

## SU(2) and SU(3) chiral perturbation theory analyses on meson and baryon masses in 2+1 flavor lattice QCD

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We investigate the quark mass dependence of meson and baryon masses obtained from 2+1 flavor dynamical quark simulations performed by the PACS-CS Collaboration. With the use of SU(2) and SU(3) chiral perturbation theories up to NLO, we examine the chiral behavior of the pseudoscalar meson masses and the decay constants in terms of the degenerate up-down quark mass ranging from 3 MeV to 24 MeV and two choices of the strange quark mass around the physical value. We discuss the convergence of the SU(2) and SU(3) chiral expansions and present the results for the low energy constants. We find that the SU(3) expansion is not convergent at NLO for the physical strange quark mass. The chiral behavior of the nucleon mass is also discussed based on the SU(2) heavy baryon chiral perturbation theory up to NNLO. Our results show that the expansion is well behaved only up to  $m_\pi^2 \approx 0.2 \text{ GeV}^2$ .

*The XXVI International Symposium on Lattice Field Theory*

July 14 - 19, 2008

Williamsburg, Virginia, USA

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## 1. Introduction

The PACS-CS Collaboration has been performing  $N_F = 2 + 1$  lattice QCD simulation with the nonperturbatively  $O(a)$ -improved Wilson quarks and the Iwasaki gauge action at the lattice spacing of  $a = 0.09$  fm on a  $(2.9 \text{ fm})^3$  box[1, 2, 3, 4]. The DDHMC algorithm armored with several improvements allows simulations in the light quark mass region, where the resulting pseudoscalar meson mass is down to 156 MeV. In this report we focus on chiral analyses of our data based on chiral perturbation theory (ChPT). We apply the SU(2) and SU(3) ChPTs up to NLO to the pseudoscalar meson masses and the decay constants for the pion mass ranging from 156 MeV to 411 MeV. The finite size effects are taken into account at one-loop level of the ChPTs. We also examine the quark mass dependence of the nucleon mass employing the SU(2) heavy baryon ChPT up to NNLO. The simulation details are given in separated reports[1, 3].

## 2. Simulation parameters

We employ the  $O(a)$ -improved Wilson quark action with a nonperturbative improvement coefficient  $c_{\text{SW}} = 1.715$  and the Iwasaki gauge action at  $\beta = 1.9$ , corresponding to the lattice spacing of  $a = 0.09$  fm, on a  $32^3 \times 64$  lattice. Simulation parameters are summarized in Table 1, where the pion mass and the quark masses are given at each combinations of  $\kappa_{\text{ud}}$  and  $\kappa_{\text{s}}$ . The quark masses are renormalized perturbatively in the  $\overline{\text{MS}}$  scheme at the scale of  $1/a$ . The statistics of each ensemble is given by the Molecular Dynamics (MD) time.

**Table 1:** Summary of pion mass and quark masses perturbatively renormalized in the  $\overline{\text{MS}}$  scheme at the scale of  $1/a$ .

$\kappa_{\text{ud}}$	$\kappa_{\text{s}}$	$m_{\pi}$	$m_{\text{ud}}^{\overline{\text{MS}}}[\text{MeV}]$	$m_{\text{s}}^{\overline{\text{MS}}}[\text{MeV}]$	MD time
0.13781	0.13640	156	3.5	87	990
0.13770	0.13640	296	12	90	2000
0.13754	0.13640	411	24	92	2250
0.13727	0.13640	570	45	97	2000
0.13700	0.13640	702	67	103	2000
0.13754	0.13660	385	21	77	2000

## 3. SU(2) and S(3) ChPT analyses for the pseudoscalar meson sector

In principle our results should be compared with the predictions of the Wilson ChPT[5]. However, their expressions in terms of the AWI quark masses agree with those of the continuum ChPT up to NLO by a redefinition of the low energy constants (LEC)[1]. We then discuss our results based on the continuum ChPT.

### 3.1 SU(3) ChPT

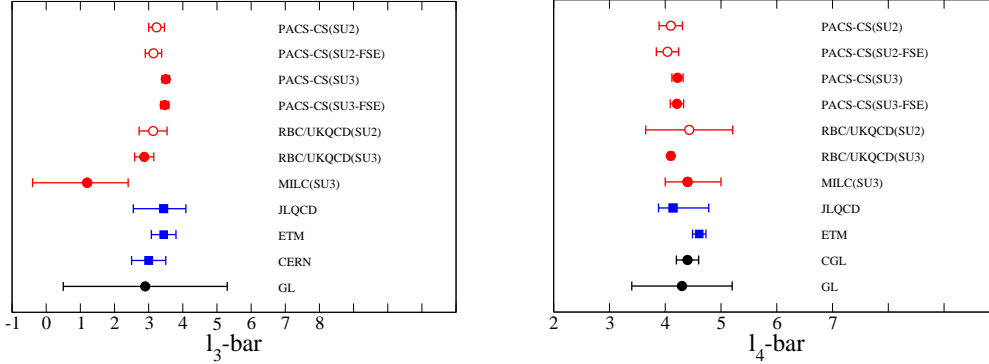
In the continuum SU(3) ChPT the one-loop expressions for  $m_{\pi}$ ,  $m_K$ ,  $f_{\pi}$ ,  $f_K$  contain six unknown LECs,  $B_0, f_0, L_4, L_5, L_6, L_8$ . We determine these parameters by applying a simultaneous

fit to  $m_\pi/2m_{\text{ud}}, m_K^2/\{m_{\text{ud}} + m_s\}, f_\pi, f_K$ , where the finite size corrections are taken into account at one-loop level[6].

The results for the LECs are listed in Table 2 where the phenomenological estimates with experimental inputs[7], the RBC/UKQCD results[8] and the MILC results[9] are also presented for comparison. We spot some discrepancies for the central values for the results of  $L_{4,5,6,8}$ . Large errors make it difficult to draw any conclusions. We instead make a comparison in terms of the SU(2) LECs obtained by the conversion from the SU(3) ones. This is shown in Fig. 1. Our results are  $\bar{l}_3 = 3.47(11)$ ,  $\bar{l}_4 = 4.21(11)$  and  $\bar{l}_3 = 3.50(11)$ ,  $\bar{l}_4 = 4.22(10)$  with and without the finite size corrections, respectively. Except for the MILC result for  $\bar{l}_3$ , all results are reasonably consistent.

**Table 2:** Results for the LECs in comparison with the phenomenological estimates, the RBC/UKQCD results and the MILC results.

	w/o FSE	w/ FSE	phenomenology	RBC/UKQCD	MILC
$L_4$	-0.04 (10)	-0.06(10)	0.0 (0.8)	0.139 (80)	0.1 (3) $\begin{pmatrix} +3 \\ -1 \end{pmatrix}$
$L_5$	1.43 (7)	1.45 (7)	1.46(10)	0.872 (99)	1.4 (2) $\begin{pmatrix} +2 \\ -1 \end{pmatrix}$
$2L_6 - L_4$	0.10 (2)	0.10 (2)	0.0 (1.0)	-0.001 (42)	0.3 (1) $\begin{pmatrix} +2 \\ -3 \end{pmatrix}$
$2L_8 - L_5$	-0.21 (3)	-0.21 (3)	0.54 (43)	0.243 (45)	0.3 (1) (1)
$\chi^2/\text{dof}$	4.2(2.7)	4.4(2.8)	—	0.7	—

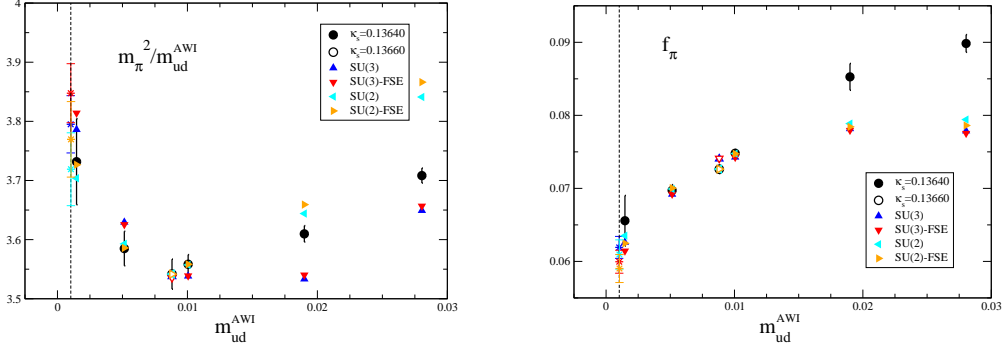


**Figure 1:** Comparison of the results for  $\bar{l}_3$  and  $\bar{l}_4$ . Black symbols denote the phenomenological estimates[10, 11]. Blue ones are for 2 flavor results[12, 13, 14]. Red closed(open) symbols represent the results for the SU(3) (SU(2)) ChPT analyses in 2+1 flavor dynamical simulations[9, 8].

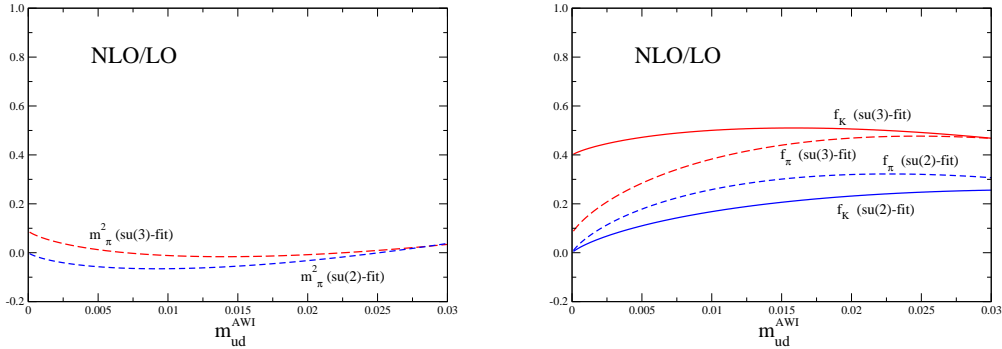
Although we find that the SU(3) ChPT fit gives reasonable values for the LECs, the value of  $\chi^2/\text{dof}$  is unacceptably large. In Fig.2 we plot the fit results for  $m_\pi^2/m_{\text{ud}}$  and  $f_\pi$ . The strange quark mass dependence between the data at  $(\kappa_{\text{ud}}, \kappa_s) = (0.13754, 0.13640)$  and  $(0.13754, 0.13660)$  is not well described. This flaw is the main cause for the large  $\chi^2/\text{dof}$ .

In order to investigate the origin of the discrepancy, we compare the NLO contributions with the LO ones in Fig. 3. While the NLO is at most 10% of the LO for the pion mass, the ratio is much larger for the decay constants, *e.g.*, for  $f_\pi$  it rapidly increases from 10% at  $m_{\text{ud}} = 0$  to 30% around  $m_{\text{ud}} = 0.01$ . The situation is worse for  $f_K$ : The NLO contribution is about 40% of the LO one even at  $m_{\text{ud}} = 0$ , most of which stems from the loops containing the strange quark. These observations

mean that the physical strange quark mass is not small enough to be well controlled up to NLO in the SU(3) ChPT.



**Figure 2:** Fit results for  $(am_\pi)^2/(am_{ud}^{AWI})$  (left) and  $f_\pi$  (right). The black symbols represent the lattice results. The red and blue triangles denote the SU(3) fit results plotted at the measured quark masses. The cyan and orange ones are for the SU(2) case. The open and filled symbols distinguish the results at  $\kappa_s = 0.13640$  and  $0.13660$ . The star symbols represent the extrapolated values at the physical point denoted by the vertical dotted line.



**Figure 3:** Ratio of the NLO contribution to the LO one in the ChPT expansions for the pion mass and the pseudoscalar meson decay constants. The strange quark mass is fixed at the physical value.

### 3.2 SU(2) ChPT

Instead of extending the SU(3) chiral expansions from NLO to NNLO, we employ the SU(2) ChPT up to NLO for further chiral analyses without increasing the data points. Our strange quark mass is close enough to the physical value to allow us an analytic expansion of the SU(2) LECs around the physical strange quark mass.

For  $m_\pi$  and  $f_\pi$  we employ the SU(2) ChPT formulae where the low energy constants  $B$  and  $f$  are linearly expanded in terms of the strange quark mass:  $B = B_s^{(0)} + m_s B_s^{(1)}$  and  $f = f_s^{(0)} + m_s f_s^{(1)}$ . The K meson is treated as a matter field in the isospin 1/2 linear representation of the SU(2) chiral transformation, which is coupled to the pions in an SU(2) invariant way. This assumption leads to

**Table 3:** Cutoff, quark masses and pseudoscalar meson decay constants determined with  $m_\pi, m_K, m_\Omega$  as physical inputs. Quark masses are renormalized in the  $\overline{\text{MS}}$  scheme at the scale of 2 GeV.

	w/o FSE	w/ FSE		w/o FSE	w/ FSE	experiment
$a^{-1}$ [GeV]	2.176 (31)	2.176 (31)	$f_\pi$	132.6 (4.5)	134.0 (4.2)	$130.7 \pm 0.1 \pm 0.36$
$m_{\text{ud}}^{\overline{\text{MS}}}$ [MeV]	2.509 (46)	2.527 (47)	$f_K$	159.2 (3.2)	159.4 (3.1)	$159.8 \pm 1.4 \pm 0.44$
$m_s^{\overline{\text{MS}}}$ [MeV]	72.74 (78)	72.72 (78)	$f_K/f_\pi$	1.201 (22)	1.189 (20)	1.223 (12)
$m_s/m_{\text{ud}}$	29.0 (4)	28.8 (4)				

the following fit formulae for  $m_K$  and  $f_K$ :

$$m_K^2 = \bar{m}_K^2 + \beta_m m_{\text{ud}}, \quad f_K = \bar{f} \left\{ 1 + \beta_f m_{\text{ud}} - \frac{3}{4} \frac{2Bm_{\text{ud}}}{16\pi^2 f^2} \ln \left( \frac{2Bm_{\text{ud}}}{\mu^2} \right) \right\}, \quad (3.1)$$

where  $\bar{m}_K^2$  and  $\bar{f}$  are also linearly expanded in terms of the strange quark mass:  $\bar{m}_K^2 = \alpha_m + \gamma_m m_s$  and  $\bar{f} = \bar{f}_s^{(0)} + m_s \bar{f}_s^{(1)}$ .

We apply a simultaneous fit to  $m_\pi^2/2m_{\text{ud}}, f_\pi$  and  $f_K$  and an independent fit to  $m_K^2$ . Evaluating the finite size effects based on the NLO formulae of the SU(2) ChPT for  $m_\pi$  and  $f_\pi$ , we obtain

$$m_{\text{ud}}^{\text{ph}} B = 0.009345(27) \text{GeV}^2, \quad f = 124.8(51) \text{MeV}, \quad \bar{l}_3 = 3.23(21), \quad \bar{l}_4 = 4.10(20), \quad (3.2)$$

without taking into account finite size effects, and

$$m_{\text{ud}}^{\text{ph}} B = 0.009332(26) \text{GeV}^2, \quad f = 126.4(47) \text{MeV}, \quad \bar{l}_3 = 3.14(23), \quad \bar{l}_4 = 4.09(19), \quad (3.3)$$

including finite size effects, where  $m_{\text{ud}}^{\text{ph}}$  is the up-down quark mass extrapolated to the physical point. The results for  $\bar{l}_3$  and  $\bar{l}_4$  are plotted in Fig. 1 for comparison. All the lattice results reside in the range  $3.0 \lesssim \bar{l}_3 \lesssim 3.5$  and  $4.0 \lesssim \bar{l}_4 \lesssim 4.5$  except the MILC result for  $\bar{l}_3$ .

The fit results for  $m_\pi^2/2m_{\text{ud}}$  and  $f_\pi$  are plotted in Fig.2. In the SU(2) case we do not observe any discrepancy around  $am_{\text{ud}} = 0.01$ . The resulting  $\chi^2/\text{dof}$  are 0.43(77) and 0.33(68) with and without the finite size corrections, respectively. These numbers are an order of magnitude smaller than the SU(3) case. In Fig.3 we illustrate the relative magnitude of the NLO contribution to the LO one in comparison with the SU(3) case. The convergences of the SU(2) chiral expansions for  $m_\pi$  and  $f_\pi$  are clearly better than the SU(3) case.

### 3.3 Results for physical quark masses and pseudoscalar decay constants

The up-down and the strange quark masses and the lattice cutoff are determined with the choice of  $m_\pi, m_K, m_\Omega$  as physical inputs. We employ the SU(2) ChPT for the chiral analysis on  $m_\pi$  and  $m_K$  as discussed in the above subsection. For the  $\Omega$  baryon we use a simple linear fit formula  $m = \alpha + \beta m_{\text{ud}} + \gamma m_s$ .

In Table 3 we summarize the results for the quark masses, the lattice cutoff and the pseudoscalar meson decay constants together with the experimental values. Our results for the quark masses are smaller than the estimates obtained by recent 2+1 flavor lattice QCD simulations[9, 8]. We note, however, that we employ the perturbative renormalization factors at one-loop level which should contain an uncertainty. For the decay constants we observe a good consistency between our results and the experimental values within the error of 2 – 3%. Here also one-loop perturbative results for the renormalization factors are used. We note that work is in progress to determine the renormalization factors non-perturbatively using the Schrödinger functional [15].

#### 4. SU(2) ChPT analysis for nucleon mass

For the nucleon mass we employ the SU(2) heavy baryon ChPT formula upto NNLO[16]:

$$\begin{aligned}
 m_N = & m_0 - 4c_1 m_\pi^2 - \frac{6g_A^2}{32\pi f_\pi^2} m_\pi^3 \\
 & + \left[ e_1(\mu) - \frac{6}{64\pi^2 f_\pi^2} \left( \frac{g_A^2}{m_0} - \frac{c_2}{2} \right) - \frac{6}{32\pi^2 f_\pi^2} \left( \frac{g_A^2}{m_0} - 8c_1 + c_2 + 4c_3 \right) \ln \frac{m_\pi}{\mu} \right] m_\pi^4 \\
 & + \frac{6g_A^2}{256\pi f_\pi^2 m_0^2} m_\pi^5 + O(m_\pi^6),
 \end{aligned} \tag{4.1}$$

which contains six new low energy constants  $m_0, c_1, c_2, c_3, g_A, e_1$ . The  $O(m_\pi^5)$  term which is obtained by the relativistic baryon ChPT[17] gives only a small contribution so that the results are little affected in the following analyses.

Since the number of our lattice data points is not sufficient for a full determination of the LECs by the ChPT fit, we choose to fit  $m_0, c_1, e_1$  while  $g_A, f_\pi, c_2, c_3$  are fixed at the phenomenologically viable values. Following Ref. [18] we set  $g_A = 1.267$ ,  $c_2 = 3.2 \text{ GeV}^{-1}$  and consider two possibilities for  $c_3$ :  $c_3 = -3.4 \text{ GeV}^{-1}$  as fit-A and  $c_3 = -4.7 \text{ GeV}^{-1}$  as fit-B. For  $f_\pi$  we use the pion decay constant extrapolated at the chiral limit with the SU(2) ChPT fit. We take two fit ranges for the data series with  $\kappa_s = 0.13640$ : Range-I is for  $0.13781 \leq \kappa_{\text{ud}} \leq 0.13727$  and range-II for  $0.13781 \leq \kappa_{\text{ud}} \leq 0.13700$ . The fit results are depicted in Fig. 4. We find that the lattice results are remarkably well described up to  $m_\pi^2 = 0.5 \text{ GeV}^2$ . Table 4 summarizes the results for the LECs together with the QCDSF/UKQCD results for comparison. The nucleon sigma term is also obtained through  $\sigma_{N\pi} = m_\pi^2 (\partial m_N / \partial m_\pi^2)$ . All the results are compatible within the  $2\sigma$  errors.

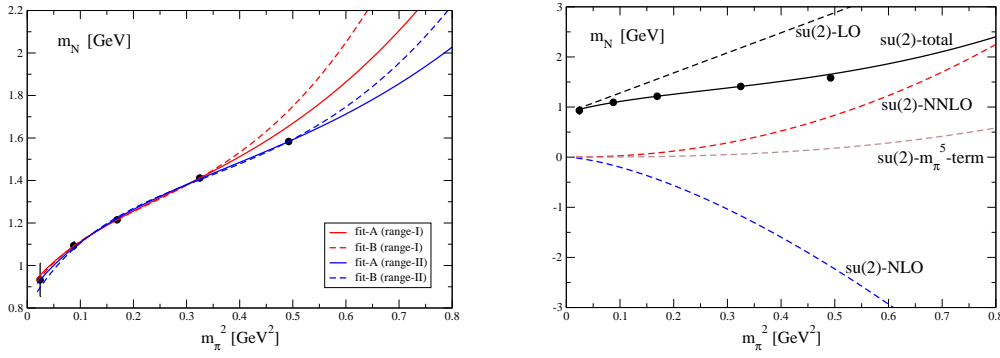
In Fig. 4 we separately draw the contribution of the LO, NLO, NNLO and  $O(m_\pi^5)$  terms in the chiral expansion. Observe that there is a drastic cancellation between the LO and NLO contributions which are both large in magnitude, and that the NNLO contribution monotonically increases as  $m_\pi$  becomes heavier. The convergence of chiral expansion in the SU(2) heavy baryon ChPT is hardly controlled beyond  $m_\pi^2 \sim 0.2 \text{ GeV}^2$ .

	range-I		range-II		QCDSF-UKQCD	
	fit-A	fit-B	fit-A	fit-B	fit-A	fit-B
$m_0$ [GeV]	0.880 (50)	0.855 (47)	0.850 (27)	0.795 (27)	0.89 (6)	0.76 (6)
$c_1$ [GeV <sup>-1</sup> ]	-1.00 (10)	-1.19 (10)	-1.08 (4)	-1.34 (4)	-0.93 (5)	-1.25 (5)
$e_1(1\text{GeV})$ [GeV <sup>-3</sup> ]	3.7 (1.4)	4.2 (1.4)	2.9 (4)	2.4 (3)	2.8 (0.4)	1.7 (0.5)
$\chi^2/\text{dof}$	0.1 (0.9)	0.0 (0.5)	0.3 (0.9)	1.2 (1.6)		
$\sigma_{N\pi}$ [MeV]	51.4 (7.6)	60.1 (7.3)	56.8 (2.7)	70.8 (2.6)		

**Table 4:** Results for  $m_0, c_1, e_1$  together with the QCDSF/UKQCD results.

#### Acknowledgment

Numerical calculations for the present work have been carried out on the PACS-CS computer under the ‘‘Interdisciplinary Computational Science Program’’ of Center for Computational Sciences, University of Tsukuba. This work is supported in part by Grants-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology (Nos. 16740147,



**Figure 4:** Fit results of the nucleon mass using the SU(2) heavy baryon ChPT formula (left) and each contribution of the LO, NLO, NNLO and  $O(m_\pi^5)$  terms in the case of fit-A with range-I (right).

17340066, 18104005, 18540250, 18740130, 19740134, 20340047, 20540248, 20740123, 20740139 ).

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