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Quark mass dependence of pseudoscalar masses and decay constants on a lattice

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Abstract. Our previous calculations of the sea- and valence-quark mass dependence of the pseudoscalar meson masses and decay constants is repeated on a $16^3 \cdot 32$ lattice, which allows for a better determination of the quantities in question. The conclusions are similar as before on the 16^4 lattice [1]. The two light dynamical quark flavours we simulate have masses in the range $m_s/4 < m_{u,d} < 2m_s/3$. The sea quark mass dependence of f_π and m_π^2/m_q is well described by the next-to-leading order (NLO) chiral perturbation theory (ChPT) formulas and clearly shows the presence of chiral logarithms. The valence quark mass dependence requires the presence of NNLO contributions in partially quenched ChPT (PQChPT)—in addition to the NLO terms. The $\mathcal{O}(a)$ lattice artifacts in these quantities turn out to be small.

1 Introduction

In Quantum Chromodynamics (QCD) – the theory of strong interactions – there are two very light quarks and one moderately light quark (u, d and s, respectively). The strong interaction dynamics at low energies can be formulated by an *effective chiral Lagrangian*, which incorporates the symmetry constraints following from the spontaneously broken chiral symmetry of the light quarks. In this low-energy effective theory, the interactions are described by a simultaneous expansion in powers of momenta and light quark masses [2,3]. The coefficients of the interaction terms in the effective chiral Lagrangian – the *Gasser-Leutwyler constants* – are free parameters, which can be constrained by experimental data and also calculated from the underlying basic QCD Lagrangian in the framework of the nonperturbative lattice regularization.

In numerical lattice QCD simulations, the quark masses are free parameters. Changing these parameters gives an excellent opportunity to precisely determine the Gasser-Leutwyler constants. In fact, chiral perturbation theory (ChPT) based on the chiral Lagrangian can be extended by changing the *valence quark masses* in quark propagators independently from the *sea quark masses* in virtual quark loops. This leads to partially quenched chiral perturbation theory (PQChPT) [4].

The aim of numerical simulations in QCD is to reach the regime of light quark masses where next-to-leading order (NLO) chiral perturbation theory gives a good approximation. In previous papers [5,6,1], our collaboration started a series of simulations with two equal-mass light quarks (qq) with the goal of extracting the values of the Gasser-Leutwyler constants conventionally denoted by L_k, $(k = 1, 2, \ldots)$. Later on, it will be possible to extend these calculations by also including the s-quark (qq+q).

In our previous paper [1], we started some larger scale simulations on a 16^4 lattice at the gauge coupling $\beta = 5.1$, which corresponds to a lattice spacing of $a \simeq 0.2\,\mathrm{fm}$. Because it became clear that interesting results can be obtained already at this relatively rough discretization scale, we decided to repeat and extend these simulations on a $16^3 \cdot 32$ lattice, which is better suited for extracting quantities like the pseudoscalar (pion) mass (m_π) and decay constant (f_π). Our work profited from the valuable experience of previous simulations by other collaborations [7–9].

Because the present work is on the same topics as [1], we shall often only refer to it without repeating its full content. In general, we use the conventions and notations of [1,6,5]. Nevertheless, we also try to make the present paper easily understandable for the reader and therefore repeat the main definitions and relations. In the next section, we deal with the sea quark mass dependence of f_π and m_π. In Sect. 3, the valence quark mass dependence is considered and the question of the magnitude of leading lattice artifacts is investigated. Section 4 is a short summary of our experience with the Monte Carlo updating algorithm. The last section contains the summary and discussion.

2 Sea quark mass dependence

We performed Monte Carlo simulations with $N_s = 2$ degenerate sea quarks on a $16^3 \cdot 32$ lattice at gauge coupling $\beta = 5.1$ and four values of the hopping parameter κ: $\kappa_0 = 0.176$, $\kappa_1 = 0.1765$, $\kappa_2 = 0.1768$ and $\kappa_3 = 0.177$. Three of these points have also been simulated previously on the 16^4 lattice in [1]. The point at $\kappa_2 = 0.1768$ is new. We collected 950–1000 gauge configurations per point, which are typically separated by 10 update cycles consisting of boson-field and gauge-field updates and noisy correction steps. (Some observations about the algorithm will be summarized in Sect. 4.)

A collection of the values of some basic quantities in these simulation points is given in Table 1: the Sommer scale-parameter in lattice units, r_0/a; the pion mass in lattice units, am_π; the quark mass parameter, $M_r = (r_0 m_\pi)^2$; the bare PCAC quark mass $Z_q am_q$, including the multiplicative renormalization factor, $Z_q = Z_P/Z_A$; the ratio of the PCAC quark masses σ_i with respect to the *reference sea quark mass* at $\kappa = \kappa_0$ and the pion decay constant in lattice units, af_π divided by the renormalization factor Z_A. (The normalization of the pion decay constant is such that the physical value is $f_\pi \simeq 93\,\mathrm{MeV}$.)

Comparing Table 1 to the corresponding one (Table 3) in [1], one can see that these quantities extracted on the $16^3 \cdot 32$ lattice differ considerably from those extracted on the 16^4 lattice. The change of r_0/a is about 2–5%. The difference in am_π increases from 3% at κ_0 to about 16% at κ_3, whereas $Z_q am_q$ differs at κ_0 by 5% and at κ_3 already by about 28%. However, as we shall see later on, considering ratios of the pion mass-square and of the pion decay constant as a function of the ratios of PCAC quark masses (denoted by σ for sea quark masses and ξ for valence quark masses), it turns out that almost all changes between the 16^4 and $16^3 \cdot 32$ lattices cancel.

In Table 1, the bare quark mass obtained from the PCAC relation is shown: $m_q \equiv m_q^{PCAC}$. (For details of its numerical determination, see Sect. 3.1.1 in [5].) Another possibility to define the quark mass is to take $am_{ren} \equiv \mu_{ren} \equiv Z_m(\mu_0 - \mu_{cr})$, where $\mu_0 = 1/(2\kappa) - 4$ is the bare quark mass in the Wilson–fermion action, μ_{cr} is its critical value corresponding to zero quark mass and Z_R is an appropriate multiplicative renormalization factor. The values of μ_0 corresponding to $\kappa_0, ..., \kappa_3$ are $\mu_{0(0)} = -1.1590909...$, $\mu_{0(1)} = -1.1671388...$, $\mu_{0(2)} = -1.1719457...$, $\mu_{0(3)} = -1.1751412...$, respectively. Comparing the values of $Z_q am_q$ or σ_i in Table 1 to the values $\mu_{0(i)}$, one can see that the relation between them is highly nonlinear. This implies the same also for the relation between the (ratios of) m_q^{PCAC} and m_{ren}. The nonlinear terms in this relation are lattice artifacts, which have to vanish in the continuum limit, but they are large at our lattice spacings.

A consequence of the strongly nonlinear relation between σ and μ_0 is that the determination of μ_{cr} (or κ_{cr}) has large uncertainty. In fact, with our four points only, we could not find a convincing extrapolation of σ to zero. A crude quadratic extrapolation gives $\mu_{cr} = -1.180(4)$ or $\kappa_{cr} = 0.1773(2)$. The uncertainty in the critical point implies an uncertainty in the extrapolation of physical quantities, too, which is necessary in a quark mass-independent renormalization scheme. In case of the lattice spacing, which can be obtained from the extrapolation of r_0/a to the critical point, Table 1 shows that the values of r_0/a increase between κ_0 and κ_2, but between κ_2 and κ_3, they are within error constants. Therefore, we take this constant value as the extrapolated one: $[r_0/a]_{cr} = 2.57(5)$. This gives, with $r_0 \equiv 0.5\,\mathrm{fm}$, for the quark mass independent lattice spacing $a = 0.195(4)\,\mathrm{fm}$.

In the ChPT formulas, the quark mass can be represented by the dimensionless quantity

$$\chi \equiv \frac{2B_0 m_q}{f_0^2}, \tag{1}$$

where B_0 is a conventional parameter with dimension mass and f_0 is the value of the pion decay constant at zero quark mass. (Its normalization here is such that the physical value is $f_0 \simeq 93\,\mathrm{MeV}$.) In what follows, we shall identify the quark mass m_q in χ with the PCAC quark mass m_q^{PCAC}. According to the previous discussion, this is a nontrivial choice because the lattice artifacts in (ratios of) the quark mass are rather different for am_q^{PCAC} than, for instance, for am_{ren}.

The sea quark mass dependence of the ratio of the pion decay constant in NLO of ChPT is:

$$Rf_{SS} \equiv \frac{f_{SS}}{f_{RR}} = 1 + 4(\sigma - 1)\chi_R(N_s L_{R4} + L_{R5}) - \frac{N_s \chi_R}{32\pi^2}\sigma \log \sigma + \mathcal{O}(\chi_R^2). \tag{2}$$

Here f_{SS} is the pion decay constant of a pion consisting of two sea quarks with mass χ_S and f_{RR} is its

Table 1. The values of some basic quantities in our simulation points. Statistical errors in last digits are given in parentheses

κ	κ_0	κ_1	κ_2	κ_3
r_0/a	2.229(63)	2.212(44)	2.621(46)	2.528(51)
am_π	0.6542(10)	0.5793(17)	0.3919(46)	0.3657(24)
$M_r = (r_0 m_\pi)^2$	2.13(12)	1.642(72)	1.055(36)	0.855(34)
$Z_q am_q$	0.07092(27)	0.05571(30)	0.02566(27)	0.02208(21)
$\sigma_i = m_{qi}/m_{q0}$	1.0	0.7856(56)	0.3618(44)	0.3113(31)
$Z_A^{-1} af_\pi$	0.2819(15)	0.2590(14)	0.2008(17)	0.1936(16)

value at some *reference quark mass* χ_R. N_s is the number of mass-degenerate sea quarks (actually $N_s = 2$), L_{Rk} ($k = 4, 5, \ldots$) are Gasser-Leutwyler constants at the scale $\mu = f_0\sqrt{\chi_R}$ and the ratio of sea quark masses to the reference quark mass is

$$\sigma \equiv \frac{\chi_S}{\chi_R}. \quad (3)$$

The analogous formula for the pion mass squares is:

$$Rn_{SS} \equiv \frac{m_{SS}^2}{\sigma m_{RR}^2} = 1 + 8(\sigma - 1)\chi_R \cdot \\ \cdot(2N_s L_{R6} + 2L_{R8} - N_s L_{R4} - L_{R5}) \\ + \frac{\chi_R}{16\pi^2 N_s}\sigma \log\sigma + \mathcal{O}(\chi_R^2). \quad (4)$$

Note that instead of the scale-dependent combinations (at $N_s = 2$),

$$L_{R45} \equiv 2L_{R4} + L_{R5} \ , \\ L_{R6845} \equiv 4L_{R6} + 2L_{R8} - 2L_{R4} - L_{R5}, \quad (5)$$

one can also use the *universal low-energy scales* $\Lambda_{3,4}$ defined by [10].

$$\Lambda_3 = 4\pi f_0 \exp(-\alpha_{6845}) \ , \\ \alpha_{6845} = 128\pi^2 L_{R6845} - \frac{1}{2}\log\frac{\chi_R}{16\pi^2} \\ \Lambda_4 = 4\pi f_0 \exp(\alpha_{45}/4) \ , \\ \alpha_{45} = 128\pi^2 L_{R45} + 2\log\frac{\chi_R}{16\pi^2}. \quad (6)$$

The free parameters in Rf_{SS} and Rn_{SS} are χ_R, $\chi_R L_{R45}$ and $\chi_R L_{R6845}$. With the small number of points we have, the linear fit with these parameters gives a good chi-square but relatively large errors: $\chi^2 = 0.8$ and

$$\chi_R = 30.8(9.4), \\ \chi_R L_{R45} = 0.1398(86), \\ \chi_R L_{R6845} = -0.0078(22). \quad (7)$$

This corresponds to

$$L_{R45} = 4.5(1.1) \cdot 10^{-3}, \ \frac{\Lambda_4}{f_0} = 23.3(8.2), \\ L_{R6845} = -2.54(21) \cdot 10^{-4}, \ \frac{\Lambda_3}{f_0} = 7.64(14). \quad (8)$$

Consistent results with smaller errors can be obtained if one takes the value of $\chi_R = 35.8(3.3)$ from the fit of the valence quark mass dependences (see next section) and performs two linear fits with the parameters $\chi_R L_{R45}$ and $\chi_R L_{R6845}$, respectively. The resulting parameters are

$$\chi_R L_{R45} = 0.1443(15), \\ L_{R45} = 4.03(37) \cdot 10^{-3}, \ \frac{\Lambda_4}{f_0} = 21.4(1.5), \\ \chi_R L_{R6845} = -0.00896(86), \\ L_{R6845} = -2.50(34) \cdot 10^{-4}, \ \frac{\Lambda_3}{f_0} = 8.21(27) \quad (9)$$

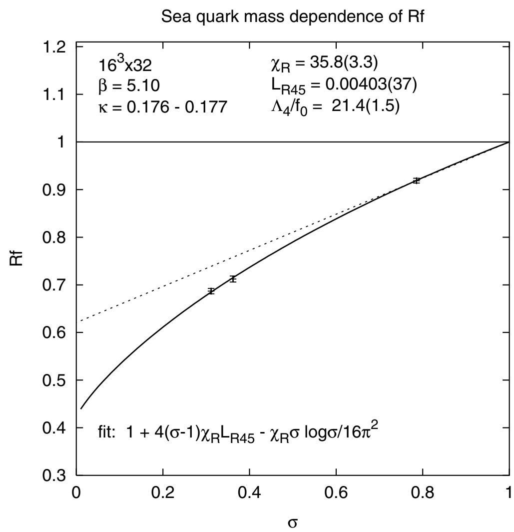

Fig. 1. Sea quark mass dependence of the pion decay constant. The straight dashed line connects the first two points

and the fits are shown in Figs. 1 and 2.

As these figures show, both Rf_{SS} and Rn_{SS} can be well fitted with the NLO ChPT formula. The fit parameters are within the expected range. For instance, the value of χ_R is rather close to the tree-level estimate $\chi_R^{estimate} \approx M_r/(r_0 f_0)^2 \simeq 40.3$. (Here we used $r_0 f_0 \simeq 0.23$.) The presence of a *chiral logarithm*, which causes the curvature, is clearly displayed in Fig. 1, where a straight line connecting the first two points is also shown. In Rn_{SS}, the measured points are consistent with the presence of a chiral logarithm but the relative errors are large because all the values including the ChPT fit are very close to 1. This implies that the deviation from the tree-level behaviour $m_{SS}^2 \propto \chi_S$ is rather small. The results for the parameters in (9) are close to the ones reported in [1]: the values for

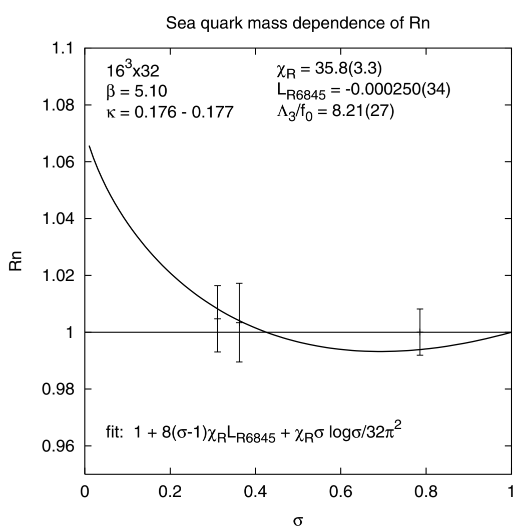

Fig. 2. Sea quark mass dependence of the pion mass-squared divided by the quark mass

Λ_4/f_0 practically coincide and the value of Λ_3/f_0 is only slightly higher now.

The extrapolated values of Rf_{SS} and Rn_{SS} at zero quark mass are, respectively:

$$Rf_0 = 0.4228(60), \qquad Rn_0 = 1.0717(69). \tag{10}$$

The value of Rf_0 together with $Z_A^{-1} a f_\pi$ from Table 1 and $r_0 = 0.5\,\mathrm{fm}$ imply, for the pion decay constant, at zero quark mass (f_0)

$$Z_A^{-1} f_0 = 121(5)\,\mathrm{MeV}. \tag{11}$$

This result for $N_s = 2$ light quarks compares well with the phenomenological value $f_0 = 93\,\mathrm{MeV}$ if, as expected, $Z_A = \mathcal{O}(1)$.

3 Valence quark mass dependence

We consider, for fixed sea quark mass χ_S, the valence quark mass dependence of f_π and m_π^2 as a function of the quark mass ratio

$$\xi \equiv \frac{\chi_V}{\chi_S}. \tag{12}$$

In our numerical data, we determined the pseudoscalar mass and decay constant in relatively wide ranges of the valence quark mass ratios, typically $\frac{1}{2} \le \xi \le 2$. At the smaller quark masses ($\kappa = \kappa_{2,3}$), however, for $\xi < 1$ *exceptional gauge configurations* appear, which blow up the statistical errors and clearly influence the mean values themselves. Therefore, in most cases, we restrict our fits to valence quark masses larger than the sea quark mass ($\xi > 1$).

In the partially quenched situation, several types of ratios can be constructed because the pseudoscalar meson can be the bound state of two valence quarks (VV) and also a valence quark and a sea quark (VS). The PQChPT formulas for the ratios of decay constants are:

$$\begin{aligned} Rf_{VV} \equiv \frac{f_{VV}}{f_{SS}} &= 1 + 4(\xi-1)\chi_S L_{S5} \\ &\quad - \frac{N_s\chi_S}{64\pi^2}(1+\xi)\log\frac{1+\xi}{2} \\ &\quad + D_{fVV}\chi_S^2(\xi-1) + Q_{fVV}\chi_S^2(\xi-1)^2 \\ &\quad + \mathcal{O}(\chi_S^2\log\xi, \chi_S^3) \end{aligned} \tag{13}$$

and

$$\begin{aligned} Rf_{VS} \equiv \frac{f_{VS}}{f_{SS}} &= 1 + 2(\xi-1)\chi_S L_{S5} \\ &\quad + \frac{\chi_S}{64N_s\pi^2}(\xi - 1 - \log\xi) \\ &\quad - \frac{N_s\chi_S}{128\pi^2}(1+\xi)\log\frac{1+\xi}{2} \\ &\quad + \frac{1}{2}D_{fVV}\chi_S^2(\xi-1) + Q_{fVS}\chi_S^2(\xi-1)^2 \\ &\quad + \mathcal{O}(\chi_S^2\log\xi, \chi_S^3). \end{aligned} \tag{14}$$

The analogous formulas for the valence quark mass dependence of the (squared) pseudoscalar meson masses are:

$$\begin{aligned} Rn_{VV} \equiv \frac{m_{VV}^2}{\xi m_{SS}^2} &= 1 + 8(\xi-1)\chi_S(2L_{S8} - L_{S5}) \\ &\quad + \frac{\chi_S}{16N_s\pi^2}[\xi - 1 + (2\xi-1)\log\xi] \\ &\quad + D_{nVV}\chi_S^2(\xi-1) + Q_{nVV}\chi_S^2(\xi-1)^2 \\ &\quad + \mathcal{O}(\chi_S^2\log\xi, \chi_S^3) \end{aligned} \tag{15}$$

and

$$\begin{aligned} Rn_{VS} &\equiv \frac{2m_{VS}^2}{(\xi+1)m_{SS}^2} \\ &= 1 + 4(\xi-1)\chi_S(2L_{S8} - L_{S5}) \\ &\quad + \frac{\chi_S}{16N_s\pi^2}\xi\log\xi \\ &\quad + \frac{1}{2}D_{nVV}\chi_S^2(\xi-1) + Q_{nVS}\chi_S^2(\xi-1)^2 \\ &\quad + \mathcal{O}(\chi_S^2\log\xi, \chi_S^3). \end{aligned} \tag{16}$$

In these formulas the Gasser-Leutwyler coefficients, L_{Sk} ($k = 4, 5, \ldots$), are defined at the scale $f_0\sqrt{\chi_S}$ and, in addition to the NLO terms, also the tree-graph (i.e. counterterm) contributions of the NNLO are included. Their general form is taken from [11] and is discussed in more detail in Sect. 2.1 of [1]. The left-out terms of NNLO, which come from two-loop integrals, are generically denoted here by $\mathcal{O}(\chi_S^2\log\xi)$.

In addition to the *single ratios*, Rf_{VV}, Rf_{VS}, Rn_{VV} and Rn_{VS}, it is useful to consider the so-called *double ratios*, which do not depend on any of the NLO coefficients L_{Sk}. The PQChPT formulas for the double ratios are:

$$\begin{aligned} RRf \equiv \frac{f_{VS}^2}{f_{VV}f_{SS}} &= 1 + \frac{\chi_S}{32N_s\pi^2}(\xi - 1 - \log\xi) \\ &\quad + Q_{fd}\chi_S^2(\xi-1)^2 + \mathcal{O}(\chi_S^2\log\xi, \chi_S^3) \end{aligned} \tag{17}$$

and

$$\begin{aligned} RRn &\equiv \frac{4\xi m_{VS}^4}{(\xi+1)^2 m_{VV}^2 m_{SS}^2} \\ &= 1 - \frac{\chi_S}{16N_s\pi^2}(\xi - 1 - \log\xi) \\ &\quad + Q_{nd}\chi_S^2(\xi-1)^2 + \mathcal{O}(\chi_S^2\log\xi, \chi_S^3). \end{aligned} \tag{18}$$

In the PQChPT formulas (13)-(18), there are altogether 11 parameters. Three of them appear at NLO, namely with $N_s = 2$,

$$\chi_R\ , \qquad \chi_R L_{R5}\ , \qquad \chi_R L_{R85} \equiv \chi_R(2L_{R8} - L_{R5}), \tag{19}$$

and the rest in NNLO:

$$\chi_R^2 D_{fVV,nVV}\ , \qquad \chi_R^2 Q_{fVV,fVS,fd,nVV,nVS,nd}. \tag{20}$$

At the smallest quark mass, fits with the NLO formulas are reasonable but for the larger quark masses the NNLO contributions are required unless the fits are restricted to a small range around $\xi = 1$.

An acceptable global fit with 11 parameters can be achieved if the valence quark mass dependence at all four sea quark masses is simultaneously considered. In this case, one has to choose a *reference sea quark mass*, χ_R, and take into account the relation between the NLO parameters

$$L_{Sk} = L_{Rk} - c_k \log \frac{\chi_S}{\chi_R}, \tag{21}$$

where the relevant constants are:

$$c_5 = \frac{1}{128\pi^2}\ , \qquad c_{85} \equiv 2c_8 - c_5 = -\frac{1}{128\pi^2}. \tag{22}$$

Fitting all six valence quark mass dependences, (Rf_{VV}, Rf_{VS}, RRf, Rn_{VV}, Rn_{VS}, RRn), there are reasonably good 11 parameter (linear) fits with $\chi^2 \simeq 200 \simeq$ degrees of freedom. A typical set of the resulting fit parameters is shown in Table 2.

Comparing Table 2 with the corresponding one (Table 4) in [1], one can see that most values are, within statistical errors, the same. This is also true for the NLO parameters defined at the scale $4\pi f_0$, which are now

$$\alpha_5 \equiv 128\pi^2 L_{R5} + \log \frac{\chi_R}{16\pi^2} = 2.06(42),$$

$$\alpha_{85} \equiv 2\alpha_8 - \alpha_5 \equiv 128\pi^2 L_{R85} - \log \frac{\chi_R}{16\pi^2} = 0.583(45). \tag{23}$$

Table 2. Values of best fit parameters for the valence quark mass dependence. Quantities directly used in the fitting procedure are in boldface

$\boldsymbol{\chi_R}$	35.8(3.3)		
$\boldsymbol{\chi_R L_{R5}}$	0.1003(76)	L_{R5}	$2.80(39) \cdot 10^{-3}$
$\boldsymbol{\chi_R L_{R85}}$	−0.0256(12)	L_{R85}	$-0.714(65) \cdot 10^{-3}$
$\boldsymbol{\chi_R^2 D_{fVV}}$	−0.109(42)	D_{fVV}	$-8.5(4.4) \cdot 10^{-5}$
$\boldsymbol{\chi_R^2 Q_{fVV}}$	−0.014(29)	Q_{fVV}	$-1.1(2.3) \cdot 10^{-5}$
$\boldsymbol{\chi_R^2 Q_{fVS}}$	−0.0177(94)	Q_{fVS}	$-1.39(81) \cdot 10^{-5}$
$\boldsymbol{\chi_R^2 Q_{fd}}$	−0.0180(31)	Q_{fd}	$-1.41(13) \cdot 10^{-5}$
$\boldsymbol{\chi_R^2 D_{nVV}}$	−0.134(21)	D_{nVV}	$-10.46(93) \cdot 10^{-5}$
$\boldsymbol{\chi_R^2 Q_{nVV}}$	−0.087(13)	Q_{nVV}	$-6.77(30) \cdot 10^{-5}$
$\boldsymbol{\chi_R^2 Q_{nVS}}$	−0.0394(44)	Q_{nVS}	$-3.07(24) \cdot 10^{-5}$
$\boldsymbol{\chi_R^2 Q_{nd}}$	0.0077(48)	Q_{nd}	$0.60(26) \cdot 10^{-5}$

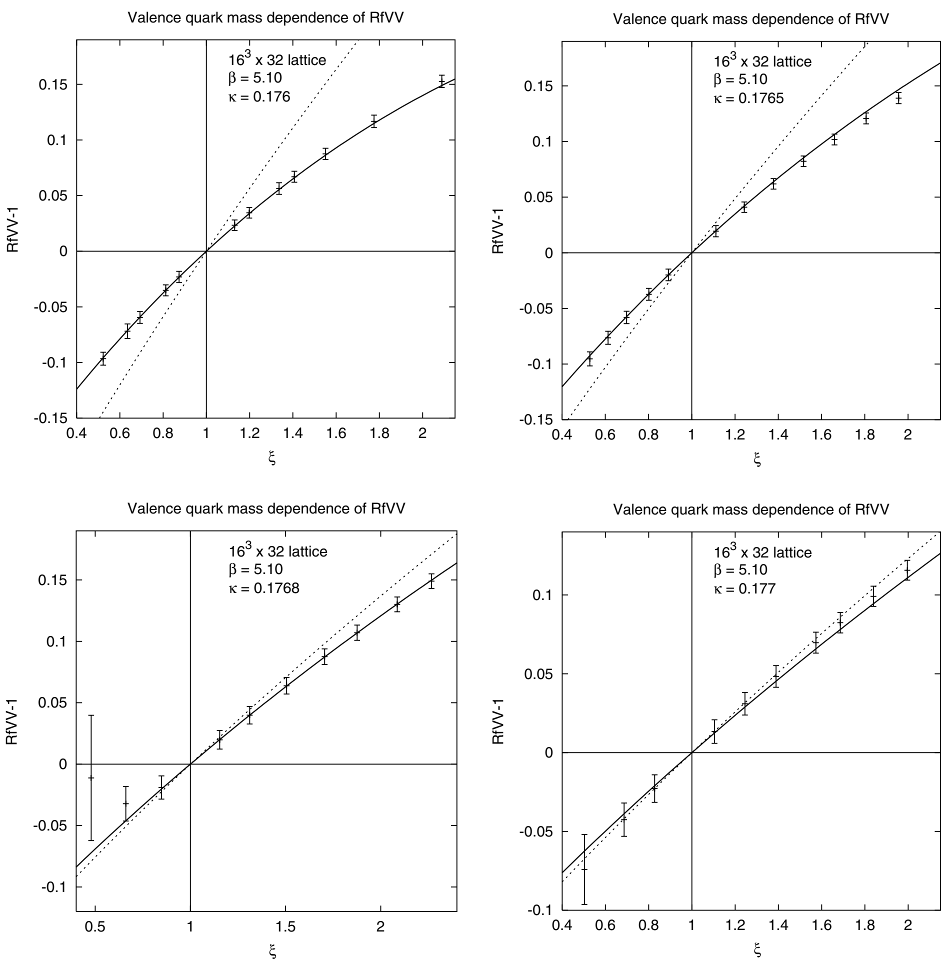

Fig. 3. The linear fit for Rf_{VV} for different sea quark masses. The NLO contributions alone are shown by dashed lines

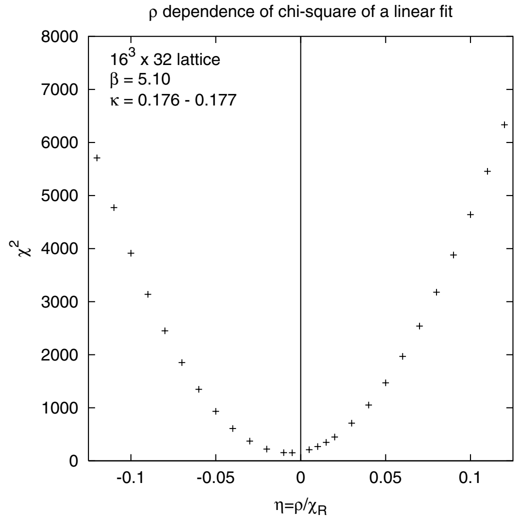

Fig. 4. χ^2 of the linear fit of the ratios Rf_{VV}, Rf_{VS}, RRf, Rn_{VV}, Rn_{VS} and RRn for all four sea quark masses at fixed values of the $\mathcal{O}(a)$ parameter ρ in the chiral Lagrangian

The value of α_5 is practically the same as in Table 5 of [1], whereas α_{85} is slightly smaller now.

The tree-graph NNLO contributions play an important role in the global fits of the valence quark dependences, especially at the two larger sea quark masses ($\kappa = \kappa_0$ and $\kappa = \kappa_1$). At the two smaller sea quark masses, NNLO is substantially less important. This is illustrated in Fig. 3, where the 11 parameter fit for Rf_{VV} is shown together with the NLO contributions alone.

3.1 $\mathcal{O}(a)$ terms

The fits above have been performed with the continuum formulas – without $\mathcal{O}(a)$ or any other lattice artifacts. The fits are reasonably good and the resulting parameters are quite similar to those obtained in [1], where the $\mathcal{O}(a)$ terms have been taken into account in the (PQ)ChPT Lagrangian according to [12]. It has been observed already in [1] that the parameter in the chiral Lagrangian characterizing the magnitude of $\mathcal{O}(a)$ effects,

$$\rho \equiv \frac{2W_0 a c_{SW}}{f_0^2}, \tag{24}$$

is rather small compared with the quark mass parameter χ in (1). Fitting the ratio $\eta_S \equiv \rho_S/\chi_S$ separately for the individual sea quark mass values, we obtained increasing values for increasing sea quark masses: $0.02 \le \eta_S \le 0.07$.

The parameter ρ should be independent of the quark mass because the quark masses are the other expansion parameters in the chiral Lagrangian. This means that a quark mass dependent ρ_S incorporates some higher order effects proportional to some power of am_q. (For instance, a linearly increasing value of η_S corresponds to $\rho_S \propto (am_q)^2$.) Because the observed values of ρ are small anyway, it is interesting to consider the behaviour of the chi-square as a function of ρ if the linear fits are performed for fixed ρ . Because of the presence of another new parameter describing $\mathcal{O}(a)$ effects in the chiral Lagrangian, the linear fit has 12 parameters for $\rho \neq 0$ (instead of 11 for $\rho = 0$). As is shown by Fig. 4, the χ^2 of the fit has a minimum near $\rho = \eta = 0$ and becomes extremely large already at $|\eta| \simeq 0.1$. where the absolute value of ρ is 10% of the value of the reference quark mass parameter χ_R. Another way to investigate the importance of $\mathcal{O}(a)$ effects in our data is to consider the following combination of double ratios:

$$RRn + 2\,RRf - 3 = (Q_{nd} + 2Q_{fd})\chi_S^2(\xi - 1)^2 + \mathcal{O}(\chi_S^2 \log\xi, \chi_S^3). \tag{25}$$

As this formula shows, this combination vanishes in next-to-leading order and only NNLO and higher orders contribute to it. On the lattice, there could also be $\mathcal{O}(a)$ contributions, which can be parametrized as

$$\begin{aligned} RRn + 2\,RRf - 3 = {} & 16\rho\, L_{S4W6}\frac{(\xi-1)^2}{\xi(\xi+1)} - \rho\,\frac{(\xi-1)^2}{\chi_S\xi(\xi+1)} \\ & + \rho\,\frac{[2(1-\xi^2) + \log\xi + 3\xi^2\log\xi]}{32\pi^2\xi(\xi+1)} \\ & + \rho\,\frac{(\xi - 1 - \xi\log\xi)}{32\pi^2\xi} \\ & + \mathcal{O}(\rho^2, \chi^2). \end{aligned} \tag{26}$$

Here only the linear piece of the $\eta_S = \rho/\chi_S$-dependence is kept because η_S is small. $L_{S4W6} \equiv L_{S4} - W_{S6}$ is a new parameter appearing in the $\mathcal{O}(a)$ terms of the chiral Lagrangian [12].

The linear fits with $\chi_S^2 Q_{n2f} \equiv \chi_S^2(Q_{nd}+2Q_{fd})$ in (25) and with ρ in (26), respectively, are shown in case of the smallest sea quark mass ($\kappa = \kappa_3$) by Fig. 5. As this figure shows, the NNLO fit with $\chi_S^2 Q_{n2f}$ is better ($\chi^2 = 1.3$) than the one with the leading $\mathcal{O}(a)$ term proportional to ρ ($\chi^2 = 7.2$). For simplicity, the parameters $\chi_S = 11.7$ and

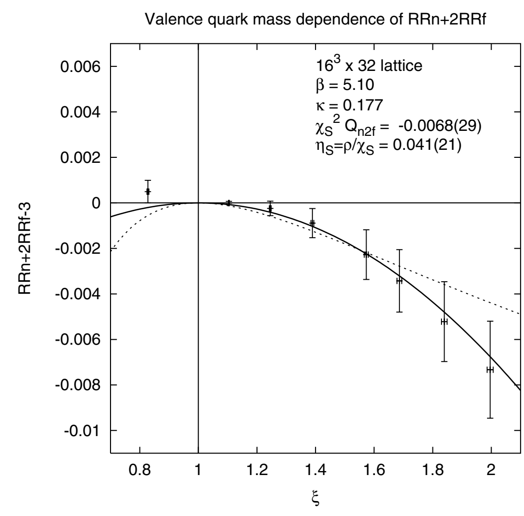

Fig. 5. Comparing the NNLO fit (full line) with the leading $\mathcal{O}(a)$ fit (dashed line) for $(RRn + 2\,RRf - 3)$ at $\kappa = \kappa_3$

$L_{S4W6} = 0.001$ are fixed in this latter case, but taking other values does not change the qualitative picture.

At the larger sea quark mass values, the fits with the leading $\mathcal{O}(a)$ terms behave similarly to Fig. 5. This supports the fact that the $\mathcal{O}(a)$ terms are not important in our numerical data. As shown by Fig. 4, good fits can only be obtained at rather small values of $\eta = \rho/\chi$. In contrast, the NNLO contributions are very important, especially at our larger sea quark masses.

4 Studies of the updating algorithm

The numerical simulations have been performed by the two-step multi-boson (TSMB) algorithm [13]. This dynamical fermion update algorithm is based on the *multi-boson representation* of the fermion determinant [14], and in its present form, it incorporates several modern ideas of fermionic updating: the *global correction step* in the update [15], the final *reweighting correction* [16] and the *determinant breakup* [17].

Our error analysis is based on measuring the autocorrelations of the quantities in question [18,19], therefore, we can estimate the *computation cost* based on the integrated autocorrelations $\tau_{\rm int}$. In our previous papers [5,20, 21], we proposed an approximate formula for the cost,

$$C_{\tau_{\rm int}} \simeq F\,(am_q)^{-2}\,\Omega, \tag{27}$$

where am_q is the quark mass in lattice units and Ω the number of lattice points. The overall factor F depends on the quantity under investigation. If we count the cost in terms of the number of floating-point operations necessary to perform an update sequence with length $\tau_{\rm int}$, then the present simulations on $16^3 \cdot 32$ lattice are consistent with

$$F_{\rm plaquette} \simeq 7\cdot 10^6, \qquad F_{m_\pi} \simeq 10^6, \qquad F_{f_\pi} < 4\cdot 10^5. \tag{28}$$

In case of f_π, we only have an upper limit on $\tau_{\rm int}$ because the gauge configurations stored for the measurements were statistically independent. These numbers are somewhat smaller than our previous estimates in [5,20,21], which is due to a better tuning of algorithmic parameters. In particular, these simulations were done with a determinant breakup $N_b = 4$, which means that the fermion determinant of the two degenerate flavours ($N_f = 2$) were reproduced by $4 \otimes (N_f = \frac{1}{2})$ flavours. Another important point is the frequent call of the global heatbath update of the multiboson fields, which every time gives a statistically independent boson configuration.

If we take the plaquette expectation value as the worst case, then at the present quark masses and lattice spacing, this cost estimate is similar to previous estimates (see, for instance, the formula of A. Ukawa [22]), but considering the more interesting cases of m_π or f_π, there is a substantial improvement by an order of magnitude or more. In addition, toward large volumes, smaller quark masses and/or smaller lattice spacings, the scaling of the cost estimate in (27) is better: for fixed lattice spacing, the cost increases as $m_q^{-2}\Omega$ and decreasing the lattice spacing and keeping the physical parameters fixed, the cost behaves as a^{-6}. This has to be compared with the estimated behaviour in [22], $m_q^{-3}\Omega^{5/4}$ and a^{-7}, respectively.

5 Summary

The quark mass dependence of the pseudoscalar mass and decay constant in our numerical data can be well fitted with the continuum (PQ)ChPT formulas. It has been already observed on the 16^4 lattice in [1] that the $\mathcal{O}(a)$ lattice artifacts at our gauge coupling $\beta = 5.1$, corresponding to a lattice spacing $a \simeq 0.2\,\mathrm{fm}$, are small and one can obtain reasonable fits by omitting them. This conclusion is strengthened by the new $16^3 \cdot 32$ data and, therefore, here we based our estimates of the chiral Lagrangian parameters on fits with the continuum formulas.

The use of the ratios of the PCAC quark mass as the variable in comparing the simulation data to chiral perturbation theory is essential. Taking other quark mass definitions, for instance $\mu_{ren} \equiv Z_m(\mu_0 - \mu_{cr})$, would be the source of large lattice artifacts at our lattice spacing.

The sea quark mass dependence of f_π and m_π^2/m_q can be well described in our quark mass range $0.855 \le M_r \le 2.13$, which roughly corresponds to $\frac{1}{4}m_s \le m_q \le \frac{2}{3}m_s$, by the NLO ChPT formulas. The obtained estimates of the relevant Gasser-Leutwyler constants are, according to Sect. 2,

$$\frac{\Lambda_3}{f_0} = 8.21(27), \qquad\qquad \frac{\Lambda_4}{f_0} = 21.4(1.5). \tag{29}$$

The functional dependence of the ratio of f_π as a function of the ratio of quark masses clearly shows the presence of chiral logarithms (see Fig. 1). This observation is in agreement with the results in a recent paper of the UKQCD Collaboration [23], which came out during the writing of this paper.

In the valence quark mass dependence of the same quantities, in addition to the NLO terms, the higher order NNLO contributions appear to be important – especially at our two larger sea quark masses. But, as shown by Fig. 3, the importance of the NNLO terms is considerably reduced at the two lighter sea quark masses. Our best estimates for the relevant Gasser-Leutwyler constants at the scale $4\pi f_0$ are, according to (23).

$$\alpha_5 = 2.06(42), \qquad\qquad 2\alpha_8 - \alpha_5 = 0.583(45). \tag{30}$$

The errors quoted in (29) and (30) are only the statistical ones. In order to decrease the systematic errors, simulations at still smaller sea quark masses would be useful. Because our lattice volume is relatively large ($L \simeq 3\,\mathrm{fm}$), finite volume effects can be expected to be small (see [24, 25]). For the moment, we have no direct handle on the magnitude of the remaining nonzero lattice spacing effects. These should be determined by performing simulations at smaller lattice spacings.

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