Tuning of the strange quark mass with optimal reweighting

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Upshot

- reweighting is viable for tuning $\mathbf{m_s}$ (cheaper than doing new simulations)
- optimal strategy combines reweighting of light and strange quarks and change the sum of bare quark masses
- reweighting module for openQCD available at `http://www-ai.math.uni-wuppertal.de/~leder/mrw/`

Why (mass) reweighting?

- Physics:
  - Tuning of quark masses, e.g., $\mathbf{m_s}$ in a 2+1 simulation
  - Quark mass dependence, QED effects, finite chemical potential, ...
- Algorithms:
  - Stabilization of the HMC algorithm (twisted mass reweighting in openQCD [Lüscher and Palombi (2008); Lüscher and Schaefer (2013)])
  - Alternative update algorithms [Finkenrath, Knechtli and Leder, Comp. Phys. Comm. (2013)]

Reweighting

- Observable in lattice QCD:

$$\langle \mathcal{O} \rangle_a = \frac{1}{Z_a} \int \mathrm{D}[U]\, P_a(U)\, \mathcal{O}_a(U)$$

  - with weight $P_a(U) = e^{-S_g(\beta,U)} \prod_{i=1}^{n_f} \det(D_0(U) + m_i)$
  - bare parameter set $a = \{\beta, m_1, m_2, \dots, m_{n_f}\}$
  - and normalization $\int \mathrm{D}[U] P(U)/Z \equiv 1$
- Observable at $b = \{\beta', m_1', m_2', \dots, m_{n_f}'\}$:

$$\langle \mathcal{O} \rangle_b = \frac{\langle \mathcal{O}_b W \rangle_a}{\langle W \rangle_a}, \quad W = \frac{P_b}{P_a}$$

  - with *reweighting factor* W

Mass reweighting - Fluctuations

- Numerical evaluation of $W = 1/\det(A)$:

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

  - with N_η Gaussian distributed random vectors $\eta^{(i)}$
  - *stochastic error* $\delta_\eta^2(A) = \mathrm{var}(W_{N_\eta})/(N_\eta |W|^2)$
- *ensemble fluctuations* $(A = I + \epsilon D^{-1} X)$:

$$\sigma_W^2 \equiv \mathrm{var}(W)/\langle W \rangle^2 = \epsilon^2 \mathrm{var}(\mathrm{Tr}(D^{-1}X)) + O(\epsilon^3)$$

- Reduction of stochastic fluctuations: [Hasenbusch (2001); Hasenfratz, Hoffmann and Schaefer (2008)]
  - factorization of W based on interpolation $\epsilon \longrightarrow \epsilon/N$

Mass reweighting - Factors

- one flavor: $m_s \longrightarrow m_s - \Delta m$

$$W_{m_s, m_s - \Delta m} = \frac{\det(D_{m_s - \Delta m})}{\det(D_{m_s})} = \frac{1}{\det(A_{1f})}$$

  with $A_{1f} = I + \Delta m D^{-1}_{m_s - \Delta m}$ and $D_m = D_0 + m$
- two flavors: $m_l \leq m_s$, $m_l \longrightarrow m_l - \gamma \Delta m$, $m_s \longrightarrow m_s + \Delta m$

$$W_{2f}^{(\gamma)} = W_{m_l, m_l - \gamma\Delta m} W_{m_s, m_s + \Delta m} = \frac{1}{\det(A_{2f})}$$

  with $A_{2f} = (D_{m_l - \gamma\Delta m} D_{m_s + \Delta m})^{-1} D_{m_l} D_{m_s} =$
  $I + \Delta m (D_{m_s + \Delta m} D_{m_l - \gamma \Delta m})^{-1} (\gamma \Delta m + \gamma D_{m_s} - D_{m_l})$

Mass reweighting - Correlations

- tune γ in $W_{2f}^{(\gamma)}$ to minimize σ_W^2
- degenerate case $m_l = m_s = m$: $\gamma = 1$, isospin

$$W_{2f}^{(1)} = W_{m, m+\Delta m} W_{m, m-\Delta m} = \frac{1}{\det(A_\pm)}$$

  with $A_\pm = I + \Delta m^2 (D_m^2 - \Delta m^2)^{-1}$, $\sigma_W^2 \propto \Delta m^4$
- $m_l < m_s$ (strange quark): minimum for $0 \leq \gamma^* \leq 1$ numerically we find

$$\gamma^* = 0.82(1)$$

[Finkenrath, Knechtli and Leder, Nucl. Phys. B877 (2013)]

Strange quark mass reweighting

- $n_f = 2 + 1$, $m_u = m_d$, m_s
- light quarks: D_{m_l} can become singular along mass interpolation, add twisted mass $D_{m_l} \rightarrow D_{m_l} + i\gamma_5 \mu$

$$(m_l, 0) \xrightarrow{(i)} (m_l, \mu) \xrightarrow{(ii)} (m_l', \mu) \xrightarrow{(iii)} (m_l', 0)$$

- mass and twisted mass reweighting:

$$W_s = W_1 W_2 W_3$$

- two flavor mass reweighting $(W_{2f}^{(\gamma)})$ at constant μ (ii):

W_1: up and strange	W_2: down and strange
$m_u \longrightarrow m_u' = m_u - \gamma\Delta m$	$m_d \longrightarrow m_d' = m_u - \gamma\Delta m$
$m_s \longrightarrow m_s' = m_s + \Delta m$	$m_s + \Delta m \longrightarrow m_s' = m_s + 2\Delta m$

- twisted mass reweighting combines (i) and (iii) for light quark doublet:

$$W_3 = \det\left(\frac{D(m_l,\mu)^\dagger D(m_l,\mu)}{D(m_l,0)^\dagger D(m_l,0)} \cdot \frac{D(m_l',0)^\dagger D(m_l',0)}{D(m_l',\mu)^\dagger D(m_l',\mu)} \right)$$

  $\sigma_{W_3}^2 \propto \mu^4 \Delta m^2$. $W_3 = 1$ if $\mu = 0$.

`mrw` module for openQCD

`http://www-ai.math.uni-wuppertal.de/~leder/mrw/`

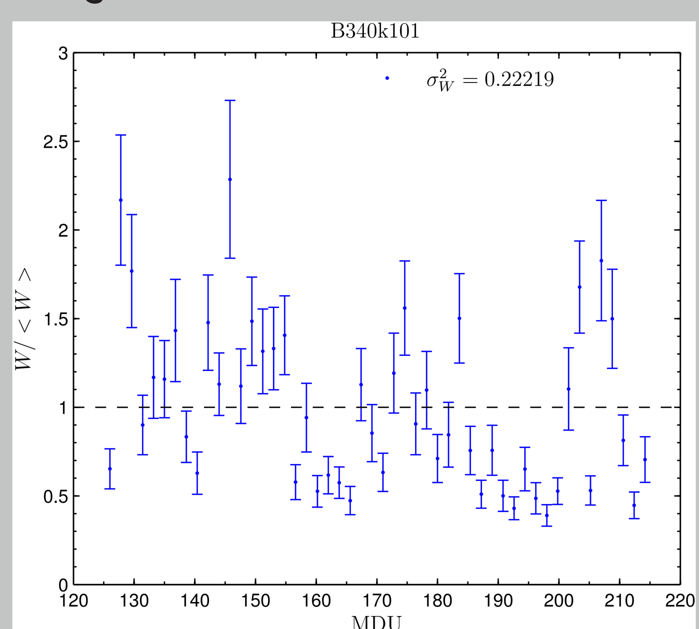
- mass and twisted-mass reweighting
- openQCD reweighting type I and II (even-odd precond.) with interpolation
- factorization with non-equidistant interpolations
- mass reweighting with twisted-mass term only on even sites
- isospin mass reweighting
- strange quark mass reweighting
- several check routines for all parts of the module
- openQCD:
  - Simulation program for lattice QCD with open boundary conditions and twisted mass reweighting (`http://luscher.web.cern.ch/luscher/openQCD/`)

Numerical results

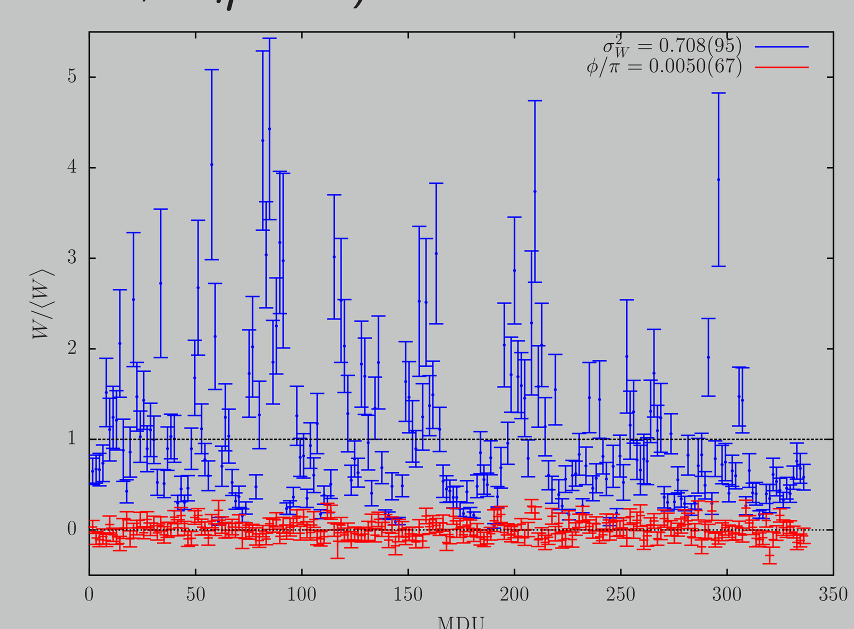
Exploratory $n_f = 2 + 1$ ensembles: 64×32^3, $a = 0.085$ fm

m_π [MeV]	m_K [MeV]	Δm [MeV]	γ	μ
340	460	-5.8	0.80	0.0
300	480	5.8	0.80	0.001

- W_1, W_2: 2×48 ($N = 8$, $N_\eta = 6$) inversions at $\sim m_u$ and at $\sim m_s$
- W_3: 3×24 inversions at $\sim m_u$ ($N = 4$, $N_\eta = 6$)



W_s for $m_s - 12$ MeV



W_s for $m_s + 12$ MeV

Scaling of the variance and cost

- Ensemble fluctuations (should be smaller than one):

$$\sigma_W^2 = 0.71 \left(\frac{\Delta m}{5.8\ \mathrm{MeV}}\right)^2 \left(\frac{240\ \mathrm{MeV}}{m_\pi}\right)^2 \frac{TL^3}{(3.2\ \mathrm{fm})^4}$$

  - $2\Delta m$: reweighting distance of strange quark in MeV
  - m_π: pion mass after reweighting in MeV
  - TL^3: volume in $(\mathrm{fm})^4$
- Cost:
  - cost per configuration: $\sim 30\%$ of one trajectory
  - autocorrelation typically large: reweigthing only every **n**th configuration

Outlook

- study of volume and quark mass dependence of reweighting factors