Isospin Effects by Mass Reweighting

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Most of today's lattice simulations are performed in the isospin symmetric limit of the light quark sector. Mass reweighting is a technique to include effects of isospin breaking in the sea quarks at moderate numerical cost. We will give a summary of our recent results on fine lattices with light quark masses and will show how light quark masses can be extracted by introducing suitable tuning conditions for the bare mass parameters.

In general the reweighting factor introduces additional fluctuations and thus increases the statistical uncertainties. In the case of isospin reweighting this factor is a ratio of fermion determinants. The stochastic evaluation of the determinants potentially leads to stochastic noise in observables. We show the quark mass and the volume dependence of these fluctuations.

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1. Introduction

Mass Reweighting [1] is an interesting and efficient method to correct and to include effects of quark masses. It can be used for tuning, e.g. the strange quark mass m_s in a 2+1 simulation or the isospin splitting in the up-quark mass m_u and the down-quark mass m_d. Moreover it can be applied to understand the mass behavior of observables. For small corrections it is applicable and more efficient than new simulations. Mass reweighting involves the evaluation of fermion determinants which can be rewritten by an integral representation. This integral representation can be estimated by Monte Carlo integration which needs around 100 inversions of the Dirac operator to control the stochastic noise efficiently.

The reweighting factor enters the measurement of an observable by [2]

$$\langle O \rangle_W = \frac{\langle OW \rangle}{\langle W \rangle} = \langle O\tilde{W} \rangle \tag{1.1}$$

where the mass reweighting factor for n_f flavors of quarks

$$W = \prod_{i=1}^{n_f} \frac{\det D_{m_{new,i}}}{\det D_{m_{old,i}}} \tag{1.2}$$

is normalized with $\tilde{W} = W/\langle W \rangle$. Here, the Dirac operator is given by the clover improved Wilson Dirac operator $D_m = D + m$. The reweighting factor can be rewritten as a determinant of a ratio matrix M with

$$W = \frac{1}{\det \prod_{i=1}^{n_f} \left[D_{m_{new,i}}^{-1} D_{m_{old,i}} \right]} = \frac{1}{\det M}. \tag{1.3}$$

In general lattice simulations are done in the isospin symmetric limit in the light quark sector by setting the light quark masses to the average light quark mass $m_{ud} = 0.5(m_u + m_d)$. The idea is to use mass reweighting to introduce isospin breaking. The reweighting is performed by splitting up the light quark masses by keeping the average quark mass constant $2m_{ud} = m_u + m_d = const$ and it follows with the mass shift $\Delta m_{ud} = m_d - m_u$

$$m_u = m_{ud} - 0.5 \cdot \Delta m_{ud} \leftarrow \quad m_{ud} \quad \rightarrow m_{ud} + 0.5 \cdot \Delta m_{ud} = m_d. \tag{1.4}$$

This leads to the isospin reweighting factor

$$W_{iso} = \frac{1}{\det \left[D_{m_u}^{-1} D_{m_{ud}} D_{m_d}^{-1} D_{m_{ud}} \right]} = \frac{1}{\det M_{iso}}. \tag{1.5}$$

Now, the determinant of the non–hermitian matrix M can be rewritten by an integral representation given by

$$\frac{1}{\det M} = \int D[\eta] \exp\{-\eta^\dagger M \eta\} \tag{1.6}$$

which holds for $\lambda(M + M^\dagger) > 0$ [3] and the normalized integral measure is given by $D[\eta] = \prod_{j=1}^{n} dx_j dy_j / \pi$ with $\eta_j = x_j + iy_j$. The integral eq. (1.6) can be estimated stochastically

$$\frac{1}{\det M} = \frac{1}{N_\eta} \sum_{i=1}^{N_\eta} e^{-\eta_i^\dagger (M-I)\eta_i} + \mathcal{O}(1/\sqrt{N_\eta}) \tag{1.7}$$

Table 1: The table shows the analyzed CLS - ensembles generate with $n_f = 2$ - $\mathcal{O}(a)$ improved Wilson fermions with $m_{ud} = m_u = m_d$ [4]. We used ensembles of three different lattice spacings a with pion masses m_π from 580 MeV down to 192 MeV and lattice volume V/a^4. The number of configurations N_{cnfg} are seperated by MDUs/config with R_{act} the relative number of active links. The maximal reweighting range is given by the quark mass shift in the $\overline{MS}$-scheme $\Delta m_{R,max}$. The renormalized mass is defined as in [4].

ID	V/a^4	a [fm]	m_π [MeV]	N_{cnfg}	MDUs/config $\cdot R_{act}$	$\Delta m_{R,max}$ [MeV]
A5	64×32^3	0.076	330	202	$20 \cdot 1$	4.43(60)
E4	64×32^3	0.066	580	100	$16 \cdot 0.37$	7.1(17)
D5	48×24^3	"	440	503	$8 \cdot 1$	5.9(10)
E5	64×32^3	"	440	99	$160 \cdot 0.37$	6.01(96)
F7	96×64^3	"	270	350	$16 \cdot 0.37$	5.01(38)
G8	128×64^3	"	192	90	$8 \cdot 1$	5.86(56)
O7	96×48^3	0.049	270	98	$40 \cdot 1$	5.63(40)

by drawing N_η pseudofermion fields η distributed via the normalized function $\propto \exp\{-\eta^\dagger \eta\}$ and I the unit matrix with dimension of M. Note for every drawn field η n_f–inversions of the Wilson Dirac operator D_{m_i} have to be performed.

In general mass reweighting introduces fluctuations which increase the statistical error. These fluctuations are the ensemble fluctuations, introduced by the ensemble average in eq. (1.1), and the stochastic fluctuations, introduced by the stochastic estimation of the integral eq. (1.6). The fluctuations are given by the variance averaged over the ensemble and the pseudofermions η. We will define the variance of the integral representation eq. (1.6) by $\sigma^2 = \langle\langle ww^\dagger \rangle_\eta\rangle - \langle\langle w \rangle_\eta\rangle\langle\langle w^\dagger \rangle_\eta\rangle$ with the stochastic estimate $w(U,\eta) = 1/N_\eta \sum_i \exp\{-\eta_i^\dagger(M-I)\eta_i\}$. By performing the η–average $\langle\rangle_\eta$ (i.e. all η_i independently) the fluctuations are given for finite N_η by

$$\sigma^2 = \frac{1}{N_\eta}\left\langle \frac{1}{\det(M+M^\dagger-I)} \right\rangle + \frac{N_\eta-1}{N_\eta}\left\langle \frac{1}{\det MM^\dagger} \right\rangle - \left\langle \frac{1}{\det M} \right\rangle\left\langle \frac{1}{\det M^\dagger} \right\rangle \qquad (1.8)$$

which holds for $\lambda(M+M^\dagger-I) > 0$. The stochastic fluctuations for one configuration are given by neglecting the ensemble average $\langle\rangle$ and vanish for $N_\eta \to \infty$. Moreover by introducing a mass interpolation between the start and the target mass the stochastic fluctuations can be further controlled, i.e. if no Dirac operator has a zero eigenvalue during the interpolation the condition $\lambda(M+M^\dagger) > 1$ can be insured [5]. In this case the number of inversions is $N_{inv} \propto N \cdot N_\eta$, where N is the number of interpolation steps. Note for many reweighting cases it is effecient to use the even-odd preconditioned Wilson–Dirac operator (e.g. see [6]), however we do not find an improvement in the case of isospin reweighting. The ensemble fluctuations can be tamed by including additional quarks into the reweighting process, e.g. in the case of isospin reweighting the fluctuations are minimized by keeping the average quark mass $m_{ud} = 0.5(m_u + m_d)$ constant during the reweighting.

Here, we will discuss mass reweighting by introducing an isospin breaking in the light quarks. We will show the scaling of the different fluctuations (ensemble and stochastic) and how the up– and down–quark mass can be extracted from the analyzed ensembles (see tab. 1).
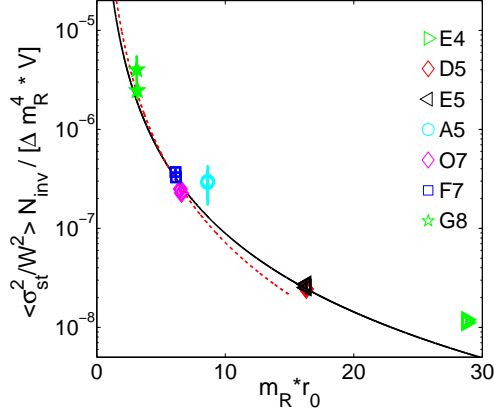
Figure 1: The relative stochastic fluctuations of the isospin reweighting factor is shown as a function of the renormalized quark mass. σ_{st}^2 is the average of the stochastic variance estimated using $N_\eta = 6$.

2. Isospin Reweighting

The isospin reweighting factor eq. (1.5) can be expanded in Δm_{ud}^2

$$W_{iso} = \frac{\det D_{m_u} \det D_{m_d}}{\det D_{m_{ud}}^2} = 1 + \Delta m_{ud}^2 \mathrm{Tr}(D_{m_{ud}}^{-2}) + \mathscr{O}(\Delta m_{ud}^4) \tag{2.1}$$

by using $\det M = \exp\{\mathrm{Tr}(\ln(M))\}$. The fluctuations σ^2 in eq. (1.8) of the isospin reweighting factor can be expanded in Δm_{ud}^2. It can be shown that the stochastic fluctuations σ_{st}^2 decouple from the ensemble fluctuations σ_{ens}^2 with $\sigma^2 = \sigma_{st}^2 + \sigma_{ens}^2$. The stochastic fluctuations in the isospin reweighting case are given by

$$\sigma_{st,rel}^2(N_{inv}) = \left\langle \frac{\sigma_{st}^2(N_{inv})}{W^2} \right\rangle = \frac{\Delta m_{ud}^4}{N_{inv}} \left\langle \mathrm{Tr} \frac{1}{\left(D_{m_{ud}} D_{m_{ud}}^\dagger\right)^2} \right\rangle + \mathscr{O}\left(\Delta m_{ud}^6\right). \tag{2.2}$$

The ensemble fluctuations are

$$\frac{\sigma_{ens}^2}{\langle W \rangle^2} = \Delta m_{ud}^4 \, \mathrm{var}\left(\mathrm{Tr}\left[\frac{1}{D_{m_{ud}}^2} \right] \right) + \mathscr{O}\left(\Delta m_{ud}^6\right) \tag{2.3}$$

with the variance $\mathrm{var}(O) = \langle O^2 \rangle - \langle O \rangle^2$. Note this is true because the Dirac operator is γ_5-hermitian. Now, the cost can be derived by demanding that the stochastic fluctuations do not dominate the ensemble fluctuations, e.g. that $\sigma_{st,rel}^2(N_{inv})/\sigma_{ens}^2 \overset{!}{\sim} 0.1$.

By using the analyzed ensembles, listed in table 1, it is possible to deduce numerically the scaling behavior of the fluctuations in the quark mass and the volume. However in the case of the stochastic fluctuations the trace of the Wilson Dirac operator is known in chiral perturbation theory, e.g. as in [7], by $\langle \mathrm{Tr} \frac{1}{(DD^\dagger)^2} \rangle \propto \frac{\Sigma V}{m_R^3}$. The numerical analysis is consistent with this behavior. It follows for the stochastic fluctuations (see fig. 1)

$$\sigma_{st,rel}^2 \approx k_{st} \frac{\Delta m_R^4 V}{N_{inv} m_R^{r'}} \frac{1}{r_0^{r'}} \tag{2.4}$$
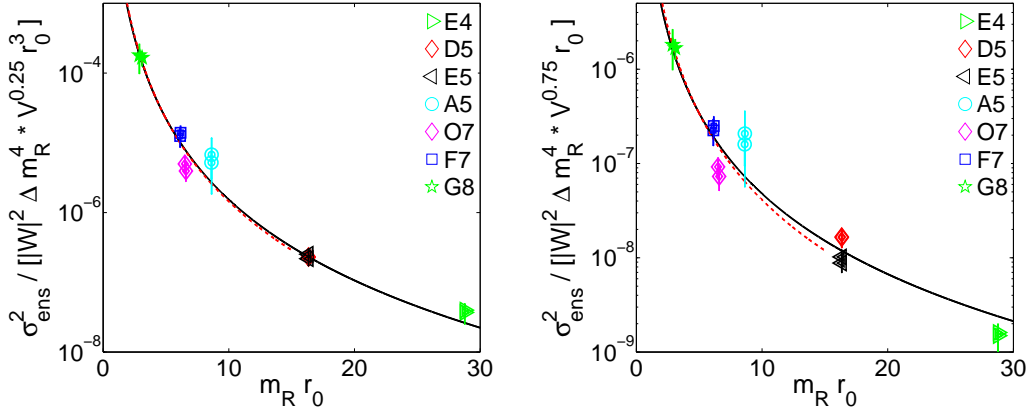
Figure 2: The scaling of the ensemble fluctuations for different volume behaviors is shown. The left figure shows the quark mass behavior for a volume behavior of $\sqrt[4]{V}$ and the right figure for a volume behavior of $V^{3/4}$.

by using the scale r_0 [8] to form dimensionless quantities. By fixing the volume behavior to V we perform a fit (black, solid) to the quark mass behavior by using the ensembles E4 (green, triangle), D5 (red, diamond), E5 (black, triangle), A5 (cyan, circle), O7 (magenta, diamond), F7 (blue, square) and G8 (green, star). For each ensemble we compute σ_{st}^2 and σ_{ens}^2 for two values of $\Delta m = \Delta m_{max}/2, \Delta m_{max}$ (see tab. 1). The quark mass behavior is given by $r' = 2.63(5)$. For the red lines the quark mass behavior and the volume behavior is fixed to V/m_q^3 and only ensembles with pion masses $< 340 \text{MeV}$ are included. The data show a good agreement with the expectation from chiral perturbation theory for pion masses $< 340 \text{MeV}$.

The leading term of the ensemble fluctuations eq. (2.3) is proportional to $\text{var}(\text{Tr}D^{-2})$. Numerically we observe a weak volume dependence V^q with $q < 1$. Similar to the stochastic fluctuations the ensemble fluctuations can be written as

$$\sigma_{ens}^2 \approx k_{ens} \frac{\Delta m_R^4 V^q}{m_R^r} \frac{1}{r_0^{r-4-q}}. \tag{2.5}$$

In general the simultaneous deduction of the volume and the quark mass behavior is difficult. A varied volume behavior changes simultaneously the mass behavior. A good fit is given for a volume scaling of $q = 0.25$ (see left figure 2) which gives a mass behavior of $r = 3.85(13)$ for all ensembles (black line) and $r = 3.94(31)$ for ensembles with pion masses $< 340 \text{MeV}$ (red dashed line). A weaker volume behavior is also supported by comparison of D5 and E5 ensembles, which gives $q \sim 0.46$. However by assuming a similar quark mass behavior as in the case for the stochastic fluctuations with $r = 3$ the scaling in the volume is roughly given by $q \sim 0.75$. In the right figure 2 we fixed the volume behavior to $q = 0.75$ which gives a mass behavior of $r = 2.83(13)$ by including every ensemble (black line) and $r = 3.04(31)$ by including ensembles with pion masses smaller than $< 340 \text{MeV}$ (red, dashed line). We conclude that the volume behavior is given by $q \simeq 0.25 \ldots 0.75$ by a simultaneous variation of the quark mass behavior from $r \simeq 4 \ldots 3$.

The cost of isospin reweighting can be estimated from the ratio

$$\sigma_{st,rel}^2(N_{inv})/\sigma_{ens}^2 \sim \frac{k'_{st}}{k'_{ens}} \frac{(Lm_\pi)^2 L}{N_{inv} \cdot r_0} \qquad \text{with} \qquad \frac{k'_{st}}{k'_{ens}} = 1e-3 \tag{2.6}$$
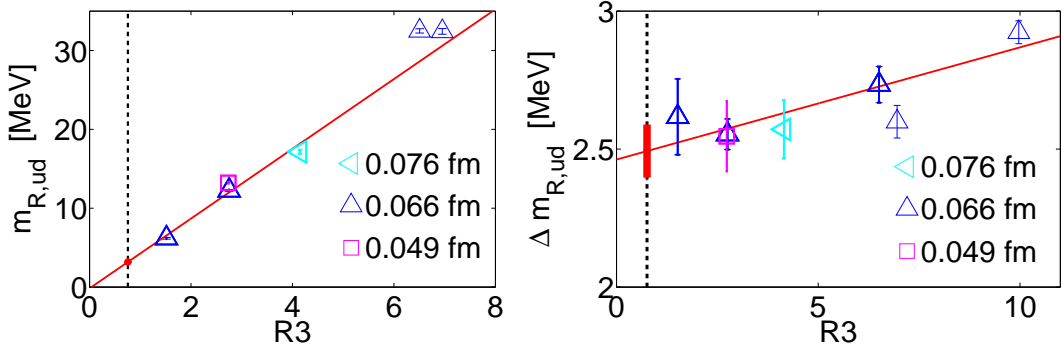
Figure 3: The figures show the average quark mass m_{ud} (left) and the mass splitting $m_d - m_u$ plotted versus R_3 after fixing R_1 and R_2. The masses are renormalized in the $\overline{\text{MS}}$–scheme at $2\,\text{GeV}$.

for $q = 0.25$ and $r = 4$. For the G8 ensemble follows $N_{inv} \approx 200$ for a ratio of 0.1.

3. Quark Masses

The continuum limit can be performed on a line of constant physics. This line can be defined by keeping dimensionless ratios of physical quantities constant. These fix the bare mass parameters, here, a quenched strange quark with m_s, the isospin mass split Δm_{ud} and the average light quark mass m_{ud}. We take the ratios

$$R_1 = \frac{0.5(m_{K^0}^2 + m_{K^\pm}^2)}{(0.5(f_{K^0} + f_{K^\pm}))^2} \quad , \quad R_2 = \frac{m_{K^0}^2 - m_{K^\pm}^2}{(0.5(f_{K^0} + f_{K^\pm}))^2} \quad \text{and} \quad R_3 = \frac{m_{\pi^\pm}^2}{(0.5(f_{K^0} + f_{K^\pm}))^2} \quad (3.1)$$

with the meson masses, the pion $m_{\pi^\pm}$, the neutral kaon m_{K^0} and the charged kaon $m_{K^\pm}$ and the kaon decay constants f_{K^0} and $f_{K^\pm}$. The physical values of the ratios are taken from [9] and we assume $0.5(f_{K^0} + f_{K^\pm}) = 155$ MeV. Now, the strategy is to use R_1 to fix m_s, which is done in [4] and R_2 to fix the isospin splitting Δm_{ud}. Afterwards the ratio R_3 is used to extrapolate the light quarks towards the physical limit.

We measure the PCAC mass on the analyzed ensembles (see tab. 1) and convert them into the $\overline{\text{MS}}$-renormalization scheme. The dimensionless ratios R_2 and R_3 are given in the lowest order chiral perturbation theory up to $\mathcal{O}(\Delta m_{ud}^2, m_{ud}^2)$ by $R_2 = \frac{B}{F^2}\Delta m_{ud}(1 + Cm_{ud})$ and $R_3 = \frac{2B}{F^2}m_{ud}$ with constants B, C and F^2. Now, it is possible to perform extrapolations towards the physical point in the light quark masses. For the average light quark mass this is shown in the left figure of fig. 3 by assuming $m_{ud}(R_3) \approx a_1 R_3$. By using the F7 and G8 ensemble the average light quark mass at the physical point at finite lattice spacing of $a = 0.066$ fm is given by $m_{ud,R} = 3.19(11)$ MeV. For the mass split in the light quarks (see right plot in figure 3) we assumed $\Delta m_{ud}(R_3) \approx b_0 + b_1 R_3$. By using the data of the E5, F7 and G8 ensemble it follows for the mass splitting $\Delta m_{ud} = 2.49(10)$ MeV at finite lattice spacing $a = 0.066$ fm.

The isospin effects enter the observable by the isospin reweighting factor which scales proportional to Δm_{ud}^2. In the case of the PCAC mass the statistical error is too big compared to the effect of the isospin reweighting correction. A determination of this effect is only possible for larger

statistics. Neclecting the sea quark effects proportional to Δm_{ud}^2, by setting the isospin reweighting factor to one, the isospin quark mass split is given by $\Delta m_{ud} = 2.52(10)$ MeV. However the isospin reweighting effects increases for smaller quark masses and we want to reduce the statistical error to figure out the isospin effects for example in the pion mass. In order to perform a continuum limit the statistics has to be increased and other ensembles have to be included.

4. Conclusion

Isospin mass reweighting needs a moderate numerical effort. The analysis shows that the cost scales with $(LM_{PS})^2 L$ for a volume scaling of the ensemble fluctuations with $\sqrt[4]{V}$ and is around 200 inversions of the Dirac operator for the G8 ensemble which has a pion mass of 192 MeV at a volume of $V/a^4 = 128 \times 64^3$. By using the introduced dimensionless ratios R_1, R_2 and R_3 it is possible to extract the light quark masses. The isospin mass spliting is $\Delta m_{ud} = 2.49(10)$ MeV and the average quark mass is $m_{ud,R} = 3.19(11)$ MeV at finite lattice spacing of $a = 0.066$ fm. Although a more careful analysis is needed to extract competitive numbers it shows that the tuning conditions are suitable to extract the light quark masses. In order to extract continuum physics the statistics has to be improved and QED-effects have to be included. A software package for mass reweighting [10] (see also [11]) is publicly available in the framework of the *openQCD* code[12].

Acknowledgements

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