically

$$W_{\rm rat} = \lim_{N \to \infty} \frac{1}{N} \sum_{j=1}^{N} \exp\{-(\eta_{\rm e}^j, [(1+Z)^{-\frac{1}{v}} - 1]\eta_{\rm e}^j)\} \ , \tag{55}$$

where the fields $\eta_{\rm e}^j$ are N independent normally-distributed pseudofermions that live on the even sites of the lattice. From the norm bound in eq. (13) for $\hat{\mu} = 0$, and the positivity of $\tilde{R}$ (which is guaranteed if the relative error δ is small enough), it follows that

$$0 \leq 1 + Z = \hat{Q}^{2u} \tilde{R}^v = [\hat{Q}^{2\alpha} \tilde{R}]^v \leq (1+\delta)^v \ , \tag{56}$$

which yields the norm bound

$$\|Z\| \leq \Delta = (1+\delta)^v - 1 = v\delta + O(\delta^2) \ . \tag{57}$$

Therefore the Taylor series

$$(1+Z)^{-\frac{1}{v}} = 1 + \sum_{n=1}^{\infty} c_{v,n}\, Z^n \ , \tag{58}$$

$$c_{v,n} = (-1)^n \frac{\frac{1}{v}(\frac{1}{v}+1)\cdots(\frac{1}{v}+n-1)}{n!} \tag{59}$$

converges rapidly in operator norm. The exponent in eq. (55) can be estimated from the first few terms of

$$(\eta_{\rm e}^j, [(1+Z)^{-\frac{1}{v}} - 1]\eta_{\rm e}^j) = \sum_{n=1}^{\infty} c_{v,n}\, (\eta_{\rm e}^j, Z^n \eta_{\rm e}^j) \ . \tag{60}$$

It is possible to estimate the size of these terms by noting that $\|\eta_{\rm e}^j\|^2$ is very nearly equal to 12 times the number $N_{\rm e}$ of even lattice points. Taking the bound (57) into account, the following estimate is obtained

$$|(\eta_{\rm e}^j, Z^n \eta_{\rm e}^j)| \leq \|Z\|^n\, \|\eta_{\rm e}^j\|^2 \leq \Delta^n \|\eta_{\rm e}^j\|^2 \simeq 12(v\delta)^n N_{\rm e} \ . \tag{61}$$

The statistical fluctuations of the exponents in eq. (55) derive from those of the gauge field and those of the random sources $\eta_{\rm e}^j$. For a given gauge field, the variance of the exponent is equal to

$$\mathrm{tr}\,\{[(1+Z)^{-\frac{1}{v}} - 1]^2\} = \frac{1}{v^2}\mathrm{tr}\, Z^2 + O(\delta^3) \leq 12 N_{\rm e}\delta^2 + O(\delta^3) \ . \tag{62}$$

These fluctuations are guaranteed to be small if, for instance, $12N_{\rm e}\delta^2 \leq 10^{-4}$. One can then just as well set $N = 1$ in eq. (55), i.e. a sufficiently accurate stochastic estimate of $W_{\rm rat}$ is obtained in this case with a single random source.

When the stronger constraint $12N_{\rm e}\delta \leq 10^{-2}$ is satisfied, the reweighting factor $W_{\rm rat}$ deviates from 1 by at most 1%. Larger approximation errors can however be tolerated in practice as long as the fluctuations of $W_{\rm rat}$ remain small.

In prectice, the calculation of Z via eq. (54) is numerically unstable for v larger than 2. The following equivalent formula turns out to be stable and is used in the code (for $v > u > 0$):

$$Z = (\hat{Q}^2 + \nu_1^2)^{v-u} \tilde{R}^u \tilde{S}^{v-u} - 1 \ . \tag{63}$$

where we have defined the rational function of degree $[n, n]$

$$\tilde{S} = \frac{\hat{Q}^2}{\hat{Q}^2 + \nu_1^2} \tilde{R} \ . \tag{64}$$

Both rational functions are represented as partial fractions, i.e.

$$\tilde{R} = A \left\{ 1 + \sum_{k=1}^{n} \frac{\tilde{\rho}_k}{\hat{Q}^2 + \mu_k^2} \right\} \ , \qquad \tilde{S} = A \left\{ 1 + \sum_{k=1}^{n} \frac{\tilde{\sigma}_k}{\hat{Q}^2 + \mu_k^2} \right\} \ . \tag{65}$$

In fact one easily finds that the following relation holds

$$\tilde{\sigma}_k = \frac{\tilde{\rho}_k \mu_k^2}{-\nu_1^2 + \mu_k^2} \ . \tag{66}$$

6.2 Reweighting factor W_{rtm}

Let us choose a rational approximation R of order $[n, n]$ for $(\hat{D}^\dagger \hat{D} + \hat{\mu}^2)^{-\alpha}$ of the form

$$R = A \prod_{j=1}^{n} \frac{\hat{D}^\dagger \hat{D} + \nu_j^2}{\hat{D}^\dagger \hat{D} + \mu_j^2} \ , \tag{67}$$

$$\nu_1 > \nu_2 > \cdots > \nu_n \ , \qquad \mu_1 > \mu_2 > \cdots > \mu_n \ , \tag{68}$$

and a rational approximation $\tilde{R}$ of order $[n, n]$ for $(\hat{D}^\dagger \hat{D})^{-\alpha}$ of the form

$$\tilde{R} = \tilde{A} \prod_{j=1}^{n} \frac{\hat{D}^\dagger \hat{D} + \tilde{\nu}_j^2}{\hat{D}^\dagger \hat{D} + \tilde{\mu}_j^2} \ , \tag{69}$$

$$\tilde{\nu}_1 > \tilde{\nu}_2 > \cdots > \tilde{\nu}_n \ , \qquad \tilde{\mu}_1 > \tilde{\mu}_2 > \cdots > \tilde{\mu}_n \ . \tag{70}$$

Let us rewrite eq. (51) as

$$W_{\mathrm{rtm}} = \det[R^{-1} \tilde{R}]^{-1} \ . \tag{71}$$

Notice that the operator $R^{-1}\tilde{R}$ is also a rational function of $\hat{Q}^2 = \hat{D}^\dagger \hat{D}$. It is convenient to break up this rational function in factors of the type

$$\tilde{P}_{k,l} = \prod_{j=k}^{l} \frac{(\hat{D}^\dagger \hat{D} + \mu_j^2)(\hat{D}^\dagger \hat{D} + \tilde{\nu}_j^2)}{(\hat{D}^\dagger \hat{D} + \nu_j^2)(\hat{D}^\dagger \hat{D} + \tilde{\mu}_j^2)} \ . \tag{72}$$

If $n = 12$, for example, the reweighting factor $W_{\rm rtm}$ can be factorized as

$$W_{\rm rtm} = \text{constant} \times \det \tilde{P}_{1,5}^{-1} \ \det \tilde{P}_{6,9}^{-1} \ \det \tilde{P}_{10,12}^{-1} \ . \tag{73}$$

Each of the above determinants is estimated stochastically

$$\det \tilde{P}_{k,l}^{-1} = \lim_{N\to\infty} \frac{1}{N} \sum_{j=1}^{N} \exp\{-(\eta_{\rm e}^{j}, [\tilde{P}_{k,l} - 1]\eta_{\rm e}^{j})\} \ , \tag{74}$$

where the fields $\eta_{\rm e}^{j}$ are N independent normally-distributed pseudofermions that live on the even sites of the lattice. It is useful to consider the partial fraction decomposition

$$\tilde{P}_{k,l} = 1 + \sum_{j=k}^{l} \left(\frac{\sigma_j}{\hat{D}^\dagger \hat{D} + \nu_j^2} + \frac{\tilde{\sigma}_j}{\hat{D}^\dagger \hat{D} + \tilde{\mu}_j^2} \right) \ , \tag{75}$$

$$\sigma_j = \frac{(\tilde{\nu}_j^2 - \nu_j^2)(\mu_j^2 - \nu_j^2)}{\tilde{\mu}_j^2 - \nu_j^2} \prod_{\substack{m=l,\ldots,k \\ m\neq j}} \frac{(\tilde{\nu}_m^2 - \nu_j^2)(\mu_m^2 - \nu_j^2)}{(\tilde{\mu}_m^2 - \nu_j^2)(\nu_m^2 - \nu_j^2)} \ , \tag{76}$$

$$\tilde{\sigma}_j = \frac{(\tilde{\nu}_j^2 - \tilde{\mu}_j^2)(\mu_j^2 - \tilde{\mu}_j^2)}{\nu_j^2 - \tilde{\mu}_j^2} \prod_{\substack{m=l,\ldots,k \\ m\neq j}} \frac{(\tilde{\nu}_m^2 - \tilde{\mu}_j^2)(\mu_m^2 - \tilde{\mu}_j^2)}{(\tilde{\mu}_m^2 - \tilde{\mu}_j^2)(\nu_m^2 - \tilde{\mu}_j^2)} \ . \tag{77}$$

Typically σ_j and $\tilde{\sigma}_j$ are found to have opposite signs. Also, for small values of j, $|\sigma_j|$ and $|\tilde{\sigma}_j|$ are of the same order of magnitude, therefore it is convenient for numerical stability to use the following representation

$$\tilde{P}_{k,l} = 1 + \sum_{j=k}^{l} \frac{(\sigma_j + \tilde{\sigma}_j)(\hat{D}^\dagger \hat{D}) + \sigma_j \tilde{\mu}_j^2 + \tilde{\sigma}_j \nu_j^2}{(\hat{D}^\dagger \hat{D} + \nu_j^2)(\hat{D}^\dagger \hat{D} + \tilde{\mu}_j^2)} \ . \tag{78}$$

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