APPLICATION OF MASS REWEIGHTING IN (2+1)-FLAVOR QCD WITH MÖBIUS DWF

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Bigger picture

- Study of chiral phase transition with chiral fermions in (2+1)-flavor QCD thermodynamics. Pisarski-Wilczek : The chiral transition ($N_f = 2+1$) belongs to the O(4) universality class if the $U_A(1)$ symmetry is still broken at Tc, which is estimated to be between 130-135 MeV. However, if the $U_A(1)$ symmetry is restored at Tc, there is a possibility of a first-order transition ($O(2) \times O(4)$) in the chiral limit. [1]
- Möbius Domain Wall fermions (MDWF) : Exact chiral symmetry ($SU(2)_L \times SU(2)_R$) and chiral anomaly on finite lattice spacing at $L_s \to \infty$ in 4-d for vanishing quark masses.
- "Almost" chiral fermions for finite L_s.[2, 3] [See Poster by Y. Aoki]

Reweighitng factor calculation

The partition function of Lattice QCD can be written as,

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{O}\, detM(m_l)[detM(m_s)]^{1/2} \exp\left[-\beta S_g[U]\right] \quad . \qquad (1)$$

Reweighting of an observable for $m_{l1} \to m_{l2}$,

$$\begin{aligned}\langle \mathcal{O} \rangle_2 &= \frac{1}{Z_2} \int DU\ \mathcal{O}\ detM(m_{l_2})[detM(m_s)]^{1/2} \exp[-S_g] \\ &= \frac{Z_1}{Z_2}\frac{1}{Z_1} \int DU \left[O\frac{detM(m_{l_2})}{detM(m_{l_1})}\right]\ detM(m_{l_1})[detM(m_s)]^{1/2} \exp[-\beta S_g]\end{aligned}$$

Hence, the reweighting factor from $m_{l_1} \to m_{l_2}$ and the observable for new m_{l_2},

$$\omega = \left[\frac{detM(m_{l_2})}{detM(m_{l_1})}\right] \quad , \ \langle \mathcal{O} \rangle_2 = \frac{\sum_n \omega_i \mathcal{O}_n}{\sum_n \omega_n} \qquad (2)$$

Detail of the calculation

The 4-dimensional DW operator is written as,

$$D_4^{Ls} = \frac{1+m}{2} + \frac{1-m}{2}\gamma_5 sgn_{tanh}^{(Ls)}(H_K) \qquad (3)$$

The sign function can be parametrize as,

$$sgn_{tanh}^{(Ls)} = \tanh(L_s \tanh^{-1}(x)) \qquad (4)$$

$$sgn_{polar}^{(Ls)} = \frac{(1+\tanh x)^L s - (1-\tanh x)^L s}{(1+\tanh x)^L s + (1-\tanh x)^L s} \qquad (5)$$

Where, H_K can be written as,

$$H_K = \frac{(b+c)\gamma_5 D_W(-M_0)}{2+(b-c)D_W(-M_0)}, \text{ Where,, D}_\text{W}\text{, is the Wilson Dirac Operator} \qquad (6)$$

we employ normalize complex Gaussian noise vectors $[\xi^\dagger, \xi]$ to estimate the reweighting factor,

$$\omega = \frac{\det D_4^{L_s}(m_1)}{\det D_4^{L_s}(m2)} \qquad (7)$$

$$\omega = detA^{-1} = \frac{\int D\xi^\dagger D\xi\ \exp[-\xi^\dagger A\xi]}{\int D\xi^\dagger D\xi\xi^\dagger\xi]},\ A = M(m_{l_2})^{-1}M(m_{l_1}) \qquad (8)$$

Summary

- We discuss the application of light quark mass reweighting in Lattice QCD simulations with Möbius Domain Wall fermions to take care of the m_{res} effect on the observable.
- Our demonstration reveals that as the value of the m_{res} increases, the reweighting factor begins to fluctuate more. The efficacy of reweighting with limited statistics depends on this point.
- If the reweighting factor shows excessive fluctuations, a larger sample size is necessary to achieve an effective reweighting. Hence, for smaller light quark masses this will likely to be fail.

References

[1]R. D. Pisarski and F. Wilczek, "Remarks on the chiral phase transition in chromodynamics", Phys. Rev. D **29**, 338–341 (1984).

[2]I. Kanamori et al., "Thermodynamics with Möbius domain wall fermions near physical point (II)", **LATTICE2022**, 176 (2023).

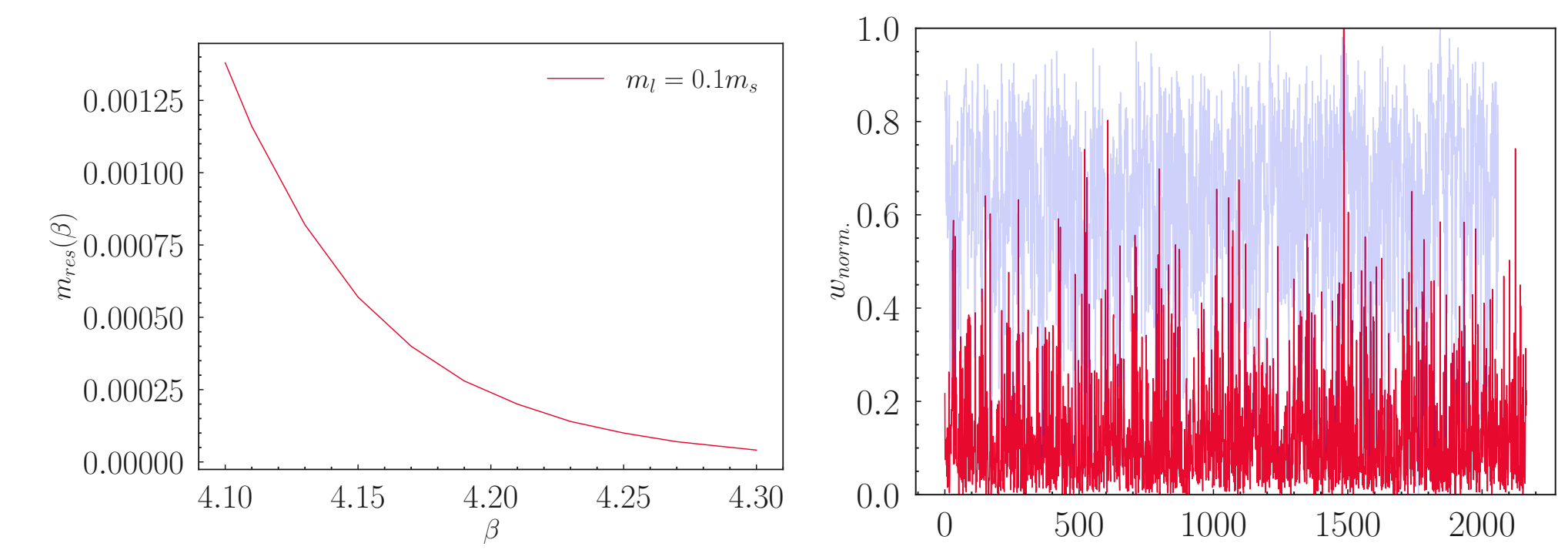
[3]Y. Aoki et al., "Thermodynamics with Möbius domain wall fermions near physical point (I)", **LATTICE2022**.

[4]T. Aoyama, I. Kanamori, K. Kanaya, H. Matsufuru, and Y. Namekawa, "Bridge++ 2.0: Benchmark results on supercomputer Fugaku", PoS **LATTICE2022**, 284 (2023).

[5]A. Hasenfratz, R. Hoffmann, and S. Schaefer, "Reweighting towards the chiral limit", Phys. Rev. D **78**, 014515 (2008).

Lattice Parameters and m_{res} effect

- Lattice size : $N_\sigma \times N_\tau = 32^3 \times 16$ and $L_s = 12$.
- $m_l = 0.1 m_s$, input quark mass tuning using the $m_l^{new} = m_l^{old} - m_{res}$.
- Perform reweighting $m_l^{old} \to m_l^{new}$. Code Base : Bridge++ [4].

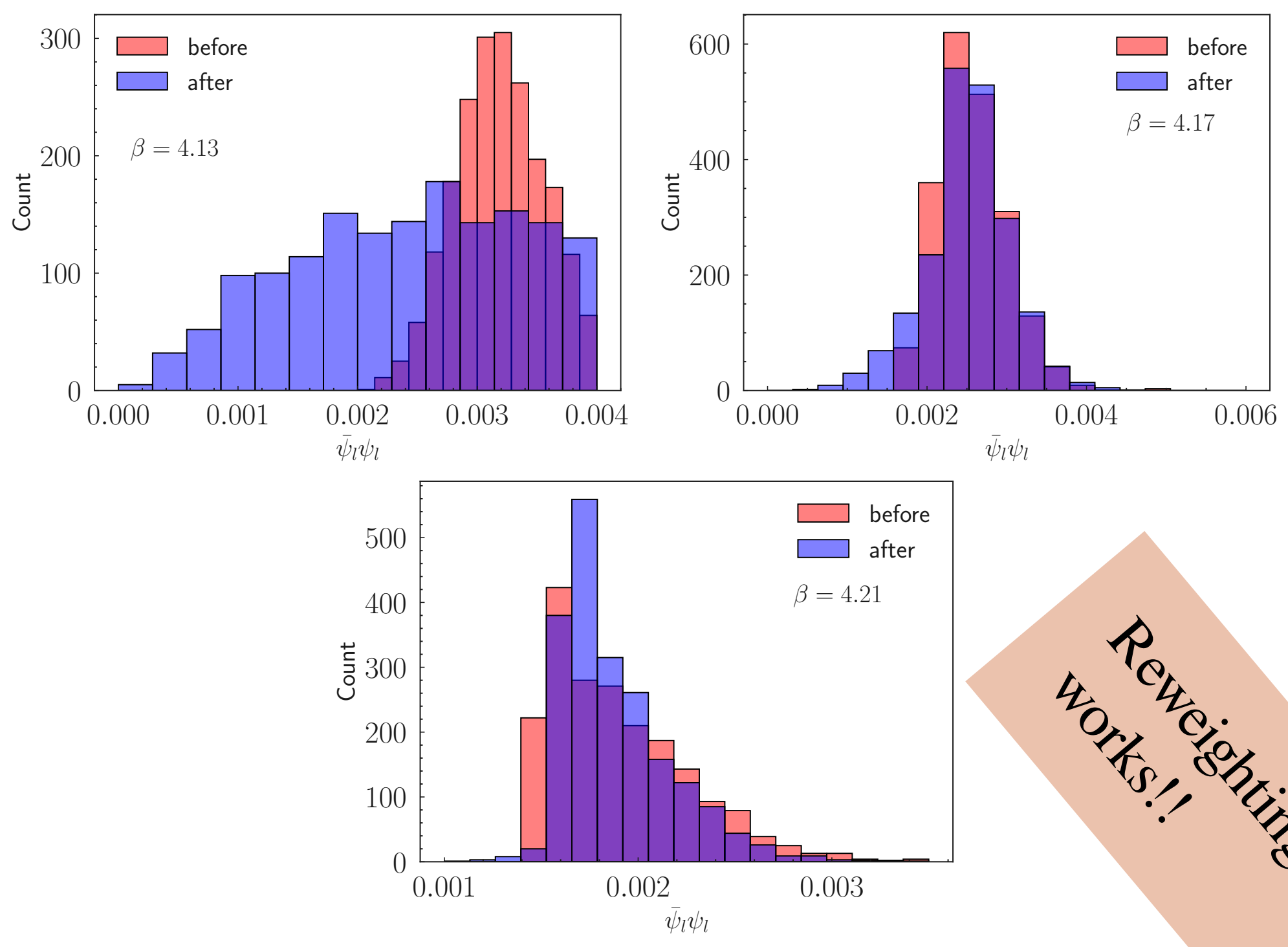


- reweighting factor fluctuate more for larger m_{res}.
- This method seems to fail when m_{res} corrections are more than 20% of the m_l^{old} within the current statistics.

Fig. 1: m_{res} vs β (left) for $\beta \in \{4.10 : 4.30\}$ and fluctuation of reweighting factor for $\beta = 4.10$ and 4.17(right).

- Statistics uncertainity of the reweighted quantity ?? $\langle \omega^2 \mathcal{O}^2 \rangle - \langle \mathcal{O}\omega \rangle^2$.
- Errors depend on the fluctuation of the reweighting factor and also with its correlation with the observable [5].
- For ex. $\beta = 4.13$, $m_l = m_s/10, m_s = 0.043913$. $m_l^{old} = 0.0043913, m_l^{new} = 0.00357$ reweighting successful!!
- Limitation : For ex. $\beta = 4.13$, $m_l = m_s/27, m_s = 0.04309$. $m_l^{old} = 0.0016, m_l^{new} = 0.00078$ would fail in current statistics.

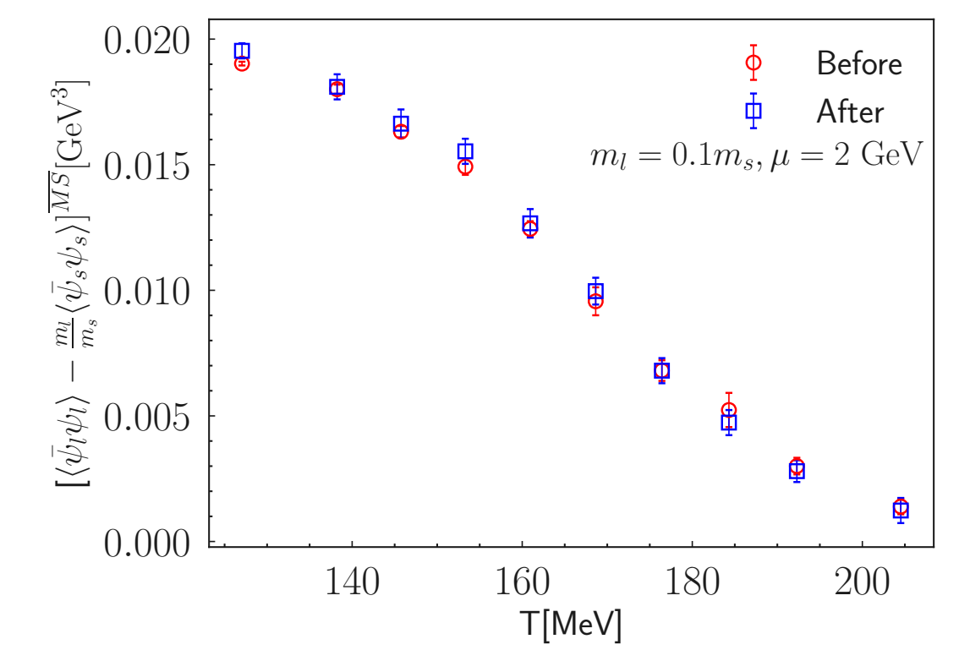
Reweighting of chiral condensate



Reweighting works!!

We use reweighting on the gauge ensembles generated by the JLQCD collaboration for 9 β values ranges from $\beta \in [4.10 : 4.30]$ with corresponding $m_l \in [0.00484742 : 0.00270836]$ and $m_{res} \in [0.00138 : 0.000041]$ [2, 3]. To make reweighting effective, we require a significant overlap between the observables being considered. We show the light quark chiral condensate for three β values here.

Fig. 2: Histogram of light quark chiral condensate for three β values



- Perform measurements of $\langle\bar{\psi}_l\psi_l\rangle$ after adjusting the valence quark mass by taking care of the m_{res} effect. Then perform reweighting on $\langle\bar{\psi}_l\psi_l\rangle$.
- Subtracted chiral condensate $\langle\bar{\psi}_l\psi_l\rangle - \frac{m_l}{m_s}\langle\bar{\psi}_s\psi_s\rangle]$ before and after reweighting.

Fig. 3: Subtracted chiral condensate before and after reweighting.

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