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Tuning of the strange quark mass with optimal reweighting

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Quark mass reweighting can be used to tune the mass of dynamical quarks. The basic idea is to use gauge field ensembles generated at some bare mass parameters to evaluate observables at different bare sea quark masses. This involves the computation of so called reweighing factors which are given as ratios of fermion determinants. In the case of simulations including the strange quark, reweighting can be used to improve the approach towards physical quark masses. Optimal reweighting strategies combine a change of the strange quark mass with a change of the light quark masses in order to minimize the fluctuations of the reweighting factor. We present numerical test of such strategies for recent CLS2 simulations and a software package for mass reweighting based on openQCD.

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1. Why mass reweighting?

Lattice QCD simulations proceed to generate ensembles at small lattice spacings and light quark masses close to or at their physical values. This is possible because of the algorithmic improvements of the last decade. Nevertheless, the cost to generate *independent* gauge configurations grows, particularly so because of the growing autocorrelation times when the lattice spacing is lowered [1]. The problem is further aggravated by the inclusion of a sea strange quark, which leads to an enlarged mass tuning problem (see for example [2]).

In such a situation it might be more cost efficient to change the masses of a given ensemble using reweighting instead of generating a new one. This is because although reweighting is expensive it only has to be done for independent gauge configurations and therefore its cost does not increase with the autocorrelation times. Also the naively expected linear scaling with the volume might be much milder in reality [3, 4].

Reweighting simply means changing the probability $P_a(U)$ ("weight") of each gauge configuration U in the expectation value

$$\langle \mathscr{O} \rangle_a = \frac{1}{Z_a} \int \mathrm{D}[U]\, P_a(U)\, \mathscr{O}(U)\,, \quad P_a(U) = \mathrm{e}^{-S_g(\beta,U)} \prod_{i=1}^{n_f} \det(D(U) + m_i + i\gamma_5\mu_i)\,. \tag{1.1}$$

Here we assume n_f quark flavors with (possibly degenerate) bare masses m_i and twisted masses μ_i, the gauge action S_g only depends on β and normalization $\int \mathrm{D}[U]P(U)/Z \equiv 1$. The subscript on the expectation value and the probability distribution specifies the bare parameter set $a = \{\beta, m_1, m_2, \ldots, m_{n_f}, \mu_1, \ldots, \mu_{n_f}\}$. Now an observable at bare parameter set $b = \{\beta', m'_1, m'_2, \ldots, m'_{n_f}, \mu'_1, \ldots, \mu'_{n_f}\}$ is obtained from

$$\langle \mathscr{O} \rangle_b = \frac{\langle \mathscr{O} W \rangle_a}{\langle W \rangle_a}\,, \quad W = \frac{P_b}{P_a}\,. \tag{1.2}$$

If one restricts oneself to changes in the masses (hence $\beta' = \beta$), as we do here, the reweighting factor W can be written as

$$W = \frac{1}{\det(A)}\,, \quad A = \prod_{i=1}^{n_f} \frac{D + m_i + i\gamma_5\mu_i}{D + m'_i + i\gamma_5\mu'_i}\,. \tag{1.3}$$

The next section specifies the stochastic estimator used for the determinant in (1.3). In section 3 follows a summary of the properties of three important cases of mass reweighting. From these properties an optimal strategy for the tuning of the strange quark mass is derived in section 4. Section 5 briefly describes a publicly available implementation of this strategy and in section 6 numerical tests and cost estimates are presented.

2. Fluctuations

The numerical estimation of reweighting factors of the form (1.3) uses the Monte-Carlo evaluation of an integral representation of the determinant of a complex matrix [5, 6]

$$W_{N_\eta}(A) = \frac{1}{N_\eta} \sum_{k=1}^{N_\eta} e^{-\eta^{(k)\dagger}(A-I)\eta^{(k)}}\,, \tag{2.1}$$

with N_η Gaussian distributed random vectors $\eta^{(i)}$ and $W_{N_\eta} \to W$ for $N_\eta \to \infty$ if $\lambda(A+A^\dagger) > 0$ [5, 6]. Let us assume A can be written as $A = I + \varepsilon B$ with $\varepsilon||B|| \ll 1$. Then the stochastic error of this estimator may be expanded

$$\delta_\eta^2(A) = \mathrm{var}_\eta(W_{N_\eta})/(N_\eta|W|^2) = \frac{1}{N_\eta}[\varepsilon^2 \mathrm{Tr}(BB^\dagger) + \mathrm{O}(\varepsilon^3)]\,. \tag{2.2}$$

A similar expansion is obtained for the fluctuations of the reweighting factor in the expectation value (1.1)

$$\sigma_U^2 = \mathrm{var}_U(W)/\langle W\rangle^2 = \varepsilon^2 \mathrm{var}_U(\mathrm{Tr}(B)) + \mathrm{O}(\varepsilon^3)\,. \tag{2.3}$$

It has been noticed that the stochastic estimator (2.1) may be plagued by large fluctuations and/or long tails in the distribution. The reason is that its variance may not be defined even if the mean is, i.e., the variance is only defined for $\lambda(A+A^\dagger) > 1$ [7]. There have been several attempts to control the variance [8, 9, 10]. Here we use a factorization of the determinant in N factors with $\varepsilon' \propto \varepsilon/N$ [5, 6]. Since the factorization has been described thoroughly elsewhere and for better readability we skip the details here and stick to the formulas with $N = 1$. The generalization is straightforward.

3. Mass reweighting factors

3.1 One flavor

The simplest case of mass reweighting is the change of the mass of one quark flavor of mass m_s to mass $m_s + \Delta m$. Using the shorthand $D_m = D + m$, the corresponding reweighting factor is ($\mu_s = 0$)

$$W_{1\mathrm{f}}(m_s, \Delta m) = \frac{\det(D_{m_s+\Delta m})}{\det(D_{m_s})} = \frac{1}{\det(A_{1\mathrm{f}})}\,, \quad A_{1\mathrm{f}} = I - \Delta m D^{-1}_{m_s+\Delta m}\,, \tag{3.1}$$

and the stochastic error and the fluctuations scale (asymptotically) with Δm^2.

3.2 Two flavors

Now we consider the simultaneous change of the mass of two quark flavors s and l. Without loss of generality we assume $m_l \leq m_s$ and a change $m_l \to m_l - \gamma\Delta m$ while $m_s \to m_s + \Delta m$. The corresponding reweighting factor is ($\mu_s = \mu_l = 0$)

$$W_{2\mathrm{f}}^{(\gamma)}(m_l, m_s, \Delta m) = \frac{\det(D_{m_l-\gamma\Delta m} D_{m_s+\Delta m})}{\det(D_{m_l} D_{m_s})} = \frac{1}{\det(A_{2\mathrm{f}})}\,, \quad A_{2\mathrm{f}} = I + \Delta m \frac{\gamma\Delta m + \gamma D_{m_s} - D_{m_l}}{D_{m_s+\Delta m} D_{m_l-\gamma\Delta m}}\,, \tag{3.2}$$

and the stochastic error and the fluctuations scale (asymptotically) with Δm^2. However, if $m_l = m_s = m$ and $\gamma = 1$ one finds $A_{2\mathrm{f}} = I + \Delta m^2 (D_m^2 - \Delta m^2)^{-1}$ and a scaling $\propto \Delta m^4$ (see the isospin reweighting in [6, 4]). In this case the noise and the fluctuations of decreasing the mass of one quark are compensated by increasing the mass of the second one. For $\gamma = 0$ the reweighting factor reduces to the one flavor case: $W_{2\mathrm{f}}^{(0)}(m_l, m_s, \Delta m) = W_{1\mathrm{f}}(m_s, \Delta m)$. Therefore, in the general case $m_l < m_s$, an optimal $0 \leq \gamma^* \leq 1$ may be found that minimizes the fluctuations of $W_{2\mathrm{f}}^{(\gamma)}$. With light quarks around the strange quark mass an optimal value of $\gamma^* \approx 0.82$ was found [5].

A generalization of eq. (3.2) for finite μ_s and/or μ_l is straightforward. Note that, in general, in this case the reweighing factor is complex.

	(m,μ)	(i)	(ii)	(iii)	(iv)
up	$(m_l,0)$	$\to(m_l,\mu)$	$\to(m_l-\gamma\Delta m,\mu)$		$\to(m_l-\gamma\Delta m,0)$
down	$(m_l,0)$	$\to(m_l,-\mu)$		$\to(m_l-\gamma\Delta m,-\mu)$	$\to(m_l-\gamma\Delta m,0)$
strange	$(m_s,0)$		$\to(m_s+\Delta m,0)$	$\to(m_s+2\Delta m,0)$	
type		tm (sec. 3.3)	2f (sec. 3.2)	2f (sec. 3.2)	tm (sec. 3.3)

Table 1: Optimal reweighting strategy for strange quark mass reweighting.

3.3 Twisted mass reweighting

Twisted mass reweighting was introduced [3] and implemented [11] in order to stabilize the HMC at small quark masses. In the context of mass reweighting it can be used to ensure the convergence of the stochastic estimator (2.1) [5]. For a doublet of quarks of mass $m_1 = m_2 = m$ and $\mu_1 = \mu = -\mu_2$ the corresponding reweighting factor is

$$W_{\rm tm}(m,\mu,\mu') = \frac{\det(D_m D_m^\dagger + \mu'^2)}{\det(D_m D_m^\dagger + \mu^2)} = \frac{1}{\det(A_{\rm tm})}\,, \qquad A_{\rm tm} = I + \frac{\mu^2-\mu'^2}{D_m D_m^\dagger + \mu'^2}\,, \tag{3.3}$$

where we used $(D_m + i\gamma_5\mu)^\dagger = \gamma_5(D_m - i\gamma_5\mu)\gamma_5$. The stochastic error and the fluctuations scale (asymptotically) with $(\mu^2-\mu'^2)^2$.

4. Optimal strange quark mass reweighting

As pointed out in the introduction, in a $n_f = 2+1$ simulation with up, down, strange quark masses $\{m_l, m_l, m_s\}$ it might be necessary to tune the strange quark mass of an ensemble in order to improve the approach to the physical point. We have seen in section 3 that it is advantageous to combine the change of the mass of one quark with an opposite change of another one. Furthermore, if light quarks are reweighted, a finite twisted mass serves as a safeguard against zero crossings of small eigenvalues. Taken together, these lessons lead us to propose the following reweighting strategy:

(i) the light quarks are reweighted to a finite μ,

(ii) the up and the strange quark are reweighted together in opposite directions,

(iii) the down and the strange quark are reweighted together by the same amount,

(iv) the light quarks are reweighted to zero twisted mass.

The four steps are summarized in Table 1. In the stochastic estimation the twisted mass reweighting in step (i) and (iv) can be combined so that the total reweighting factor W_s can be written as a product of three factors

$$W_s = W_{\rm (ii)}\,W_{\rm (iii)}\,W_{\rm (i+iv)} \quad \leftarrow \quad (W_{\rm (ii)})_{N_\eta}\,(W_{\rm (iii)})_{N_\eta}\,(W_{\rm (i+iv)})_{N_\eta}\,, \tag{4.1}$$

and each of these factors is estimated according to (2.1). The total change in the masses is

$$\{m_l, m_l, m_s\} \to \{m_l-\gamma\Delta m,\, m_l-\gamma\Delta m,\, m_s+2\Delta m\}\,.$$

If the ensemble is generated at finite μ in the light quark sector, as for example in [2], step (i) can be omitted. Depending on which kind of twisted mass reweighting is used in the production of the ensemble, the last factor is then given by

$$W_{\text{(i+iv)}} = \begin{cases} W_{\text{tm}}(m_l,0,\mu)\,W_{\text{tm}}(m_l-\gamma\Delta m,\mu,0) & \text{none} \\ W_{\text{tm}}(m_l-\gamma\Delta m,\mu,0) & \text{type I in [11]}\ . \\ W_{\text{tm}}(m_l,\mu,\sqrt{2}\mu)\,W_{\text{tm}}(m_l-\gamma\Delta m,\mu,0) & \text{type II in [11]} \end{cases} \tag{4.2}$$

The reweighting factors for step (ii) and (iii) are explicitly given by

$$W_{\text{(ii)}} = W_{2\text{f}}^{(\gamma)}(m_l,m_s,\Delta m)\,, \quad \text{with } \mu_l = \mu \tag{4.3}$$

$$W_{\text{(iii)}} = W_{2\text{f}}^{(\gamma)}(m_l,m_s+\Delta m,\Delta m)\,, \quad \text{with } \mu_l = -\mu\,, \tag{4.4}$$

and $\gamma \approx \gamma^*$. As mentioned before for $\mu_l \neq 0$ the reweighting factor $W_{2\text{f}}^{(\gamma)}$ is complex. But since the product $W_{\text{(ii)}}W_{\text{(iii)}}$ is manifestly real, the phases of the two factors cancel.

5. Public code for mass reweighting

The numerical results presented in the next section have been obtained with the mrw-package [12], an extended version of the openQCD package [13]. Keeping the structure of openQCD the extension is implemented as a module (`mrw`). It provides a main program that reads in openQCD style input files, documentation and sample input files. The mrw-package is publicly available at `https://github.com/bjoern-leder/mrw`. In detail it adds the following features to openQCD:

- one flavor mass and twisted-mass reweighting [5, 6]
- interpolation (factorization) for twisted mass reweighting type I and II
- factorization with non-equidistant interpolations [5, 6]
- isospin mass reweighting [5, 6]
- strange quark mass reweighting of section 4
- several check routines for all parts of the new module

6. Numerical test and cost

The optimal strange quark mass reweighting proposed in section 4 has been tested on two $n_f = 2+1$ ensembles from the effort described in [2], see Table 2. While the first one is off the quark mass trajectory described in section 2.3 of [2], the second one sits on it.[1] The lattice spacing is approximated to $a = 0.086\,\text{fm}$ [2] and the lattice size is 64×32^3.

[1] This trajectory is defined by $\sum_i m_i = \text{const}$. Note that for $\gamma \neq 1$ the optimal strange quark reweighting takes the ensemble off, whereas for $\gamma = 1$ it would move the ensemble along this trajectory.

ID in [2]	m_π [MeV]	m_K [MeV]	$\Delta\overline{m}_s$ [MeV]	γ	μ
–	330 (380)	450 (430)	-12	0.80	0.0
B105	280 (200)	460 (480)	12	0.80	0.001

Table 2: Ensembles used in the numerical test. In parentheses are the meson masses after reweighting. $\Delta\overline{m}_s$ is the difference of the renormalized strange quark masses before and after the reweighting. The first ensemble was part of an exploratory study and is not listed in [2].

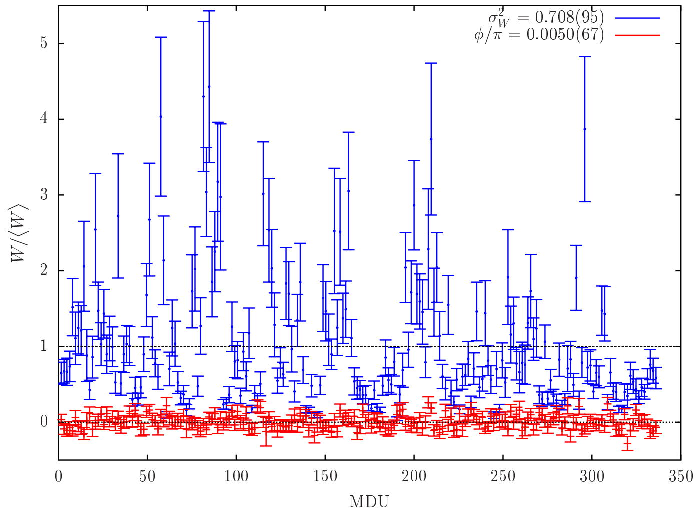

Figure 1: Strange quark reweighting factor W_s for ensemble B105.

In Figure 1 the reweighting factor W_s (eq. (4.1)) is plotted for the ensemble B105. The phase is also plotted and is compatible with zero as expected. The fluctuations of the reweighting are sizable, but the change in the meson masses is large: 5% (30%) for the kaon (pion). By using a smaller value for γ this change can be made more balanced. Assuming a scaling of the fluctuations $\propto \Delta m^2 V^q/\overline{m}_l$ the feasibility of such a reweighting at different parameters can be projected using the following formula

$$\sigma^2_{W_s} = 0.71\left(\frac{\Delta\overline{m}_s}{12\,\mathrm{MeV}}\right)^2\left(\frac{240\,\mathrm{MeV}}{\overline{m_\pi}}\right)^2\frac{V^q}{(3.3\text{ fm})^{4q}}, \quad q = 1/4\ldots 3/4.$$

where $\Delta\overline{m}_s$ is the difference of the renormalized strange quark masses and $\overline{m_\pi}$ is the mean of the pion masses before and after the reweighting, and V is the physical volume [4]. The uncertainty in the volume scaling is currently under investigation.

The cost for estimating the reweighting factors $W_{\mathrm{(ii)}}$, $W_{\mathrm{(iii)}}$, $W_{\mathrm{(i+iv)}}$ is roughly independent of the ensemble parameters. It is fixed by demanding the stochastic noise to be much smaller than the fluctuations [5]. The error bars in Figure 1 indicate the stochastic error for each configuration. The total number of Gaussian noise vectors was 48 for $W_{\mathrm{(ii)}}$ and $W_{\mathrm{(iii)}}$, and 24 for $W_{\mathrm{(i+iv)}}$. Since the stochastic error is large in Figure 1 these numbers have to be increased in an application of the method.

The numerical cost per configuration (core hours) is $\sim 30\%$ of one trajectory of length 2 MDU. But since the autocorrelation times of observables $\tau_{\mathcal{O}}$ are typically much larger than this, reweighting is only needed every $n = \tau_{\mathcal{O}}/2 \gg 1$ trajectories, effectively cutting the cost to $\sim (30/n)\%$.

7. Outlook

In the first numerical test presented in the last section a value for γ^* is used that was determined in another setup and at different quark masses. A dedicated tuning needs only a small number of configurations and has the potential to lower the fluctuations significantly. Furthermore the cost per configuration can be reduced by combining the reweighting factors $W_{(\mathrm{ii})}$, $W_{(\mathrm{iii})}$ into one estimator. Finally, the mrw-package will be upgraded to openQCD-1.4, including support for periodic boundary conditions.

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