Reweighting factors provided by the module `mrw`

Björn Leder

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1 Introduction

This module provides routines to compute estimators for mass and twisted-mass reweighting factors. See reference [1] for details on the definition and properties of the estimators. We will denote with $D(m, \mu)$ the Wilson-Dirac operator with bare mass m and twisted-mass μ. We will repeatedly and tacitly use the property $D(m, \mu)^\dagger = \gamma_5 D(m, -\mu)\gamma_5$.

Before describing in Section 4 the implemented reweighting factors and how to selected them in the input file, we shortly define the used stochastic estimator (Section 2) and in detail list the occuring ratios of Dirac operators (Section 3). At the end of Section 3 we also discuss the possible interpolations used in the estimator to factorize the determiant. At the end (Section 5) we desribe the user routines provided by the package.

2 Stochastic estimator

The estimator for the reweighting factor W is given by the product of $N \geq 1$ factors

$$W = \prod_{l=0}^{N-1} W_l \,, \quad W_l = \frac{1}{\det M_l} \,. \tag{1}$$

Each factor is estimated by an average over N_η random vectors

$$W_{l,N_\eta} = \sum_{k=1}^{N_\eta} w_{l,k} \,, \quad -\ln w_{l,k} = {\eta^{(l,k)}}^\dagger (M_l - I)\eta^{(l,k)} \,. \tag{2}$$

Under mild conditions (on M_l) W_{l,N_η} is an unbiased estimator for W_l, see [1].

3 Ratios

The matrix M_l is given by ratios of Dirac operators $D_i = D(m_i, \mu_i)$. We classify them by the maximal inverse power p of D and whether the reweighting is in the mass or the twisted-mass parameter

$$M_l \equiv M_l^{(p,s)} \,, \quad p \in \{1, 2, 4\} \,, \quad s \in \{\mathrm{m}, \mathrm{tm}\} \,, \tag{3}$$

and similar $w_{l,k} \equiv w_{l,k}^{(p,s)}$. The tag "m" corresponds to mass, and "tm" to twisted-mass reweighting. The occurring mass (m_i) and twisted-mass (μ_i) parameters and the reweighting distances δ_i (introduced below) depend on l

$$m_i \equiv m_i(l)\,, \quad \mu_i \equiv \mu_i(l)\,, \quad \delta_i \equiv \delta_i(l)\,. \tag{4}$$

However, for clarity we drop subscripts k, l and the dependence on l for now and until Section 3.5, where we discuss the l dependence (interpolations).

3.1 $M^{(1,\cdot)}$

For mass reweighting we consider

$$M^{(1,\mathrm{m})} = \frac{D_1 + \delta_1}{D_1} = I + \delta_1 D_1^{-1}\,, \tag{5}$$

and for twisted-mass reweighting

$$M^{(1,\mathrm{tm})} = \frac{D_1 + i\delta_1\gamma_5}{D_1} = I + i\delta_1 D_1^{-1}\gamma_5\,. \tag{6}$$

In terms of the solution ψ_1 of

$$D_1^\dagger \psi_1 = \eta\,, \tag{7}$$

we can write the scalar products in (2) as

$$-\ln w^{(1,s)} = \begin{cases} \delta_1 \psi_1^\dagger \eta\,, & s = \mathrm{m}\,, \\ i\delta_1 \psi_1^\dagger \gamma_5 \eta\,, & s = \mathrm{tm}\,, \end{cases} \tag{8}$$

3.2 $M^{(2,\cdot)}$

Here we combine two factors of the previous section, i.e., for mass reweighting

$$M^{(2,\mathrm{m})} = \frac{D_1 + \delta_1}{D_1}\frac{D_2 + \delta_2}{D_2} = I + \delta_1 D_1^{-1} + \delta_2 D_2^{-1} + \delta_1\delta_2 (D_2 D_1)^{-1}\,, \tag{9}$$

and for twisted-mass reweighting

$$M^{(2,\mathrm{tm})} = \frac{D_1 + i\delta_1\gamma_5}{D_1} \cdot \left(\frac{D_2 + i\delta_2\gamma_5}{D_2}\right)^\dagger\,, \tag{10}$$

$$= I + i\delta_1 D_1^{-1}\gamma_5 - i\delta_2 \gamma_5 {D_2^\dagger}^{-1} + \delta_1\delta_2 (D_2^\dagger D_1)^{-1}\,. \tag{11}$$

In terms of the solutions $\psi_{1,2,3}$ of

$$D_1^\dagger \psi_1 = \eta\,, \quad D_2^\dagger \psi_2 = \eta\,, \quad D_2 \psi_3 = \eta\,, \tag{12}$$

we can write the scalar products in (2) as

$$-\ln w^{(2,s)} = \begin{cases} \delta_1 \psi_1^\dagger \eta + \delta_2 \eta^\dagger \psi_3 + \delta_1\delta_2 \psi_1^\dagger \psi_3\,, & s = \mathrm{m}\,, \\ i\delta_1 \psi_1^\dagger \gamma_5 \eta - i\delta_2 \eta^\dagger \gamma_5 \psi_2 + \delta_1\delta_2 \psi_1^\dagger \psi_2\,, & s = \mathrm{tm}\,. \end{cases} \tag{13}$$

3.2.1 Special cases of $M^{(2,\mathrm{m})}$

In the special case $D_2 = D_1$ and $\delta_2 = -\delta_1$ Eqs. (9) and (13) reduce to

$$M^{(iso,\mathrm{m})} = I + (\delta_1(m_2 - m_1 + i\gamma_5(\mu_2 - \mu_1)) - \delta_1^2)D_1^{-2}\,, \tag{14}$$

$$-\ln w^{(iso,\mathrm{m})} = (\delta_1(m_2 - m_1) - \delta_1^2)\psi_1^\dagger\psi_3 + i\delta_1(\mu_2 - \mu_1)\psi_1^\dagger\gamma_5\psi_3\,. \tag{15}$$

Another special case is $D_2 = D_1^\dagger$ and $\delta_2 = \pm\delta_1$. Then

$$M^{(\pm,\mathrm{m})} = \begin{cases} I + 2\delta_1\mathrm{Re}(D_1^{-1}) + \delta_1^2(D_1^\dagger D_1)^{-1}\,, & \delta_2 = \delta_1\,, \\ I + 2i\delta_1\mathrm{Im}(D_1^{-1}) - \delta_1^2(D_1^\dagger D_1)^{-1}\,, & \delta_2 = -\delta_1\,, \end{cases} \tag{16}$$

and correspondingly

$$-\ln w^{(\pm,\mathrm{m})} = \begin{cases} 2\delta_1\mathrm{Re}(\psi_1^\dagger\eta) + \delta_1^2\psi_1^\dagger\psi_1\,, & \delta_2 = \delta_1\,, \\ 2i\delta_1\mathrm{Im}(\psi_1^\dagger\eta) - \delta_1^2\psi_1^\dagger\psi_1\,, & \delta_2 = -\delta_1\,, \end{cases} \tag{17}$$

3.2.2 Special cases of $M^{(2,\mathrm{tm})}$

In the special case $D_2 = D_1$ and $\delta_2 = \delta_1$ Eqs. (11) and (13) reduce to

$$M^{(iso,\mathrm{tm})} = I + d_1(D_1^\dagger D_1)^{-1}\,, \tag{18}$$

$$-\ln w^{(iso,\mathrm{tm})} = d_1\psi_1^\dagger\psi_1\,, \tag{19}$$

where we used $\gamma_5 D_1^\dagger D_1 = D_1 D_1^\dagger\gamma_5$ and d_1 is the reweighting distance of the symmetric operator $D_1^\dagger D_1$

$$d_1 = (2\mu_1\delta_1 + \delta_1^2) = (\mu_1 + \delta_1)^2 - \mu_1^2\,. \tag{20}$$

Finally, in the special case $D_2 = D_1$ and $\delta_2 = -\delta_1$ we obtain

$$M^{(-,\mathrm{tm})} = I + 2i\delta_1\mathrm{Im}(D_1^{-1}i\gamma_5) - \delta_1^2(D_1^\dagger D_1)^{-1}\,, \tag{21}$$

$$-\ln w^{(-,\mathrm{tm})} = 2i\delta_1\mathrm{Im}(\psi_1^\dagger i\gamma_5\eta) - \delta_1^2\psi_1^\dagger\psi_1\,. \tag{22}$$

3.3 $M^{(4,\mathrm{tm})}$

Here we combine two reweighting factors that are of the the special kind (18)

$$M^{(4,\mathrm{tm})} = \frac{D_1^\dagger D_1 + d_1}{D_1^\dagger D_1}\,\frac{D_2^\dagger D_2 + d_2}{D_2^\dagger D_2} = (I + d_1(D_1^\dagger D_1)^{-1})(I + d_2(D_2^\dagger D_2)^{-1})\,, \tag{23}$$

with the reweighting distance of the symmetric operator $D_{1,2}^\dagger D_{1,2}$

$$d_{1,2} = (2\mu_{1,2}\delta_{1,2} + \delta_{1,2}^2) = (\mu_{1,2} + \delta_{1,2})^2 - \mu_{1,2}^2\,. \tag{24}$$

In general, by factoring out we obtain

$$M^{(4,\mathrm{tm})} = I + d_1(D_1^\dagger D_1)^{-1} + d_2(D_2^\dagger D_2)^{-1} + d_1 d_2(D_1^\dagger D_1)^{-1}(D_2^\dagger D_2)^{-1} \tag{25}$$

$$= I + [d_1 D_2^\dagger D_2 + d_2 D_1^\dagger D_1 + d_1 d_2](D_1^\dagger D_1)^{-1}(D_2^\dagger D_2)^{-1}\,. \tag{26}$$

The case $d_2 = -d_1$ is especially favorable here, since then

$$M^{(4,\mathrm{tm})} = I + [d_1(\Delta + \mu_2^2 - \mu_1^2) - d_1^2](D_1^\dagger D_1)^{-1}(D_2^\dagger D_2)^{-1} . \tag{27}$$

with

$$\Delta = D(m_2, 0)^\dagger D(m_2, 0) - D(m_1, 0)^\dagger D(m_1, 0) . \tag{28}$$

If additionally the μ-reweighting is such that

$$\mu_2^2 - \mu_1^2 = hd_1 , \tag{29}$$

this further reduces to

$$M^{(4,\mathrm{tm})} = I + [d_1\Delta + d_1^2(h-1)](D_1^\dagger D_1)^{-1}(D_2^\dagger D_2)^{-1} . \tag{30}$$

For $m_1 = m_2$ we have $\Delta = 0$ and the leading fluctuations thus scale like $(h-1)^2 d_1^4$. For $m_1 \neq m_2$ the leading fluctuations will scale like $d_1^2(m_2 - m_1)^2$.

There are several possible solutions to the conditions $d_2 = -d_1$ and (29):

1. For $m_2 = m_1$, $\mu_2 = \sqrt{2}\mu$, $\mu_1 = 0$, $\delta_2 = (1-\sqrt{2})\mu$ and $\delta_1 = \mu$, which coincides with the openQCD μ-reweighting factor W_2, we find $d_1 = \mu$ and $h = 2$ [2].

2. For $m_1 \neq m_2$ we can set $\delta_2 = -\delta_1$. Demanding $d_1 = -d_2$ leads to $\mu_2 = \mu_1 + \delta_1$ and $\mu_2^2 - \mu_1^2 = d_1$, i.e., $h = 1$.

Introducing ψ_4, the solution to $D_2\psi_4 = \psi_1$, the scalar product in (2) can be evaluated as

$$-\ln w^{(4,\mathrm{tm})} = d_1\psi_1^\dagger\psi_1 + d_2\psi_2^\dagger\psi_2 + d_1 d_2\psi_4^\dagger\psi_4 , \tag{31}$$

where we used $D_1^\dagger D_2 D_2^\dagger D_1 = D_2^\dagger D_2 D_1^\dagger D_1$. If $d_2 = -d_1$ and $m_1 = m_2$ we can use (27) with $\Delta = 0$ and therefore only need ψ_4

$$-\ln w^{(4,\mathrm{tm})} = (d_1(\mu_2^2 - \mu_1^2) - d_1^2)\psi_4^\dagger\psi_4 , \tag{32}$$

3.4 Even-odd twisted mass reweighting

In Eqs. (6), (10) and (11) D can be replaced by the even-odd preconditioned Dirc operator $\hat{D} = D_{\mathrm{ee}} - D_{\mathrm{eo}}D_{\mathrm{oo}}^{-1}D_{\mathrm{oe}}$. Assuming the twisted-mass to be non-zero only on the even sites, all subsequent results for twisted-mass reweighting remain the same. Therefore all twisted-mass reweighting factors come in two versions, without and with even-odd preconditioning.

3.5 Interpolations

Lets consider first the one flavor mass/twisted-mass reweighting Eqs. (5) and (6). We consider here only pure mass/twisted-mass interpolations. An interpolation in N steps $l = 0, \ldots, N-1$ between ensemble and target mass (twisted-mass), m_0 and m (μ_0 and μ), respectively, is given by

$$\{m_1(l), \mu_1(l), \delta_1(l) : \; m_1(0) = m \,, \; m_1(N-1) = m_0 - \delta_1(N-1) \,, \; \mu_1(l) \equiv \mu_0\} , \tag{33}$$

for mass reweighting and by

$$\{m_1(l), \mu_1(l), \delta_1(l):\ \mu_1(0) = \mu\,,\ \mu_1(N-1) = \mu_0 - \delta_1(N-1)\,,\ m_1(l) \equiv m_0\}\,, \tag{34}$$

for twisted-mass reweighting. For $N \geq 2$ the reweighting differences are given by

$$\delta_1(l) = x_1(l+1) - x_1(l)\,, \quad x \in \{m, \mu\}\,. \tag{35}$$

For such interpolations the product in (1) yields

$$\prod_{l=0}^{N-1} W_l^{(1,s)} = \begin{cases} \det\left(\frac{D(m,\mu_0)}{D(m_0,\mu_0)}\right) & s = \mathrm{m} \\ \det\left(\frac{D(m_0,\mu)}{D(m_0,\mu_0)}\right) & s = \mathrm{tm} \end{cases} \tag{36}$$

Furthermore the interpolation should be such that $\delta_1(l) \to 0$ as $N \to \infty$ for all l. These conditions are satisfied for the family of interpolations ($x \in \{m, \mu\}$)

$$x_1(l) = x + S_l^p \frac{x_0 - x}{S_N^p}\,, \quad \delta_1(l) = (l+1)^p \frac{(x_0 - x)}{S_N^p}\,, \quad S_n^p = \sum_{k=1}^{n} k^p\,. \tag{37}$$

We focus here on integer powers $p = 0, 1, 2, 3, 4$ because for those S_n^p can be easily computed

$$S_n^0 = n\,, \quad S_n^1 = S_n^0\,(n+1)/2\,, \quad S_n^2 = S_n^1\,(2n+1)/3\,, \tag{38}$$

$$S_n^3 = \left(S_n^1\right)^2\,, \quad S_n^4 = S_n^2\,(3n^2 + 3n - 1)/5\,, \tag{39}$$

and powers $p > 4$ are not needed in practice.

In the case of two flavor reweighting Eqs. (9) and (10) the product in (1) can be factored into two products containing only terms with D_1 and D_2, respectively. It is straight forward to see that choosing an interpolation as above for $m_{1,2}(l)$ and $\mu_{1,2}(l)$ yields the correct result. Note that in the implemented estimators the value of p is the same for D_1 and D_2, but in general it does not have to be the same.

In the case of the μ-reweighting Eq. (18) and Eq. (23) the interpolation is conveniently defined for the twisted mass squared $\mu_1^2(l)$. To avoid ambiguities we assume here $\mu_1(l) \geq 0$. The interpolation is given by

$$\{m_1(l), \mu_1^2(l), d_1(l):\ \mu_1^2(0) = \mu^2\,,\ \mu_1^2(N-1) = \mu_0^2 - d_1(N-1)\,,\ m_1(l) \equiv m_0\}\,, \tag{40}$$

and for $N \geq 2$

$$d_1(l) = \mu_1^2(l+1) - \mu_1^2(l)\,. \tag{41}$$

All conditions are satisfied by the interpolations Eq. (37) with $x \to \mu^2$ and $\delta \to d$. The reweighting distance $\delta_1(l)$ is given by solving Eq. (20)

$$\delta_1(l) = -\mu_1(l) + \sqrt{\mu_1^2(l) + d_1(l)}\,. \tag{42}$$

The interpolation $\mu_2^2(l)$ is analogous.

4 Computation of reweighting factors with program `ms5`

Common reweighting factors, their mass interpolations (l dependence of $m_{1,2}$, $\mu_{1,2}$, $\delta_{1,2}$) and how-to select them in the input file.

The number of reweighting factors to be computed is set by `nrw` in the `Configurations` section of the input file. Each reweighting factor has to be specified in a corresponding section. In general, in each section the type of reweighting `mrwfact`, the number of mass/twisted-mass interpolation steps N (`nm`), the type of interpolation, i.e., the power p in Eq. (37) (`pwr`) and the number of noise sources N_η (`nsrc`) has to be specified, e.g.,

```
[Reweighting factor 0]
mrwfact   TMRW        # or TMRW1,TMRW1_EO,...
...
nm        2
pwr       1
nsrc      12
```

In the case of mass reweighting `MRW,MRW_ISO,MRW_TF` it is neccessary to indicate wether the twisted-mass term is defined only on the even sites or not

```
tmeo       0
```

Depending on whether one or two/three inversions are needed, i.e., whether routine `mrw1[eo]` or `mrw2[eo]`/`mrw3[eo]` is used (see Secs. 5.2, 5.3 and 5.4), one or two solvers have to be chosen

```
isp       1 [0]
```

Also the number of values written to the `.ms5.dat`-file differs in the two cases. If `mrw1` is used, $4NN_\eta$ `double` numbers per reweighting factor are written, i.e., per source field:

```
  complex_dble return, double sqnp, double sqne
```

whereas $9NN_\eta$ `double` numbers per reweighting factor in the case of `mrw2`/`mrw3`:

```
  complex_dble return, complex_dble lnw1[2],
  double sqnp[2], double sqne
```

In the case of `mrw3` the imaginary part of the return value is identical zero.

4.1 One flavor mass/twisted-mass: `MRW,TMRW,TMRW_EO`

We consider reweighting factors as in Eqs. (5) and (6).

```
[Reweighting factor 0]
mrwfact       MRW
kappa0        0.13515
mu0           0.00
kappa         0.13519
...

[Reweighting factor 1]
mrwfact       TMRW
kappa0        0.13515
mu0           0.0
mu            0.005
...
```

In both cases the mass $m_0 = 1/(2\kappa_0) - 4$ and twisted-mass μ_0 of the ensemble are given by `kappa0` and `mu0`. It follows the target mass $m = 1/(2\kappa) - 4$ in terms of the target `kappa`, or the target twisted-mass μ (`mu`). The routine `mrw1` is used and therefore only one solver needs to be specified.

4.2 `openQCD` μ-reweighting type I: `TMRW1`,`TMRW1_EO`

We consider a reweighting factor as in Eq. (10). Choosing $\mu_2(l) = \mu_1(l)$, $m_2(l) = m_1(l)$ the special case of Eq. (18) applies for all factors and the interpolation is given by Eq. (40). Here μ and μ_0 have to be non-negative.

```
[Reweighting factor 1]
mrwfact       TMRW1
kappa0        0.13515
mu0           0.005
mu            0.0
...
```

The needed entries and their meaning are equivalent to the case `TMRW` in Sec. 4.1.

Since `mrw1` also computes $\psi_1^\dagger \psi_1$, cf. Eq. (19), we can obtain

$$\prod_{l=0}^{N-1} W_l^{(d,\mathrm{tm})} = \det\left(\frac{D(m_0,\mu)^\dagger D(m_0,\mu)}{D(m_0,\mu_0)^\dagger D(m_0,\mu_0)}\right) . \tag{43}$$

For $\mu = 0$, $N = 1$ this is equivalent to the `openQCD` μ-reweighting type I [2].

4.3 `openQCD` μ-reweighting type II: `TMRW2`,`TMRW2_EO`

We consider a reweighting factor as in Eq. (23).

```
[Reweighting factor 1]
mrwfact       TMRW2
kappa0        0.13515
mu0           0.005
mu            0.0
kappa         0.135
...
```

This computes the combination of a twisted-mass reweighting of a doublet of quarks from μ_0 to μ at the ensemble mass $m_0 = 1/(2\kappa_0) - 4$ (set by `kappa0`) and a twisted-mass reweighting from μ_0 to $\mu' = \sqrt{(2\mu_0^2 - \mu^2)}$ at $m = 1/(2\kappa) - 4$ (set by `kappa`). Without loss of generality and to avoid ambiguities we assume $\mu_0 > \mu$.

$$\prod_{l=0}^{N-1} W_l^{(4,\mathrm{tm})} = \det\left(\frac{D(m_0,\mu)^\dagger D(m_0,\mu)}{D(m_0,\mu_0)^\dagger D(m_0,\mu_0)} \cdot \frac{D(m,\mu')^\dagger D(m,\mu')}{D(m,\mu_0)^\dagger D(m,\mu_0)}\right) . \tag{44}$$

For $\mu = 0$, $N = 1$, $m = m_0$ this is equivalent to the `openQCD` μ-reweighting type II [2].

The interpolation for $\mu_1^2(l)$ is as in Eq. (40). Here μ and μ_0 have to be non-negative. In order to minimize stochastic noise we choose $\mu_2^2(l)$ such that $d_2(l) = -d_1(l)$ and $\mu_2^2(l) - \mu_1^2(l) = \mu_0^2 - \mu^2 + d_1(l)$, cf. Section 3.3.

The routine `mrw3` is used and therefore two solvers have to be specified: for the solve with m_0 and the solve with m.

Logarithmic interpolation A logarithmic interpolation between μ_0 and 0 in n steps is obtained for

$$d_1(l) = \mu_0^2 q^{l+1} , \quad \mu_1^2(l) = \mu_0^2 - \sum_{i=0}^{l} d_1(l) = \mu_0^2 \left(2 - \frac{1-q^{l+2}}{1-q} \right) , \tag{45}$$

for $l = 0, \ldots, n-2$ and in the last step

$$d_1(n-1) = \mu_1^2(n-2) \approx \mu_0^2 q^{n-1} , \quad \mu_1^2(l) = 0 . \tag{46}$$

Here q is a positive constant $q \leq 0.5$. To minimize the stochastic noise we set again in all steps $\mu_2^2(l) = \mu_0^2 + \mu_1^2(l) + d_1(l)$, $d_2(l) = -d_1(l)$, cf. Section 3.3.

This can be realized by combining n `TMRW2,TMRW2_EO` reweighting factors with `nm` set to one. For the steps $l = 0, \ldots, n-2$ `pwr` set to $-(l+1)$ and `mu0`, `mu` set to μ_0. For the last step `pwr` is set to $-(n-1)$, `mu0` to μ_0 and `mu` to zero.

4.4 Rectangle μ-detour: `TMRW3,TMRW3_EO`

We consider a reweighting factor as in Eq. (10).

```
[Reweighting factor 1]
mrwfact      TMRW3
kappa0       0.13515
mu0          0.0
mu           0.05
kappa        0.135
...
```

This computes the combination of a twisted-mass reweighting from μ_0 to μ at the ensemble mass $m_0 = 1/(2\kappa_0) - 4$ (set by `kappa0`) and a twisted-mass reweighting from μ to μ_0 at $m = 1/(2\kappa) - 4$ (set by `kappa`). If $\mu_1(l)$ is an interpolation between μ_0 and μ and $\mu_2(l)$ an interpolation between $-\mu_0$ and $-\mu$ we obtain

$$\prod_{l=0}^{N-1} W_l^{(2,\mathrm{tm})} = \det \left(\frac{D(m_0,\mu)}{D(m_0,\mu_0)} \frac{D(m,\mu_0)}{D(m,\mu)} \right) . \tag{47}$$

To minimize the stochastic noise the interpolations are such that $\mu_1(l)$ is given by an interpolation as in Eq. (34) and $\mu_2(0) = -\mu_0$, $\mu_2(l) = -(\mu_1(l) + d_1(l))$ and $\delta_2(l) = \delta_1(l)$. The routine `mrw2` is used and therefore two solvers have to be specified: for the solve with m_0 and the solve with m.

4.5 Rectangle μ-detour for doublet: `TMRW4,TMRW4_EO`

We consider a reweighting factor as in Eq. (23).

```
[Reweighting factor 1]
mrwfact      TMRW4
kappa0       0.13515
mu0          0.0
mu           0.05
kappa        0.135
...
```

This computes the combination of a twisted-mass reweighting of a doublet of quarks from μ_0 to μ at the ensemble mass $m_0 = 1/(2\kappa_0) - 4$ (set by `kappa0`) and a twisted-mass reweighting from μ to μ_0 at $m = 1/(2\kappa) - 4$ (set by `kappa`)

$$\prod_{l=0}^{N-1} W_l^{(4,\mathrm{tm})} = \det\left(\frac{D(m_0,\mu)^\dagger D(m_0,\mu)}{D(m_0,\mu_0)^\dagger D(m_0,\mu_0)} \cdot \frac{D(m,\mu_0)^\dagger D(m,\mu_0)}{D(m,\mu)^\dagger D(m,\mu)}\right) . \tag{48}$$

The interpolation for $\mu_1^2(l)$ is as in Eq. (40). Here μ and μ_0 have to be non-negative. In order to minimize stochastic noise we choose $\mu_2^2(0) = \mu_0^2$, $\mu_2^2(l) = \mu_1^2(l-1)$ for $l > 0$ and $d_2(l) = -d_1(l)$. In each step one has $\mu_2^2(l) - \mu_1^2(l) = d_1(l)$, cf. Section 3.3.

The routine `mrw3` is used and therefore two solvers have to be specified: for the solve with m_0 and the solve with m.

4.6 Isospin reweighting: `MRW_ISO`

We consider a reweighting factor as in Eq. (9).

```
[Reweighting factor 0]
mrwfact       MRW_ISO
kappa0        0.13519
mu0           0.05
kappa         0.13515
...
```

This computes the combination of a mass reweighting from the ensemble mass $m_0 = 1/(2\kappa_0) - 4$ (set by `kappa0`) to $m_0 - \Delta m$ and $m_0 + \Delta m$, where $\Delta m = m_0 - m$ and $m = 1/(2\kappa) - 4$ (set by `kappa`)

$$\prod_{l=0}^{N-1} W_l^{(2,\mathrm{m})} = \det\left(\frac{D(m_0+\Delta m,\mu_0) D(m_0-\Delta m,\mu_0)}{D(m_0,\mu_0) D(m_0,\mu_0)}\right) . \tag{49}$$

To minimize the stochastic noise the interpolations are such that $m_1(l)$ is given by an interpolation as in Eq. (33) and $m_2(l) = m_1(l) + \delta_1(l) + \Delta m$, $\delta_2(l) = -\delta_1(l)$.

The routine `mrw2` is used and therefore two solvers have to specified: for the solve with $m_1(l)$ and the solve with $m_2(l)$.

4.7 Two flavor reweighting: `MRW_TF`

We consider a reweighting factor as in Eq. (9).

```
[Reweighting factor 0]
mrwfact       MRW_TF
kappa0        0.13519
kappa         0.135
mu0           0.05
mu            0.0
gamma         1.0
kappa2        0.135
...
```

This is the most general selection for mass reweighting. It computes the combination of a mass reweighting from ensemble mass $m_r = 1/(2\kappa_0) - 4$ (set by `kappa0`) to $m_r + \gamma\Delta m$ at fixed μ_0 and from ensemble mass $m_s = 1/(2\kappa) - 4$ (set by kappa) to $m_s - \Delta m$ at fixed μ. Here $\Delta m = m_s - m$ with $m = 1/(2\kappa_2) - 4$ (set by kappa2) and γ is set by gamma.

$$\prod_{l=0}^{N-1} W_l^{(2,\mathrm{m})} = \det\left(\frac{D(m_r + \gamma\Delta m, \mu_0)}{D(m_r, \mu_0)} \frac{D(m_s - \Delta m, \mu)}{D(m_s, \mu)}\right) . \tag{50}$$

To minimize the stochastic noise the interpolations are such that $m_1(l)$ is given by an interpolation as in Eq. (33) with $m_0 = m_s$ and $m = m_s - \Delta m$. The interpolation $m_2(l)$ is then given by $m_2(l) = m_r + \gamma(m_1(l) + \delta_1(l) - m)$, $\delta_2(l) = -\gamma\delta_1(l)$.

The routine mrw2 is used and therefore two solvers have to specified: for the solve with $m_1(l)$ and the solve with $m_2(l)$.

5 Data structures and routines

5.1 Structure mrw_masses_t

Definition:

```
typedef struct
{
   double m1,mu1,d1;
   double m2,mu2,d2;
} mrw_masses_t;
```

5.2 Routine mrw1[eo]

This routine is used for reweighting factors with a ratio as in Section 3.1.

```
complex_dble mrw1[eo](mrw_masses_t ms,int tm,int isp,double *sqnp,
                      double *sqne,int *status);
```

The routine generates a new random vector η and computes the solution ψ_1, cf. Eq. (12). It returns $-\ln w^{(1,s)}$, see Eq. (8), with $s = \mathrm{m}$ if tm equals zero and $s = \mathrm{tm}$ otherwise. Additionally, sqnp is set to the square of the norm of ψ_1, i.e., $\psi_1^\dagger\psi$. Only the elements m1,mu1,d1 of ms are used and set m_1, μ_1, δ_1, respectively. The parameter isp selects the solver to be used. On exit sqne is set to the square of the norm of η and status[0-2] to the status of the solver.

5.3 Routine mrw2

This routine is used for reweighting factors with a ratio as in Section 3.2.

```
complex_dble mrw2[eo](mrw_masses_t ms,int tm,int *isp,
                      complex_dble *lnw1, double *sqnp,double *sqne,
                      int *status);
```

The routine generates a new random vector η and computes the solutions ψ_1 and ψ_2 or ψ_1 and ψ_3, cf. Eq. (12), if tm is non-zero or zero, respectively. It returns $-\ln w^{(2,s)}$, see Eq. (13), with $s = \mathrm{m}$ if tm equals zero and $s = \mathrm{tm}$ otherwise. Additionally, lnw1[0,1] is set to $\delta_1\psi_1^\dagger\eta$ ($i\delta_1\psi_1^\dagger\gamma_5\eta$) and $\delta_2\eta^\dagger\psi_3$ ($i\delta_2\psi_2^\dagger\gamma_5\eta$), and sqnp[0,1] to the square norm of ψ_1 and ψ_3 (ψ_1 and ψ_2), if the parameter tm is zero (none-zero). The elements m1,mu1,d1 and m2,mu2,d2 of ms set m_1, μ_1, δ_1 and m_2, μ_2, δ_2, respectively. The parameter `isp[0]` and `isp[1]` select the solver to be used in solving for ψ_1 and $\psi_{2,3}$, respectively. On exit `sqne` is set to the square of the norm of η and `status[0-2]` and `status[3-5]` are set to the status of the two solver calls.

5.4 Routine `mrw3`

This routine is used for reweighting factors with a ratio as in Section 3.3.

```
double mrw3[eo](mrw_masses_t ms,int *isp,complex_dble *lnw1,
                double *sqnp,double *sqne,int *status)
```

This routine generates a new random vector η. If `ms.m1!=ms.m1` it computes the solutions ψ_1, ψ_2 and ψ_4, cf. Section 3.3. It returns $-\ln w^{(4,\mathrm{tm})}$, computed as in Eq. (31). Additionally, `lnw1[0,1]` is set to $i\delta_1\psi_1^\dagger\gamma_5\eta$ and $i\delta_2\psi_2^\dagger\gamma_5\eta$, and `sqnp[0,1]` to the square norm of ψ_1 and ψ_2. The elements `m1,mu1,d1` and `m2,mu2,d2` of `ms` set m_1, μ_1, δ_1 and m_2, μ_2, δ_2, respectively. The parameter `isp[0]` and `isp[1]` select the solver to be used in solving for ψ_1 and $\psi_{2,4}$, respectively. On exit `sqne` is set to the square of the norm of η and `status[0-2]`, `status[3-5]` and `status[6-8]` are set to the status of the three solver calls.

In order to avoid big cancellations, if $d_2 = -d_1$ in (31) the difference of norm squares is computed as

$$\psi_1^\dagger\psi_1 - \psi_2^\dagger\psi_2 = \mathrm{Re}((\psi_1 - \psi_2)^\dagger(\psi_1 + \psi_2)) \,. \tag{51}$$

If `ms.m1==ms.m1` and $d_2 = -d_1$ it is possible to compute $-\ln w^{(4,\mathrm{tm})}$ using only ψ_4, cf. Eq. (32). Therefore, in this case the solve for ψ_2 is skipped and `lnw1[1]`, `sqnp[1]` and `status[3-5]` are set to zero.

References

[1] J. Finkenrath, F. Knechtli, and B. Leder, *Nucl. Phys.* **B877** (2013) 441–456, [arXiv:1306.3962].

[2] M. Lüscher and S. Schaefer, *Comput.Phys.Commun.* **184** (2013) 519–528, [arXiv:1206.2809].