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Light and strange quark masses from $N_f = 2+1$ simulations with Wilson fermions

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We present a nearly final analysis of the u/d and s quark masses, extracted using the PCAC quark masses reported in [1]. The data is based on the CLS $N_f = 2+1$ simulations with Wilson/Clover quarks and Lüscher-Weisz gauge action, at four β values (i.e. lattice spacings) and a range of quark masses. We use the ALPHA results of [2] for non-perturbative quark mass renormalisation and RG-running from hadronic to electroweak scales in the Schrödinger Functional scheme. Quark masses are quoted both in the $\overline{\text{MS}}$ scheme and as RGI quantities.

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1. Introduction and setup

Here we report of the ALPHA Collaboration's analysis of the u/d and s quark masses using Wilson fermions. The starting point is the computation of light PCAC bare quark masses (up/down and strange), performed in refs. [1, 3] with $N_f = 2+1$ dynamical sea quarks. The gauge action is the Lüscher-Weisz action with tree-level coefficients [4], and the fermion action is non-perturbatively $\mathscr{O}(a)$ improved, with the value of the clover coefficient $c_{\rm sw}$ obtained in [5]. The boundary conditions are periodic in space and open in time, as detailed in ref. [6].

Simulations have been carried out at four lattice spacings: $a \approx 0.050$, 0.064, 0.076 and 0.086 fm, corresponding to lattice couplings $\beta = 3.7$, 3.55, 3.46 and 3.40 respectively. In order to keep finite-size effects under control, all ensembles have $LM_\pi \gtrsim 4$ and the time extent varies from $T = 2L$ to $T = 3L$ (where $L^3 \times T$ is the lattice size). The pion mass M_π varies between 200 MeV and 420 MeV, and the kaon mass $M_{\rm K}$ between 420 MeV and 470 MeV. A detailed overview of the simulations can be found in ref. [1].

For each lattice coupling β we have ensembles with different values of the hopping parameters $\kappa_1 = \kappa_2$ and κ_3 (except for $\beta = 3.46$ where we only have one ensemble with three degenerate quark masses). The bare subtracted quark masses are defined as $m_{{\rm q},r} = 1/(2\kappa_r) - 1/(2\kappa_{\rm crit})$, with $\kappa_{\rm crit}$ the critical (chiral) point. The index r labels quark flavours: we use values 1 and 2 for the two degenerate light quark flavours (u and d), and 3 for the strange quark. These masses are chosen so that their mass matrix, at a given β, satisfies the condition

$$\mathrm{Tr}\, M_{\rm q} = 2m_{{\rm q},1} + m_{{\rm q},3} = \text{constant}. \tag{1.1}$$

This condition ensures that the improved bare gauge coupling

$$\tilde{g}_0^2 \equiv g_0^2 \Big(1 + \frac{1}{N_f} b_g a \,\mathrm{Tr}\, M_{\rm q} \Big) \tag{1.2}$$

is constant up to $\mathscr{O}(a^2)$ effects, for any b_g. Consequently, in the improved theory a constant $\tilde{g}_0^2(a)$ corresponds to fixed lattice spacing. However, a constant $\mathrm{Tr}\, M_{\rm q}$ does not correspond to a constant trace of the renormalised quark mass matrix $M^{\rm R}$, since [8, 9]

$$\mathrm{Tr}\, M^{\rm R} = Z_m [(1 + a\bar{d}_m \,\mathrm{Tr}\, M_{\rm q})\,\mathrm{Tr}\, M_{\rm q} + a d_m \,\mathrm{Tr}(M_{\rm q}^2)] + \mathscr{O}(a^2). \tag{1.3}$$

The d_m counter-term is proportional to squared masses and this violates a constant $\mathrm{Tr}\, M^{\rm R}$ requirement by $\mathscr{O}(a)$ effects. This is an undesirable feature, since we wish to stay on a constant-physics trajectory (up to $\mathscr{O}(a^2)$), as the bare parameters (masses) are varied. This problem can be be avoided by redefining the chiral trajectory in terms of $\phi_4 = $ const. [1], where

$$\phi_4 \equiv 8t_0 \Big(M_{\rm K}^2 + \frac{1}{2} M_\pi^2 \Big). \tag{1.4}$$

Here t_0 is a gluonic dimension-two quantity defined using the Wilson flow [10]. This requirement gives a Symanzik-improved constant physics condition. The improved bare coupling $\tilde{g}_0^2$ now suffers from $\mathscr{O}(am_q \,\mathrm{tr}\, M_q)$ discretisation effects due to higher-order χPT contributions, but these turn out to be small and can be ignored.

The values of the bare quark masses are chosen so that one is approximately at the physical value of ϕ_4. The precise value of $\phi_4^{\rm phys}$ (and $t_0^{\rm phys}$) is found a posteriori, as part of the scale setting. The small differences between the target and measured values of ϕ_4 and ϕ_2 for each ensemble can be corrected for by expanding observables in powers of Δm_q, and computing the relevant coefficients — see [1] for details. The aim is to express the computed quantities of interest (in our case the quark masses) as functions of

$$\phi_2 \equiv 8t_0 M_\pi^2, \tag{1.5}$$

with ϕ_4 held fixed at $\phi_4^{\rm phys}$, and eventually extrapolate them to $\phi_2^{\rm phys} = 8t_0^{\rm phys} m_\pi^2$ (where m_π is the physical pion mass).

Following ref. [1] we define the bare correlation functions

$$f_{\rm P}^{rs}(x_0,y_0) = -\frac{a^6}{L^3}\sum_{\vec{x},\vec{y}}\langle P^{rs}(x_0,\vec{x})P^{sr}(y_0,\vec{y})\rangle, \quad f_{\rm A}^{rs}(x_0,y_0) = -\frac{a^6}{L^3}\sum_{\vec{x},\vec{y}}\langle A_0^{rs}(x_0,\vec{x})P^{sr}(y_0,\vec{y})\rangle, \tag{1.6}$$

where the bare pseudoscalar density and axial current are

$$P^{rs}(x) = \bar{\psi}^r(x)\gamma_5\psi^s(x), \quad A_0^{rs}(x) = \bar{\psi}^r(x)\gamma_0\gamma_5\psi^s(x) + ac_{\rm A}\partial_0 P^{rs}(x) \tag{1.7}$$

(the indices r,s label quark flavours). These two-point functions are estimated with stochastic sources located near the boundaries as described in refs. [1, 3]. The $\mathcal{O}(a)$-improvement coefficient $c_{\rm A}$ has been tuned non-perturbatively in ref. [7]. The bare PCAC mass is then defined through the ratio

$$m_{rs} = \frac{f_{\rm A}^{rs}(x_0+a,y_0) - f_{\rm A}^{rs}(x_0-a,y_0)}{4f_{\rm P}^{rs}(x_0,y_0)}. \tag{1.8}$$

This PCAC quark mass is re-expressed as a dimensionless quantity through the definition

$$\phi_{rs} \equiv \sqrt{8t_0}\, m_{rs}, \tag{1.9}$$

and the corresponding renormalisation group invariant (RGI) dimensionless quantity is then given by

$$\phi_{rs}^{\rm RGI} = \frac{M}{\overline{m}(\mu_{\rm had})}\phi^{\rm R}(\mu_{\rm had}) = Z_{\rm M}\Big(1 + (\tilde{b}_{\rm A} - \tilde{b}_{\rm P})am_{rs} + (\bar{b}_{\rm A} - \bar{b}_{\rm P})a\,{\rm Tr}\,M_{\rm q}\Big)\phi_{rs} + \mathcal{O}(a^2), \tag{1.10}$$

where the renormalisation coefficient $Z_{\rm M}$ is

$$Z_{\rm M}(g_0^2) = \frac{M}{\overline{m}(\mu_{\rm had})}\frac{Z_{\rm A}(g_0^2)}{Z_{\rm P}(g_0^2, a\mu_{\rm had})}. \tag{1.11}$$

The first factor, $M/\overline{m}(\mu_{\rm had})$, is the ratio of the RGI quark mass M (in physical units) to the renormalised quark mass $\overline{m}(\mu_{\rm had})$. The second factor, $Z_{\rm A}(g_0^2)/Z_{\rm P}(g_0^2, a\mu_{\rm had})$, is the ratio of the axial current normalisation $Z_{\rm A}(g_0^2)$ to the pseudoscalar density $Z_{\rm P}(g_0^2, a\mu_{\rm had})$. The former is scale independent and depends solely on the bare gauge coupling, while the latter depends on a renormalisation scheme and a renormalisation scale which we set in the hadronic region of low energies.

The quark mass RG-running was carried out non-perturbatively up to $\mu_{\rm pt} \sim 100$ GeV in the Schrödinger Functional scheme for a theory with $N_f = 3$ massless quarks in ref. [2]. Standard step-scaling functions were obtained in the continuum, by extrapolating results computed on small lattices at fixed renormalisation scale μ. Beyond the scale $\mu_{\rm pt}$ the RG-running is done perturbatively (at 2-loops for the quark mass and 3-loops for the gauge coupling). The result quoted in ref. [2] is

$$\frac{M}{\overline{m}(\mu_{\rm had})} = 0.9148(88), \tag{1.12}$$

for $\mu_{\rm had} = 233(8)$ MeV; the error encompasses both statistical and systematic effects.

We use the axial current renormalisation parameter $Z_{\rm A}(g_0^2)$ obtained on the chirally rotated Schrödinger Functional setup in ref. [11]. The renormalisation parameter $Z_{\rm P}(g_0^2, \mu_{\rm had})$ was computed in ref. [2] for the same action and in the Schrödinger Functional scheme at fixed scale $\mu_{\rm had}$, in the range of inverse gauge couplings $\beta \in [3.40, 3.85]$. This is the range covered by the large volume ensembles of ref. [1], from which our bare PCAC masses ϕ_{rs} are extracted. The final result is summarised as

$$Z_{\rm M}(g_0) = Z_{\rm M}^{(0)} + Z_{\rm M}^{(1)}(\beta - 3.79) + Z_{\rm M}^{(2)}(\beta - 3.79)^2, \tag{1.13}$$

where

$$Z_{\rm M}^{(0)} = 2.270073 \times \frac{M}{\overline{m}(\mu_{\rm had})},\ Z_{\rm M}^{(1)} = 0.125658 \times \frac{M}{\overline{m}(\mu_{\rm had})},\ Z_{\rm M}^{(2)} = -0.464575 \times \frac{M}{\overline{m}(\mu_{\rm had})}, \tag{1.14}$$

with covariance matrix

$$\mathrm{cov}(Z_{\rm M}^{(i)}, Z_{\rm M}^{(j)}) = \begin{pmatrix} 0.164635 \times 10^{-4} & 0.215658 \times 10^{-4} & -0.754203 \times 10^{-4} \\ 0.215658 \times 10^{-4} & 0.121072 \times 10^{-2} & 0.308890 \times 10^{-2} \\ -0.754203 \times 10^{-4} & 0.308890 \times 10^{-2} & 0.953843 \times 10^{-2} \end{pmatrix}. \tag{1.15}$$

The quoted errors only contain the uncertainties from the determination of $Z_{\rm A}$ and $Z_{\rm P}$ at the hadronic scale. The error of the total running factor $M/\overline{m}(\mu_{\rm had})$ in eq. (1.12) only affects the continuum limit, and is only included after the extrapolation to vanishing lattice spacing.

As seen from equation (1.10), besides the renormalisation parameter $Z_{\rm M}$, we also need the mass-dependent improvement coefficients $(\tilde{b}_{\rm A} - \tilde{b}_{\rm P})$ and $(\bar{b}_{\rm A} - \bar{b}_{\rm P})$. We ignore the latter, as it is $\mathcal{O}(g_0^4)$ in perturbation theory. The coefficient $(\tilde{b}_{\rm A} - \tilde{b}_{\rm P})$ is known in 1-loop perturbation theory and has the value $(\tilde{b}_{\rm A} - \tilde{b}_{\rm P}) = -0.0012 g_0^2$. However, we use a preliminary value from a non-perturbative determination from the ALPHA Collaboration [14]:

$$\tilde{b}_{\rm A} - \tilde{b}_{\rm P} = \frac{1.03652(g_0^2)^3 - 0.863388(g_0^2)^4 + 0.109868(g_0^2)^5}{0.956281(g_0^2)^3 - 0.246337(g_0^2)^4 - 0.116847(g_0^2)^5}. \tag{1.16}$$

The perturbative and non-perturbative values are quite different for the ensembles used in this study, but the effect on the final result is negligible.

2. Chiral Fits

Having obtained the renormalised, dimensionless quantities $\phi_{12}^{\rm R}$ and $\phi_{13}^{\rm R}$ (where indices 1,2 refer to the degenerate light quarks and 3 is the strange quark at the physical point) we now proceed to do the chiral and continuum extrapolation. We adapt the standard χPT expressions to our specific parametrisation of our data, which leads to

$$\phi_{12}^{\mathrm{R}} = \phi_2\left[b_1 - b_2\phi_2 - c_{\log}K\left(\bar{L}_\pi - \frac{1}{3}\bar{L}_\eta\right)\right] + c_{a1}\frac{a^2}{8t_0},$$
$$\phi_{13}^{\mathrm{R}} = \frac{2\phi_4-\phi_2}{2}\left[b_1 - b_2\left(\frac{2\phi_4-\phi_2}{2}\right) - c_{\log}\frac{2}{3}K\bar{L}_\eta\right] + c_{a2}\frac{a^2}{8t_0}. \tag{2.1}$$

Note that ϕ_{12}^{R} and ϕ_{13}^{R} are functions of ϕ_2 only, ϕ_4 being held constant. They have common fit parameters b_1, b_2 and $c_{\log}$, arising from NLO χPT. The chiral logs are $\bar{L}_\pi = \phi_2 \ln\phi_2$ and $\bar{L}_\eta = \phi_\eta \ln\phi_\eta$, where $\phi_\eta \equiv (4\phi_4 - 3\phi_2)/3$ and the fit parameters relate to LEC's as

$$b_1 = \frac{1}{2B_0\sqrt{8t_0}}\left[1 - \frac{32}{8t_0 f_0^2}(2L_6 - L_4)\phi_4\right], \quad b_2 = \frac{1}{2B_0\sqrt{8t_0}}\frac{16}{8t_0 f_0^2}(2L_8 - L_5), \quad c_{\log} = \frac{1}{2B_0\sqrt{8t_0}},$$

and

$$K = \frac{1}{16\pi^2 8t_0 f_{\pi\mathrm{K}}^2}, \quad f_{\pi\mathrm{K}} \equiv \frac{2}{3}\left(f_K + \frac{1}{2}f_\pi\right). \tag{2.2}$$

The fit parameters c_{a1}, c_{a2} arise from the parametrisation of the discretisation effects in our Symanzik-improved setup. It is implied that the dominant discretisation error is mass-independent; i.e. corrections of $\mathscr{O}(a^2\phi_2)$ may be ignored. This is supported by work on Wilson χPT [12, 13]. In some test-fits, where such a mass-dependent term was also allowed, it turned out to be small.

These chiral formulae can be combined to form the ratio of the two PCAC masses,

$$\frac{\phi_{12}^{\mathrm{R}}}{2\phi_{13}^{\mathrm{R}}} = \frac{\phi_2}{2\phi_4-\phi_2}\left[1 + \frac{b_2}{b_1}\phi_4 - \frac{3b_2}{2b_1}\phi_2 - \frac{c_{\log}K}{b_1}\left(\bar{L}_\pi - \bar{L}_\eta\right)\right] + c_a\frac{a^2}{8t_0}\left(1 - \frac{2\phi_2}{2\phi_4-\phi_2}\right)$$
$$\overset{LO}{\approx} \frac{\phi_2}{2\phi_4-\phi_2}\left[1 + \frac{b_2}{b_1}\phi_4 - \frac{3b_2}{2b_1}\phi_2 - K\left(\bar{L}_\pi - \bar{L}_\eta\right)\right] + c_a\frac{a^2}{8t_0}\left(1 - \frac{2\phi_2}{2\phi_4-\phi_2}\right). \tag{2.3}$$

The ratio has the advantage of cancelling the renormalisation constants. The form of the cutoff effects has been tailored to satisfy the exact constraint

$$\left.\frac{\phi_{12}^{\mathrm{R}}}{\phi_{13}^{\mathrm{R}}}\right|_{m_l=m_h} = 1. \tag{2.4}$$

Another combination to study is

$$4\frac{\phi_{12}^{\mathrm{R}}}{2\phi_4-\phi_2} + \frac{\phi_{12}^{\mathrm{R}}}{\phi_2} = 3b_1 + 2b_2\phi_4 + c_{\log}K\left(\bar{L}_\pi - \bar{L}_\eta\right) + c_a'\frac{a^2}{8t_0}, \tag{2.5}$$

as this will show how sensitive we are to the chiral logarithms.

The analysis is carried out using the library described in [15], and standard MINPACK routines are used for χ^2 minimisation. Errors in abscissa variables – ϕ_2, ϕ_4 and K – are included in the fit. The error analysis is carried out using the Gamma method approach and automatic differentiation for error propagation (see [15] and references therein). This takes into account all existing correlations in the data, and computes autocorrelation functions (including exponential tails) to estimate the uncertainties correspondingly. Following [1], the values τ_{exp} used in the analysis are those quoted in [3], namely

$$\tau_{\mathrm{exp}} = 14(3)\frac{t_0}{a^2}. \tag{2.6}$$

This is a very conservative estimate for our data.

Doing combined fits to various combinations of the ratio $\phi_{12}^{\mathrm{R}}/(2\phi_{13}^{\mathrm{R}})$, ϕ_{13}^{R}, ϕ_{12}^{R} and eq. (2.5) shows that our most stable fits are:

fit 1: combined fit of ratio $\phi_{12}^{\mathrm{R}}/(2\phi_{13}^{\mathrm{R}})$ and ϕ_{13}^{R},

fit 2: conbined fit of eq. (2.5) and ϕ_{13}^{R}.

Our results indicate that χPT suffers at our highest pion masses, which are around 420 MeV. Therefore we introduce a cut in the pion mass at $m_\pi < 400$ MeV and $m_\pi < 300$ MeV to test how much the results change. We take the results from fit 2 with a cut at $m_\pi < 400$ MeV as our main result, and use the spread of central values in these two sets of fits to estimate the systematics. The results have been crosschecked by various independent analyses.

3. Results and outlook

Our preliminary results for the strange and u/d quark masses are

$$m_s^{\mathrm{RGI}} = 127.0(3.1)(3.2)\ \mathrm{MeV}, \quad m_{u/d}^{\mathrm{RGI}} = 4.70(15)(12)\ \mathrm{MeV}. \tag{3.1}$$

The first error includes statistics/fitting and the second error is systematic. Using 4-loop PT to convert RGI masses to $\overline{\mathrm{MS}}$ scheme at $\mu = 2$ GeV and $n_f = 3$ gives

$$m_s^{\overline{\mathrm{MS}}} = 95.5(2.5)(2.4)\ \mathrm{MeV}, \quad m_{u/d}^{\overline{\mathrm{MS}}} = 3.53(12)(9)\ \mathrm{MeV} \tag{3.2}$$

(the conversion factor is 1.330(13)). These results agree very well with the quark masses listed in PDG [16], $m_s^{\overline{\mathrm{MS}}} = 95^{+9}_{-3}$ MeV and $m_{u/d}^{\overline{\mathrm{MS}}} = 3.5^{+0.5}_{-0.2}$ MeV. The agreement with other $n_f = 2+1$ lattice results is also good: FLAG review [17] gives the lattice averages as $m_s^{\overline{\mathrm{MS}}} = 92.0(2.1)$ MeV and $m_{u/d}^{\overline{\mathrm{MS}}} = 3.373(80)$ MeV. Our result for the quark mass ratio is

$$\frac{m_s}{m_l} = 27.0(1.0)(0.4), \tag{3.3}$$

compared to the PDG value [16] $m_s/m_l = 27.3(0.7)$ and the FLAG average [17] $m_s/m_l = 27.43(31)$. Our results are still preliminary, and we will address the full error budget in a forthcoming publication. The fairly large systematic uncertainties are due to the absence of very chiral ensembles in this analysis, which could be improved on as further ensembles become available.

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