

Leading order mesonic and baryonic SU(3) low energy constants from $N_f = 3$ lattice QCD

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We determine the leading order mesonic (B_0 and F_0) and baryonic (m_0 , D and F) SU(3) chiral perturbation theory low energy constants from lattice QCD. We employ gauge ensembles with $N_f = 3$ (i.e., $m_u = m_d = m_s$) nonperturbatively improved Wilson fermions at six distinct values of the lattice spacing in the range $a \approx (0.039\text{--}0.098)$ fm, which constitute a subset of the coordinated lattice simulations (CLS) gauge ensembles. The pseudoscalar meson mass M_π ranges from around 430 MeV down to 240 MeV and the linear spatial lattice extent L from $6.4M_\pi^{-1}$ to $3.3M_\pi^{-1}$, where $LM_\pi \geq 4$ for the majority of the ensembles. This allows us to perform a controlled extrapolation of all the low energy constants to the chiral, infinite volume and continuum limits. We find the SU(3) chiral condensate and F_0 to be smaller than their SU(2) counterparts while the Gell-Mann–Oakes–Renner parameters $B_0 \approx B$ are similar. Regarding baryonic LECs, we obtain $F/D = 0.612^{(14)}_{(12)}$.

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I. INTRODUCTION

Chiral perturbation theory (ChPT) is a central tool for the description and understanding of a multitude of hadronic processes. In this context, the interplay between ChPT and lattice simulations of QCD is of particular interest: while in Nature the quark masses are fixed, in lattice simulations these (and other simulation parameters) can be varied and the precision and the range of validity of truncated ChPT expansions explored systematically. Moreover, some of the low energy constants (LECs) of this effective field theory can be constrained or determined from lattice data, which complements phenomenological fits to experimental data that are restricted to the physical quark mass point. Vice versa, ChPT augments lattice QCD simulations, providing parametrizations of the dependence of the results on the light quark masses and the simulation volume that are

consistent with the dynamical breaking of chiral symmetry as well as with the global symmetries of QCD in the massless limit.

While the light pseudoscalar masses, decay constants, the chiral condensate and related mesonic quantities have been well explored in lattice QCD simulations and confronted with SU(2) ChPT predictions—see, e.g., the recent Flavour Lattice Averaging Group (FLAG) review [1]—this is less so regarding baryonic observables. On the one hand, the lattice data are less precise for baryons, in particular toward small values of the quark masses. On the other hand, the number of independent LECs is larger and also the convergence properties of ChPT may be inferior in the baryonic sector. For instance, the mass gaps between octet and decuplet baryons are smaller than those between pseudoscalar mesons and vector meson resonances, which may necessitate the inclusion of decuplet baryons as explicit degrees of freedom, at least for some observables. Including hyperons, i.e., the Λ , the Σ and the Ξ , into the ChPT analysis, in addition to the nucleon N (or the N and the Δ resonance), provides a wealth of additional information, whereas the number of baryonic LECs of flavor SU(3) ChPT increases only moderately relative to SU(2) ChPT. This makes SU(3) ChPT a particularly popular choice in the description of processes that involve baryons. One concern regarding phenomenological applications, however, is the convergence of SU(3) ChPT at the physical point itself, where neither the mass $M_{\eta_8} \approx (\frac{4}{3}M_K^2 - \frac{1}{3}M_\pi^2)^{1/2} \approx 565$ MeV

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of the would-be η_8 pseudoscalar meson, the kaon mass $M_K \approx 494$ MeV nor the average light meson mass $\bar{M} = (\frac{2}{3}M_K^2 + \frac{1}{3}M_\pi^2)^{1/2} \approx 411$ MeV are particularly small in comparison to the chiral symmetry breaking scale $\Lambda_\chi := 4\pi F_0 < 4\pi F_\pi \approx 1160$ MeV. While this may limit the practical applicability of SU(3) ChPT regarding some observables, the corresponding LECs are well defined and can in principle be obtained from lattice QCD.

Within most lattice simulations of $N_f = 2 + 1$ (or of $N_f = 2 + 1 + 1$) QCD the mass of the light quark $m_\ell = m_u = m_d$ is varied while that of the strange quark m_s is kept approximately fixed near its physical value. In a few cases, instead $\text{tr}M = m_u + m_d + m_s$ is kept constant [2–5]. The former setting is ideal regarding SU(2) ChPT while neither choice is sufficient to determine SU(3) LECs, unless other quark mass combinations are added; in particular, one may want to reduce the trace of the mass matrix $\text{tr}M$ below its physical value. This can be achieved via a partially quenched strategy, see, e.g., Refs. [6–8], or, ideally, by realizing additional sea quark mass combinations [9,10].

So far no comprehensive lattice QCD investigation of SU(3) ChPT exists, that includes pion masses smaller than 300 MeV or addresses the continuum limit—neither for mesons nor for baryons. Here we start to close this gap with a consistent, simultaneous analysis of several observables within the framework of SU(3) ChPT: we are in the process of computing the masses M_P ($P \in \{\pi, K, \eta_8\}$) and m_B ($B \in \{N, \Lambda, \Sigma, \Xi\}$) of the light pseudoscalar mesons and baryons as well as the corresponding decay constants F_P and axial charges g_A^B from $N_f = 2 + 1$ QCD at many points in the plane spanned by the quark masses $m_\ell = m_u = m_d$ and m_s at several values of the lattice spacing a .

Here we present first results, obtained on $N_f = 3$ mass-degenerate gauge ensembles for the leading order (LO) mesonic LECs F_0 and B_0 and baryonic LECs m_0 , D and F , where D and F also enter the dependence of the octet baryon masses on the pseudoscalar meson masses at order p^3 [next-to-leading order (NLO) of heavy baryon ChPT (HBChPT) or next-to-next-to-leading order (NNLO) of covariant baryon ChPT (BChPT)]. We remark that for $m_\ell = m_s$ all the octet baryons masses are degenerate, however, this is not so for the nonflavor singlet axial charges, where two independent combinations exist. The main quantity that determines the convergence properties of ChPT is the squared average pseudoscalar mass \bar{M}^2 . The value realized in Nature corresponds to our largest quark mass values and we cover a range in \bar{M}^2 that extends down to less than one third of that: if SU(3) ChPT is applicable at the physical quark mass point then it should also apply to our lattice data, in the continuum limit.

The reliable determination of LO LECs from an extrapolation to the chiral limit requires at least NLO ChPT. Naturally, it is *a priori* unknown whether higher order ChPT may be required within the window of available pseudoscalar masses or if ChPT is applicable at all.

Including higher orders is of limited practicability in view of the finite number of data points and their statistical errors, due to the exploding number of new LECs. However, simultaneously analysing a number of different quantities that should be sensitive to the same set of LECs like baryon masses and their axial charges can serve as a consistency check and reduces the parametric uncertainty. Here we attempt exactly this, albeit only for the LO LECs. Previous analyses of lattice QCD data that aimed at determining LECs focused on one type of observable at a time. Ideally, however, one would wish to confirm that the same set of LECs can be employed consistently across a range of quantities.

This article is organized as follows. In Sec. II we collect all SU(3) ChPT expressions for the quark mass and volume dependence that are relevant for our analysis, restricting ourselves to the special case $m_\ell = m_s$. For completeness, additional expressions for the baryon mass and the axial charges are collected in Appendix A. Then, in Sec. III, we discuss properties of the gauge ensembles employed, the analysis methods used, the nonperturbative renormalization and improvement of the pseudoscalar decay constant and the axial charges as well as our continuum and chiral limit extrapolation strategy. The determination of systematic errors through a model averaging procedure is detailed in Appendix B. Finally, in Sec. IV we determine and discuss the LECs, before we conclude.

II. MESON AND BARYON SU(3) ChPT EXPRESSIONS

A. Infinite volume

Throughout this article the isospin limit $m_\ell = m_u = m_d$ is assumed and only the SU(3) symmetric case $m := m_\ell = m_s$ is considered. Our aim is to determine the LO mesonic (B_0 and F_0) and baryonic (m_0 , D and F) SU(3) ChPT LECs. The ChPT expressions in which these LECs appear are conveniently expressed in terms of the quark mass-dependent variables

$$x = \frac{2mB_0}{(4\pi F_0)^2}, \quad \xi = \frac{M_\pi^2}{(4\pi F_0)^2}, \quad \mathcal{L} = \log\left(\frac{M_\pi^2}{\mu^2}\right), \quad (1)$$

where M_π denotes the pseudoscalar meson mass and $B_0 := \Sigma_0/F_0^2$ the Gell-Mann–Oakes–Renner (GMOR) parameter, whereas $\Sigma_0 := -\langle \bar{u}u \rangle|_{m=0} > 0$ and $F_0 := F_\pi|_{m=0}$ are the quark chiral condensate and the pseudoscalar decay constant, respectively, in the SU(3) chiral limit. The LO LECs do not depend on the scale μ . For the analysis of the mesonic case, it is convenient to set $\mu^{-2} = 8t_{0,\text{ch}}$, using the Wilson scale parameter t_0 [11] in the chiral limit. From $t_{0,\text{ch}}/t_0^* = 1.037(5)$ [12] and $(8t_0^*)^{-1/2} = 478(7)$ MeV [13], where t_0^* [4] is defined as the value of t_0 at the point where $12t_0^*M_\pi^2 = 1.11$ (and $m_\ell = m_s$), we obtain $\mu = 469(7)$ MeV.

At NNLO in SU(N_f) ChPT the corrections to the GMOR relation and the pion mass-dependence of the pseudoscalar decay constant [14–16] read

$$M_\pi^2 = 2B_0 m [1 + x(a_{10} + a_{11}\mathcal{L}) + x^2(a_{20} + a_{21}\mathcal{L} + a_{22}\mathcal{L}^2)], \quad (2)$$

$$F_\pi = F_0 [1 + x(b_{10} + b_{11}\mathcal{L}) + x^2(b_{20} + b_{21}\mathcal{L} + b_{22}\mathcal{L}^2)], \quad (3)$$

where

$$a_{11} = \frac{1}{N_f}, \quad a_{22} = \frac{9}{2N_f^2} - \frac{1}{2} + \frac{3N_f^2}{8}, \quad (4)$$

$$b_{11} = -\frac{N_f}{2}, \quad b_{22} = -\frac{1}{2} - \frac{3N_f^2}{16}. \quad (5)$$

While a_{10} , b_{10} , a_{21} and b_{21} are combinations of NLO LECs, a_{20} and b_{20} are combinations of NNLO LECs. Whereas NLO and possibly NNLO corrections may turn out necessary to describe our lattice data for which $430 \text{ MeV} \gtrsim M_\pi \gtrsim 240 \text{ MeV}$, it needs to be seen whether all of these LECs can be resolved, in addition to lattice spacing effects.

The LO octet baryonic LECs are the nucleon mass in the chiral limit m_0 and the couplings F and D which parameterize the octet axial charges in the SU(3) chiral limit and also enter within the chiral expansions of other octet baryon observables, in particular the masses. In the $N_f = 3$ flavor symmetric case at $\mathcal{O}(p^3)$ in BChPT the octet baryon mass m_B is given as [17,18]

$$m_B = m_0 + \bar{b}M_\pi^2 + 2\xi M_\pi \left(\frac{5D^2}{3} + 3F^2 \right) f_B(r) \quad (6)$$

with $\bar{b} = -6b_0 - 4b_D$ being a combination of NLO LECs and $r = M_\pi/m_0$. In the extended on-mass-shell (EOMS) scheme [18–20] the loop function is given as

$$f_B(r) = -2 \left[\sqrt{1 - \frac{r^2}{4}} \arccos\left(\frac{r}{2}\right) + \frac{r}{2} \log(r) \right], \quad (7)$$

where we follow the standard convention to identify the renormalization scale with m_0 . Expanding this function for small r , i.e., for $m_0 \rightarrow \infty$, one obtains the heavy baryon ChPT (HBChPT) limit [21,22] $f_B(r) = -\pi + \mathcal{O}(r)$. The EOMS BChPT expressions are also known at NNNLO [23], however, our present lattice data cannot constrain the additional free parameters.

Regarding the axial charges g_A^B , the pion mass dependence in the SU(3) case for the nucleon and the Σ baryon at $\mathcal{O}(p^3)$ is given as [24–26]

$$g_A^N = D + F + c_N \xi + \bar{c}_N \xi \log\left(\frac{M_\pi}{m_0}\right) + d_N \xi^{3/2}, \quad (8)$$

$$g_A^\Sigma = 2F + c_\Sigma \xi + \bar{c}_\Sigma \xi \log\left(\frac{M_\pi}{m_0}\right) + d_\Sigma \xi^{3/2}, \quad (9)$$

where the coefficients,

$$\bar{c}_N = - \left[3(D + F) + \frac{1}{3}(27D^3 + 25D^2F + 45DF^2 + 63F^3) \right], \quad (10)$$

$$\bar{c}_\Sigma = - \left[6F + \frac{2}{3}F(25D^2 + 63F^2) \right], \quad (11)$$

are entirely determined by the LO LECs. Above, $d_N = d_\Sigma = 0$, however, such terms arise naturally when loop corrections that contain decuplet baryons are included [27]. For completeness, we reference the corresponding expectations (as well as those for m_B) in Appendix A. Unfortunately, these expressions, involving the additional LECs Δ , \mathcal{C} and \mathcal{H} , do not satisfactorily describe our data on g_A^B while fits to m_B suggest $\mathcal{C} \approx 0$. Including the logarithmic terms, a reasonable fit quality seems only possible when also adding the above phenomenological d_B -terms. However, such fits give very small values for F and D , that are at variance with the pion mass-dependence of m_B . Leaving \bar{c}_B as free parameters, i.e., ignoring the ChPT expectation, the data even suggest $\bar{c}_B > 0$, opposite to the expectation of Eqs. (10) and (11). Similar tensions are evident also in recent data on g_A^N within SU(2) ChPT, see, e.g., Refs. [28–30]. We interpret this as a sign of large cancellations between pion and decuplet loop effects, a full understanding of which requires to further reduce the quark mass and/or to increase the ChPT order. For the purpose of determining the LO LECs and also in view of the precision of the lattice data, we will truncate Eqs. (8) and (9) at $\mathcal{O}(p^2)$.

B. Finite volume corrections

Since ChPT also predicts the finite volume dependence, we include the associated corrections. For the pseudoscalar meson mass and decay constant in the continuum limit the dependence on the linear spatial lattice extent L is given by [31,32]

$$M_\pi^2(L) = M_\pi^2 \left[1 + x \frac{1}{N_f} h(\lambda_\pi) + \dots \right], \quad (12)$$

$$F_\pi(L) = F_\pi \left[1 - x \frac{N_f}{2} h(\lambda_\pi) + \dots \right] \quad (13)$$

with $M_\pi = M_\pi(L = \infty)$, $F_\pi = F_\pi(L = \infty)$ and to this order we can substitute x for ξ . Above, $\lambda_\pi = LM_\pi$ and

$$h(\lambda) = 4 \sum_{\mathbf{n} \neq 0} \frac{K_1(\lambda|\mathbf{n}|)}{\lambda|\mathbf{n}|}, \quad (14)$$

where $\mathbf{n} \in \mathbb{Z}^3$ and $K_n(x)$ denotes the modified Bessel function of the second kind of order n . We will not consider two-loop finite volume effects [33,34] since these contain the NLO LECs.

For the octet baryon mass the SU(2) BChPT result [35,36] easily generalizes to SU(3):

$$m_B(L) = m_B + 4m_0\xi \left(\frac{5D^2}{3} + 3F^2 \right) \cdot \int_0^\infty dy \sum_{\mathbf{n} \neq 0} K_0 \left(\lambda_\pi |\mathbf{n}| \sqrt{1 - y + \frac{y^2}{r^2}} \right), \quad (15)$$

where we truncated the expression at $\mathcal{O}(p^3)$ and $r = M_\pi/m_0$ as above. Note that corrections to the baryon mass m_B due to transitions to decuplet baryons with the mass m_{D0} were first considered in Ref. [27]. For completeness, we collect the corresponding $m_\ell = m_s$ expectations in Appendix A.

In the case of the axial charges g_A^B , the finite volume corrections given in Appendix A have a sign opposite to the trend of the lattice data. It appears that—just like in the infinite volume case—the effect of decuplet baryons needs to be included, introducing three additional LECs which cannot be resolved at present. Therefore, we combine the infinite volume $\mathcal{O}(p^2)$ ChPT expectation with the dominant ChPT finite volume term

$$g_A^B(L) = g_A^B + c_V^B \xi \frac{\exp(-LM_\pi)}{\sqrt{LM_\pi}}, \quad (16)$$

where c_V^B is a free phenomenological coefficient.

III. LATTICE SETUP

We discuss the gauge ensembles used. Subsequently, we summarize our determination of the relevant observables, including—where applicable—their renormalization and order a improvement. We then list the results for the analyzed ensembles and detail our continuum, infinite volume and chiral extrapolation strategy.

A. Gauge ensembles

In our analysis we employ ensembles generated with $N_f = 3$ flavors of nonperturbatively $\mathcal{O}(a)$ -improved Wilson fermions with the tree-level Symanzik-improved gauge action. Most of the ensembles were produced within the coordinated lattice simulations (CLS) [3] effort. Here we only focus on the subset of ensembles with degenerate quark masses $m_u = m_d = m_s$.

The ensembles come with either periodic or open boundary conditions in time [37], where the latter choice is necessary at the two finest lattice spacings to circumvent

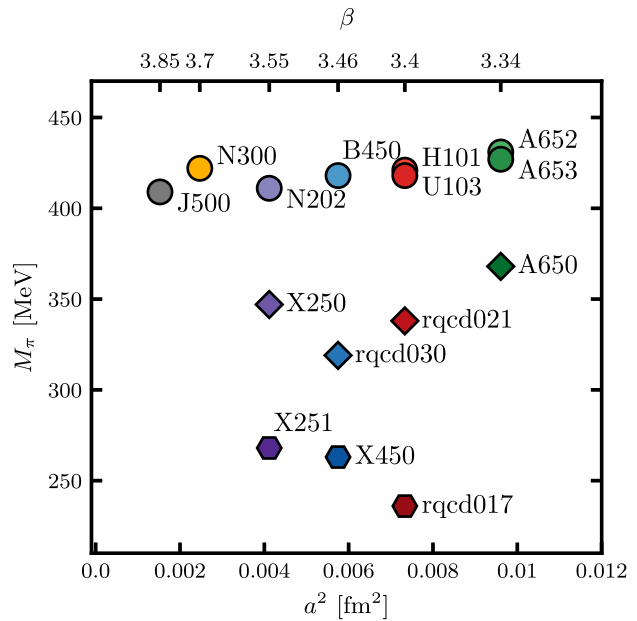


FIG. 1. The parameter landscape of the ensembles listed in Table I. The same color coding will be used throughout this article to identify the individual ensembles.

the freezing of the topological charge and thus to ensure ergodicity [38]. On ensembles with open boundary conditions measurements are taken far away from the boundaries, where translational symmetry in time is restored within statistical precision.

In total we analyzed fifteen ensembles where the simulated parameter space is illustrated in Fig. 1. More details can be found in Table I. We cover a range of six different lattice spacings $0.039 \text{ fm} \lesssim a \lesssim 0.098 \text{ fm}$, the pion masses range from around 430 MeV down to 240 MeV and volumes are realized between $3.3 \leq LM_\pi \leq 6.4$ where $LM_\pi \geq 4$ for the majority of the ensembles.

B. Analysis methods

The scale parameters t_0/a^2 and t_0^*/a^2 as well as the quark mass from the axial Ward identity (AWI), the pseudoscalar meson mass and the octet baryon mass have been obtained within an extensive RQCD analysis [12] of the light hadron spectrum on all the available CLS gauge ensembles. For the present purpose we only require these results for the subset of $m_\ell = m_s$ ensembles. Details on the computation of the two-point correlation functions $C_{2\text{pt}}(t)$, the extraction of the ground state masses and the statistical methods applied to account for autocorrelation effects and to compute covariance matrices between these quantities will be described in Ref. [12]. In Fig. 2 we show as an example the effective mass in lattice units for the nucleon

$$am_{\text{eff}}^N(t + a/2) = \log \left(\frac{C_{2\text{pt}}(t)}{C_{2\text{pt}}(t + a)} \right), \quad (17)$$

TABLE I. The gauge ensembles analyzed in this work. The rqcd xyz ensembles were generated by RQCD using the BQCD code [39], whereas all the other ensembles were generated within the CLS effort [3]. The fourth column labels periodic (p) and open (o) boundary conditions, respectively. The lattice spacings a were determined in Refs. [4,9,12].

Ensemble	β	a (fm)	Bc	$N_t \cdot N_s^3$	M_π (MeV)	LM_π	N_{config}
A652	3.34	0.098	p	$48 \cdot 24^3$	431	5.14	4995
A653			p	$48 \cdot 24^3$	427	5.09	2525
A650			p	$48 \cdot 24^3$	368	4.4	2328
H101	3.4	0.086	o	$96 \cdot 32^3$	421	5.85	2000
U103			o	$128 \cdot 24^3$	418	4.35	2475
rqcd021			p	$32 \cdot 32^3$	338	4.7	1541
rqcd017			p	$32 \cdot 32^3$	236	3.27	2468
B450	3.46	0.076	p	$64 \cdot 32^3$	418	5.15	1612
rqcd030			p	$64 \cdot 32^3$	319	3.94	1224
X450			p	$64 \cdot 48^3$	263	4.87	400
N202	3.55	0.064	o	$128 \cdot 48^3$	411	6.43	884
X250			p	$64 \cdot 48^3$	347	5.43	345
X251			p	$64 \cdot 48^3$	268	4.19	436
N300	3.7	0.05	o	$128 \cdot 48^3$	422	5.11	1520
J500	3.85	0.039	o	$192 \cdot 64^3$	409	5.2	751

together with the extracted ground state mass $am_N = am_B$, on the ensemble B450. $C_{2\text{pt}}(t)$ in this case is a baryonic two-point function. For this, the pion two-point function and the baryon three-point functions, we employ Wuppertal smearing [40] at the source and the sink, using spatially APE-smear [41] gauge transporters. The root mean squared quark smearing radii range from about 0.6 fm (for $M_\pi \approx 420$ MeV) up to about 0.75 fm (for $M_\pi \approx 230$ MeV), see Table 2 of Ref. [42].

The pion decay constant and the AWI quark mass are also obtained from two-point functions, using similar methods as for the pseudoscalar mass. However, in this case the two-point functions are only smeared at the source. We follow the strategy detailed in Refs. [43] and [44]. The calculation of the octet axial charges g_A^B for the nucleon and the Σ baryon is part of a long term project [10]. The baryon three-point functions $C_{3\text{pt}}(t, \tau, J)$, are computed

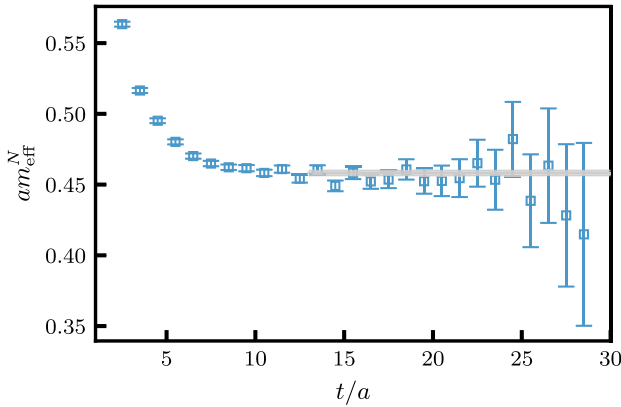


FIG. 2. Effective mass [see Eq. (17)] of the baryon on ensemble B450. The grey horizontal error band indicates the fit range and the extracted ground state mass.

using the sequential source method [45], (approximately) realizing four distinct source-sink separations $t/\text{fm} \in \{0.7, 0.8, 1.0, 1.2\}$ in order to control excited state contamination. The local current $J_{ud} = J_u - J_d$, where $J_q = \bar{q}\gamma_\mu\gamma_5 q$ is inserted at the time τ . Note that since $m_u = m_d$, no quark line-disconnected contributions appear. For definiteness with respect to the quark content we choose $N = p \sim uud$, $\Sigma = \Sigma^+ \sim uus$ and $\Xi = \Xi^0 \sim ssu$. Since the Cartan subgroup of SU(3) has rank two, in the case of exact SU(3) flavor symmetry ($m_\ell = m_s$) all the axial charges g_A^B can be written as combinations of just two fundamental charges \bar{F} and \bar{D} :

$$\begin{aligned} g_A^N &= \bar{F} + \bar{D}, & g_A^\Lambda &= 0, \\ g_A^\Sigma &= 2\bar{F}, & g_A^\Xi &= \bar{F} - \bar{D}. \end{aligned} \quad (18)$$

Here we choose g_A^N and g_A^Σ as our basis. The combinations

$$\bar{F} = \frac{1}{2} g_A^\Sigma \xrightarrow{m \rightarrow 0} F, \quad \bar{D} = g_A^N - \frac{1}{2} g_A^\Sigma \xrightarrow{m \rightarrow 0} D \quad (19)$$

approach the LECs F and D in the chiral limit.

The matrix element of interest for a baryon B can be obtained from a fit to the ratio of three-point over two-point functions

$$R^B(t, \tau, J_{ud}) = \frac{C_{3\text{pt}}^B(t, \tau, J_{ud})}{C_{2\text{pt}}^B(t)} \xrightarrow{t, \tau \rightarrow \infty} g_A^B, \quad (20)$$

see, e.g., Ref. [46], for details. As an example, we show in Fig. 3 for the ensemble N300 a simultaneous fit for $J \in \{J_u, J_d\}$,¹ to the ratios

¹We take the differences of a proton with spin-up and spin-down along the direction k .

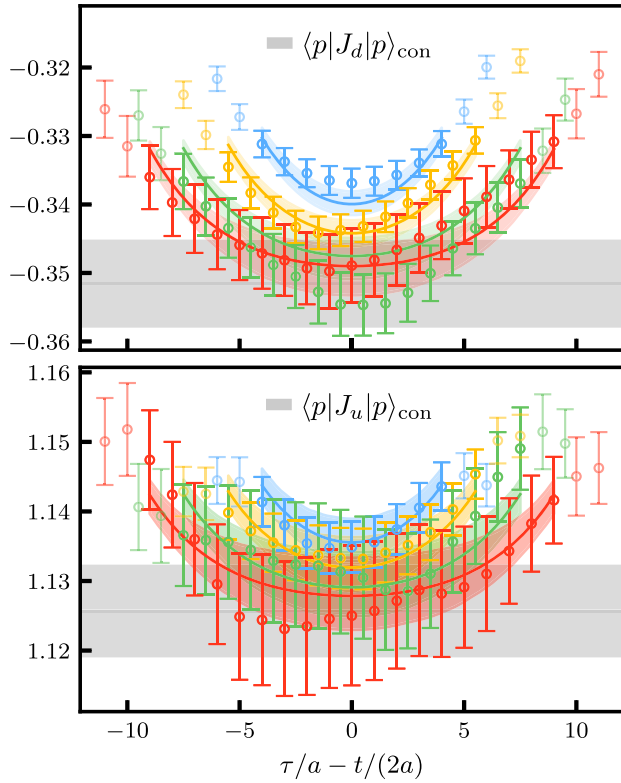


FIG. 3. Simultaneous fit to all four source-sink separations of the ratios for $\langle p|J_d|p \rangle_{\text{con}} = \bar{F} - \bar{D}$ and $\langle p|J_u|p \rangle_{\text{con}} = 2\bar{F}$ on the ensemble N300. Only the dark symbols are included in the fit. The grey band shows the ground state contribution and its error.

$$R_{\text{con}}^p(t, \tau, J) = b_{0,J} + b_{1,J} e^{-\Delta m t/2} \cosh(\Delta m(\tau - t/2)) + b_{2,J} e^{-\Delta m t} \quad (21)$$

for the proton, employing one and the same excited state mass gap Δm in both channels, where the subscript “con” indicates that we only consider the quark line-connected Wick contractions. Exploiting the fact that all the quarks are mass-degenerate, this gives the matrix elements $b_{0,J_u} = g_A^\Sigma = 2\bar{F}$ and $b_{0,J_d} = g_A^\Sigma - g_A^N = \bar{F} - \bar{D}$. The bootstrap error analysis is carried out using binned data with a bin size that is large compared to the integrated autocorrelation time, with the bootstraps matched to those of the other observables so that in the subsequent analysis all correlations can be taken into account.

C. Nonperturbative renormalization and improvement

The quark mass, the pion decay constant and the axial charges need to be renormalized. We also $\mathcal{O}(a)$ -improve these observables. Regarding the renormalization of the axial currents, we use the factors $Z_{A,\text{sub}}^i(g^2)$ of Ref. [47], obtained with the chirally rotated Schrödinger functional approach, as parametrized in their interpolation formula (C.7). The renormalization factor $Z_M(g^2) = Z_A(g^2)/Z_P(g^2)$, required to translate the AWI quark mass m^{AWI} into the

renormalization group invariant (RGI) [48,49] mass m , is given in Eq. (5.6) of Ref. [50]. We emphasize that both these factors have been computed entirely nonperturbatively. Using the improvement coefficients $b_A(g^2)$, $\tilde{b}_A(g^2)$, $b_P(g^2)$ and $\tilde{b}_P(g^2)$ [51], the observables can be renormalized and fully $\mathcal{O}(a)$ -improved at each value of the lattice coupling $g^2 = 6/\beta$ as follows:

$$m = Z_M[1 + am^{\text{latt}}(b_A - b_P + 3\tilde{b}_A - 3\tilde{b}_P)]m^{\text{AWI}}, \quad (22)$$

$$F_\pi = Z_A[1 + am^{\text{latt}}(b_A + 3\tilde{b}_A)]F_\pi^{\text{latt}}, \quad (23)$$

$$g_A^B = Z_A[1 + am^{\text{latt}}(b_A + 3\tilde{b}_A)]g_A^{B,\text{latt}}, \quad (24)$$

where $am^{\text{latt}} = (\kappa^{-1} - \kappa_{\text{crit}}^{-1})/2$ is the lattice quark mass, κ_{crit} is determined in Ref. [12] and we have assumed $m_\ell = m_s = \frac{1}{3}\text{tr}M$. The uncertainties of the renormalization factors and improvement coefficients are incorporated in the statistical analysis by means of pseudo-bootstrap distributions.

D. Lattice results

We will fit the squared pion mass M_π^2 and the pion decay constant F_π simultaneously as functions of the RGI quark mass m , whereas we parametrize the dependence of the baryon mass m_B and of the axial charges g_A^N and g_A^Σ in terms of the pion mass. Regarding the continuum limit extrapolation, the quantities t_0 and t_0^* are required, as described below in more detail. In Table II we summarize the corresponding results in lattice units for all the ensembles, with the exception of t_0^*/a^2 , listed in Table III, whose values are common to all ensembles that share the same gauge coupling. Note that no axial charges have been determined on the ensembles A652 and rqed017. However, ensemble A653 is very similar to A652 in terms of the simulation parameters while the rqed017 volume is rather small and finite volume effects can be substantial, in particular for the axial charges.

E. Extrapolation strategy

A reliable extraction of the LO SU(3) LECs in the chiral limit requires a chiral, infinite volume and continuum limit extrapolation. Ideally, one would carry out simultaneous fits to all the observables. In particular, the mesonic LEC F_0 also appears within the ChPT expansions of the baryonic observables. In principle, this is possible and we even have the full covariance matrices available between aM_π , am , aF_π , am_B , g_A^N and g_A^Σ , however, the former three observables are much more precise in terms of their statistical accuracy than the baryonic ones. Therefore, any impact of the baryonic results onto the mesonic LECs should be negligible and we opt for a two stage procedure, first determining the mesonic LECs and then using the resulting

TABLE II. Results for the ensembles used in this work. The scale parameter t_0/a^2 , the renormalized pion decay constant F_π (where $F_\pi = f_\pi/\sqrt{2}$), the pion mass M_π , the baryon mass m_B , the RGI quark mass m as well as the renormalized axial charges for the nucleon g_A^N and the Σ baryon g_A^Σ , respectively.

Ensemble	t_0/a^2	aF_π	aM_π	am_B	am	g_A^N	g_A^Σ
A652	2.1697(56)	0.04985(29)	0.2140(10)	0.5842(41)	0.02072(21)		
A653	2.1729(50)	0.04980(25)	0.21245(93)	0.5855(37)	0.02050(20)	1.1670(85)	0.8903(61)
A650	2.2878(72)	0.04598(36)	0.1835(13)	0.5469(54)	0.01547(21)	1.1489(94)	0.8822(74)
H101	2.8545(81)	0.04499(23)	0.18286(57)	0.5074(18)	0.01796(10)	1.1818(87)	0.9014(78)
U103	2.8815(57)	0.04386(57)	0.18158(60)	0.5193(30)	0.01745(10)	1.1334(74)	0.8692(72)
rqcd021	3.032(15)	0.04084(23)	0.14702(88)	0.4508(47)	0.01172(12)	1.1548(90)	0.873(12)
rqcd017	3.251(13)	0.03505(68)	0.1022(15)	0.388(13)	0.00548(21)		
B450	3.663(11)	0.03999(13)	0.16103(49)	0.4582(24)	0.016154(82)	1.1723(58)	0.8962(71)
rqcd030	3.914(15)	0.03535(18)	0.12221(68)	0.3957(90)	0.009460(80)	1.1437(89)	0.8723(70)
X450	3.9935(92)	0.03358(21)	0.10144(62)	0.3764(61)	0.006574(57)	1.175(10)	0.894(11)
N202	5.165(14)	0.03419(18)	0.13389(35)	0.3799(18)	0.013802(46)	1.1806(58)	0.9026(70)
X250	5.283(28)	0.03195(19)	0.11321(39)	0.3597(51)	0.009880(47)	1.1650(89)	0.8884(93)
X251	5.483(26)	0.02932(21)	0.08684(40)	0.3185(85)	0.005812(47)	1.165(13)	0.889(14)
N300	8.576(21)	0.02680(12)	0.10647(38)	0.3035(13)	0.011332(30)	1.1639(86)	0.884(17)
J500	14.013(40)	0.02106(11)	0.08119(34)	0.2313(26)	0.008755(21)	1.1514(50)	0.8873(84)

TABLE III. Values for t_0^*/a^2 for each β -value taken from [12].

β	3.34	3.4	3.46	3.55	3.7	3.85
$\frac{t_0^*}{a^2}$	2.219(7)	2.908(3)	3.709(3)	5.180(4)	8.634(10)	13.984(31)

value for $F_0/\sqrt{8t_{0,\text{ch}}}$ within the extraction of the baryonic LECs.

For the action, the axial current (needed for F_π , g_A^B and m) and the pseudoscalar current (needed for m), $\mathcal{O}(a)$ improvement is implemented nonperturbatively. Therefore, if we would simulate at a fixed lattice spacing a , we would have full $\mathcal{O}(a)$ improvement. However, instead we keep the unimproved, bare lattice coupling g^2 fixed which results in a correction term $\propto atrM$ for quantities aQ , that are measured in lattice units.² This term cancels when constructing dimensionless combinations $(\sqrt{8t_0}a^{-1})(aQ)$, using the scale parameter t_0/a^2 on the same ensemble. Therefore, to achieve full $\mathcal{O}(a)$ -improvement while varying the quark mass, we rescale all quantities $aQ \mapsto \sqrt{8t_0}Q$. This means that at the end of the analysis the dimensionful LECs m_0 , F_0 and B_0 will be obtained in units of $\sqrt{8t_{0,\text{ch}}}$, which can then be converted into physical units.

The continuum fit functions $X(\mathcal{M}, L, a=0)$, where $\mathcal{M} = \sqrt{8t_0}m$ and $\mathcal{M} = 8t_0M_\pi^2$, respectively, for mesonic observables $X \in \{8t_0M_\pi^2, \sqrt{8t_0}F_\pi\}$ and baryonic observables $X \in \{\sqrt{8t_0}m_B, g_A^N, g_A^\Sigma\}$, are summarized in Eqs. (1)–(9) and (12)–(16). Note that the dependence

²In fact this mass-dependent shift of the improved lattice coupling also affects the renormalization factors of the axial and pseudoscalar currents but this effect has been accounted for within the definition of the improvement coefficients \tilde{b}_A and \tilde{b}_P [51] of Eqs. (22)–(24).

$t_0 = t_{0,\text{ch}}[1 + k_1x + (k_{20} + k_{21}\mathcal{L})x^2 + \dots]$ [52] does not interfere with the universal ChPT logs and therefore neither the functional forms of the continuum formulas nor the LECs are affected by the rescaling of all dimensionful quantities in units of t_0 . Nevertheless, we remark that some of the higher order LECs, which we do not determine here, would require some knowledge about the LECs k_1 etc., that are associated with t_0 . Regarding the lattice spacing-dependence, we assume the factorization

$$X(\mathcal{M}, L, a) = X(\mathcal{M}, L, 0) \cdot \left[1 + \frac{a^2}{8t_0^*} (c_a^X + \bar{c}_a^X 8t_0 M_\pi^2) \right] \quad (25)$$

into the continuum parametrization times mass-independent and mass-dependent lattice spacing effects, where c_a^X and \bar{c}_a^X are independent fit parameters for each observable X .

We will estimate the systematic errors of the LECs by varying the fit model and by employing different cuts on the ensembles that enter the fit:

- (1) no cut: including all the available data points,
- (2) pion mass cut: excluding all ensembles with $M_\pi > 400$ MeV,
- (3) lattice spacing cut: excluding the coarsest lattice spacing, i.e., the ensembles with $a \approx 0.098$ fm,
- (4) volume cut: excluding all ensembles with $LM_\pi < 4$.

We then carry out the model averaging procedure described in Appendix B.

IV. RESULTS AND DISCUSSION

We determine the LO SU(3) mesonic LECs as well as the LO SU(3) octet baryonic LECs and compare the results with values from the literature.

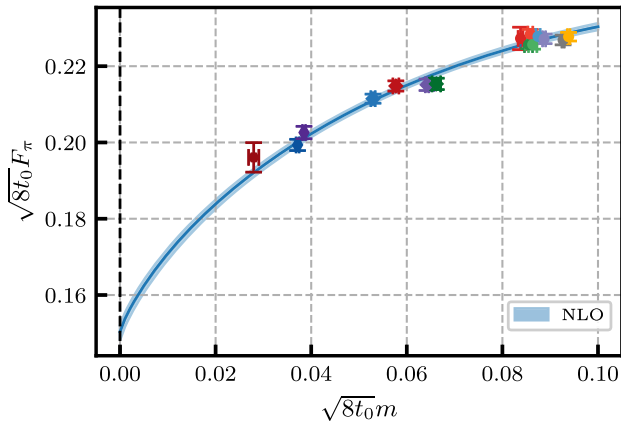


FIG. 4. Extrapolation of the pion decay constant F_π to the chiral limit. The data points are corrected for discretization and finite volume effects according to the parameters obtained from a combined fit to the pseudoscalar decay constant and mass on all the available data points employing the NLO ChPT ansatz. The blue band shows the NLO expression for the quark mass dependence.

A. Mesonic LECs

The LO mesonic LECs B_0 and F_0 are determined by simultaneous fits to the pseudoscalar mass and decay constant as functions of the quark mass, the volume and the lattice spacing as described above. The fits are carried out including the errors of and the correlations between the pion decay constant, the pseudoscalar mass and the quark mass within each ensemble. The resulting χ^2 -values are fully correlated.

Including only the mass-independent discretization terms of Eq. (25) and carrying out fits employing the NLO ChPT expressions, i.e., truncating the quark mass and the volume dependence at $\mathcal{O}(x)$, we are able to resolve all parameters reasonably well. Figures 4 and 5 illustrate the resulting quark mass-dependence of the pseudoscalar decay constant and the squared pion mass, respectively, from a combined fit to all the available data points. This fit to 30

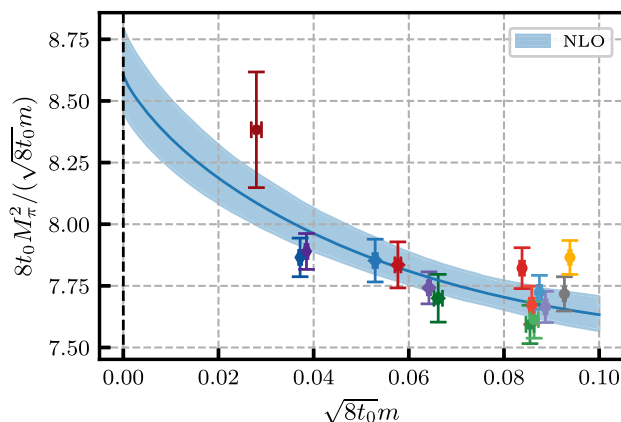


FIG. 5. The same as Fig. 4 for the ratio of the squared pion mass over the quark mass M_π^2/m .

TABLE IV. Results for the LO mesonic LECs F_0 and B_0 in units of $1/\sqrt{8t_{0,\text{ch}}} = 469(7)$ MeV obtained from fits to the NLO ChPT expression and different subsets of the parameter space spanned. The subsets are defined at the end of Sec. III E.

Fit	χ^2/N_{dof}	$\sqrt{8t_{0,\text{ch}}}F_0$	$\sqrt{8t_{0,\text{ch}}}B_0$
1	0.9322	0.1504(19)	4.302(81)
2	0.7146	0.1565(30)	4.10(14)
3	0.3444	0.1485(22)	4.118(86)
4	1.0500	0.1489(22)	4.364(89)

points requires six parameters ($\sqrt{8t_0}B_0$, $\sqrt{8t_0}F_0$, a_{10} , b_{10} , $c_a^{M_\pi}$ and $c_a^{F_\pi}$) while the coefficients of the logs, $a_{11} = 1/3$ and $b_{11} = -3/2$, are fixed, see Eqs. (4) and (5). For a better visualization of the deviations from the linear GMOR, in Fig. 5 we have divided the squared pion mass by the quark mass (all in units of $8t_0$). This ratio approaches the GMOR expectation $2B_0\sqrt{8t_{0,\text{ch}}}$ in the chiral limit. The deviation from a linear dependence is caused by b_{11} . This, as well as the curvature observed in Fig. 4 that is due to a_{11} , is in agreement with the data.

Since this simple fit describes the data very well, adding further parameters does not improve the situation: allowing for the mass-dependent discretization terms $\bar{c}_a^X \neq 0$ in Eq. (25), does not significantly change the values of χ^2/N_{dof} , F_0 or B_0 . However, the errors for the fit parameters c_A^X , a_{10} and b_{10} increase considerably and on the reduced datasets, when incorporating the cuts described at the end of Sec. III E, stable fits become impossible. Similarly, when allowing for the $\mathcal{O}(x^2)$ (NNLO) terms in the continuum fit functions (2) and (3), the statistical errors of all parameters increase while the higher order parameters are either comparable with zero or cannot be resolved reliably due to cancellations. After exploring these alternative parametrizations, we decided, in view of the range and quality of the present data, only to include the four parameter NLO continuum fit in conjunction with the two parameters that account for mass-independent $\mathcal{O}(a^2)$ effects into our analysis, and to explore the parametrization uncertainty by imposing the cuts on the data that are defined in Sec. III E. Carrying out the fits on these four sets of ensembles and performing the model averaging procedure as described in Appendix B, we obtain

$$\sqrt{8t_{0,\text{ch}}}F_0 = 0.1502_{(29)}^{(56)}, \quad \sqrt{8t_{0,\text{ch}}}B_0 = 4.22_{(16)}^{(15)}, \quad (26)$$

where the errors include the systematics. The individual results for each fit are listed in Table IV and compiled in Fig. 6, where also the final result is indicated.

B. Baryonic LECs

In analogy to the analysis of the mesonic observables, we carry out a simultaneous extrapolation of the octet baryon

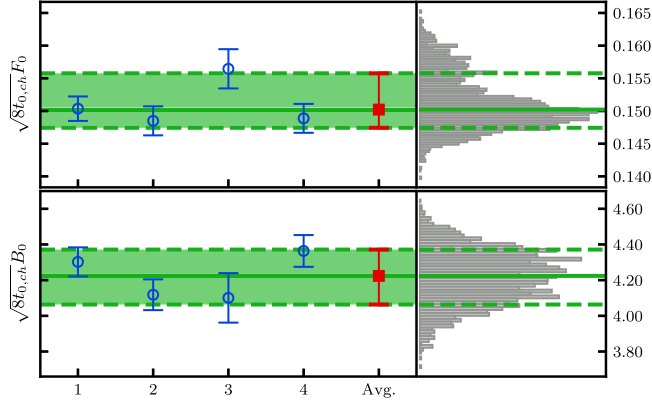


FIG. 6. Final result for F_0 and B_0 (red point and green error band) obtained from individual fits (blue points) by performing the model averaging procedure described in Appendix B. The model averaged distribution is shown as a histogram on the right where also the median and the 68% confidence level interval are indicated (green lines).

mass and the axial charges for the nucleon and the Σ baryon. The continuum expressions for the dependence of these three observables on the pion mass and the lattice extent L are given in Eqs. (6)–(9), (15) and (16). Again, lattice spacing effects are parametrized as in Eq. (25). For the decay constant F_0 , that enters in the definition of ξ , we use the result obtained in Sec. IV A. HBChPT should give the same set of LO LECs m_0 , F and D as BChPT in the EOMS prescription. To investigate the impact of different truncations of the chiral expansion, in addition to the BChPT fits, we also carry out a HBChPT analysis, replacing the loop function (7) $f_B(r) \mapsto -\pi$.

The pion mass dependence of the axial charges appears to be mild. As already pointed out at the end of Sec. II A, the logarithmic corrections suggested by ChPT without decuplet loops differ in sign from what the data suggest and this—within our window of pion masses—can only be compensated for by corrections of $\mathcal{O}(\xi^{3/2})$ and higher and/or by including effects of the decuplet baryons, adding the additional LECs Δ , \mathcal{C} and \mathcal{H} . The same observation is made regarding finite volume effects, whose sign can only be reconciled with the data if decuplet loops are included. We list the relevant formulas in Appendix A but we cannot explore these additional contributions, given the statistical error of our present data. Therefore, regarding the axial charges, we opt for the NLO [$\mathcal{O}(p^2)$] analysis and truncate Eqs. (8) and (9) at $\mathcal{O}(\xi)$. Regarding the finite volume effects, we restrict ourselves to the leading term (16), with phenomenological coefficients c_V^N and c_V^Σ . Turning to the baryon mass, we are able to employ the full NNLO [$\mathcal{O}(p^3)$] expressions, both for the pion mass-dependence and the finite volume behavior. We also found the baryon mass data to be well described when including decuplet loops, however, in this case, the LEC \mathcal{C} is found to be compatible with zero within large errors, suggesting that the impact of the decuplet on the octet baryon mass is small.

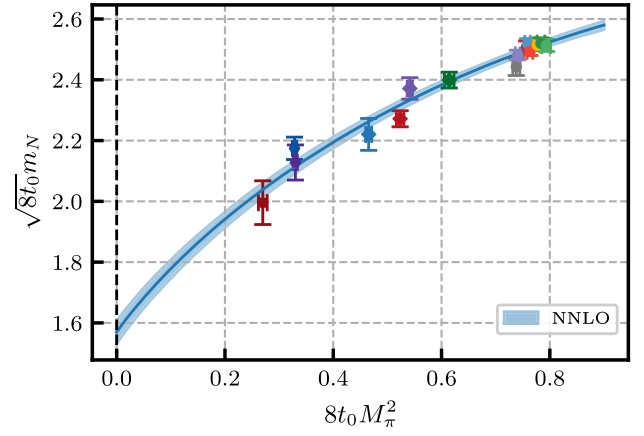


FIG. 7. Extrapolation of the nucleon mass m_N to the chiral limit. The data points are corrected for discretization and finite volume effects according to the parameters obtained from a combined fit to the nucleon mass and the two axial charges on all the available data points. The blue band shows the NNLO BChPT expression for the pion mass dependence.

In Figs. 7 and 8 the pion mass dependencies of the nucleon mass and of the axial charges are shown, respectively, for a combined fit to all the available data points. The fit is to 41 data points (15 ensembles for m_B and 13 ensembles for each of the axial charges) and requires 11 parameters, m_0 , F , D , \bar{b} , c_N , c_Σ , c_V^N , c_V^Σ , c_a^N , c_a^{Σ} and c_a^{Σ} : six (combinations of) LECs, two finite volume parameters for the axial charges and three parameters to describe discretization effects. We carry out the same variations of the dataset as in the meson case. In addition, we explore both BChPT and HBChPT for the pion mass-dependence of the baryon mass, giving eight distinct results that are collected in Table V and shown in Fig. 9. We find BChPT to give better fit qualities than HBChPT which is why the former fits dominate the averaging procedure. The BChPT results for m_0 are systematically larger than those of HBChPT

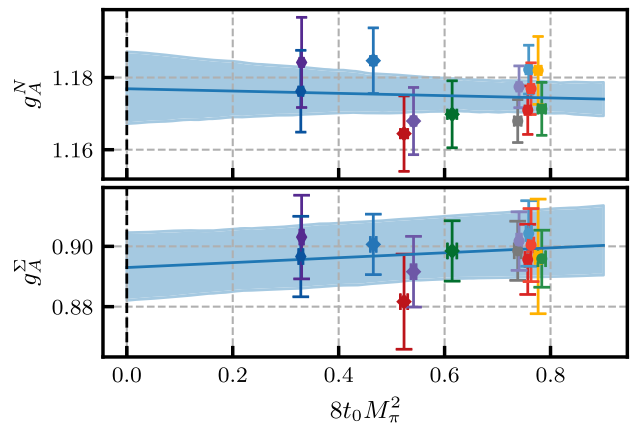


FIG. 8. The same as Fig. 7 for the axial charges of the nucleon and the Σ baryon. The blue band shows the NLO [$\mathcal{O}(p^2)$] chiral extrapolation.

TABLE V. Results for the LO baryonic LECs m_0 (octet baryon mass in the chiral limit), F and D obtained from fits to the BChPT (B) and HBChPT (H) expressions on different subsets of ensembles. The subsets are defined at the end of Sec. III E.

Fit	χ^2/N_{dof}	$\sqrt{8t_{0,\text{ch}}}m_0$	F	D
1 (H)	1.1710	1.325(49)	0.4455(59)	0.729(10)
1 (B)	0.9451	1.570(39)	0.4465(59)	0.730(10)
2 (H)	1.4793	1.447(70)	0.4489(82)	0.741(12)
2 (B)	1.2450	1.608(64)	0.4492(82)	0.742(12)
3 (H)	1.3788	1.341(51)	0.4442(61)	0.726(11)
3 (B)	1.1174	1.570(42)	0.4449(61)	0.728(11)
4 (H)	1.2265	1.339(50)	0.4447(61)	0.725(10)
4 (B)	0.9689	1.587(41)	0.4456(61)	0.727(10)

which suggests a larger curvature of the data. Since D and F are mostly determined by the axial charges, where to the order that we employ no difference between BChPT and HBChPT exists, these values are largely unaffected by the parametrization. The final, averaged results read:

$$\sqrt{8t_{0,\text{ch}}}m_0 = 1.57_{(6)}^{(5)}, \quad F = 0.447_{(7)}^{(6)}, \quad D = 0.730_{(11)}^{(11)}. \quad (27)$$

Again, the errors include the systematics of the extrapolation.

C. Comparison with other recent determinations

We employ the value $(8t_{0,\text{ch}})^{-1/2} = \mu = 469(7)$ MeV to convert our results into physical units. As explained in

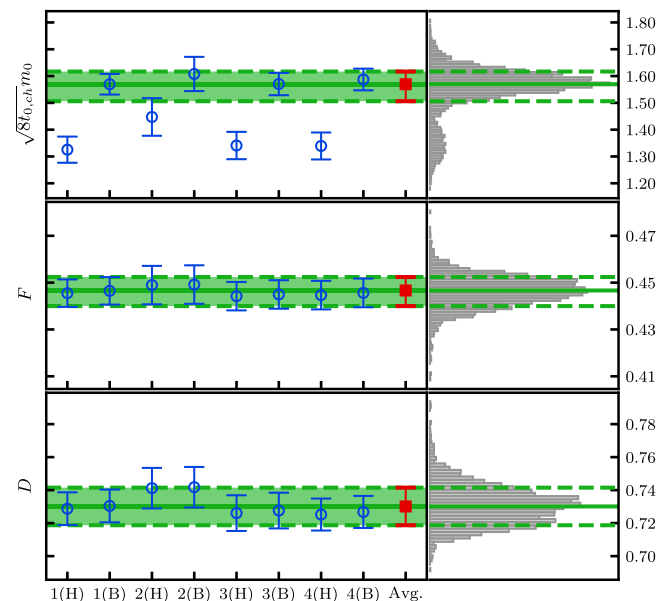


FIG. 9. The same as Fig. 6 but for m_0 , F and D . For each cut there are two data points: BChPT (B) and HBChPT (H).

Sec. II A, this value is obtained by combining $t_{0,\text{ch}}/t_0^* = 1.037(5)$ [12] with $(8t_0^*)^{-1/2} = 478(7)$ MeV [13]. The mesonic LECs (with systematic uncertainties included in the errors) then read

$$F_0 = 70_{(2)}^{(3)} \text{ MeV}, \quad \Sigma_0^{1/3}(\text{RGI}) = 214_{(5)}^{(7)} \text{ MeV}, \quad (28)$$

where $\Sigma_0 = B_0 F_0^2$. Note that $\Sigma_0(\text{RGI})$ refers to the value of the chiral condensate in the RGI scheme with $N_f = 3$ active sea quark flavors. Using version 3 of the *Mathematica* implementation of the RUNDEC package [53,54] at five loop accuracy in the quark mass anomalous dimension- and the β -functions, we obtain the conversion factor $m(\text{RGI}) = 1.330(14)(7)m(\overline{\text{MS}}, 2 \text{ GeV})$ for the quark mass between the RGI and the $\overline{\text{MS}}$ schemes.³ The first error corresponds to the uncertainty of the three-flavor Λ -parameter [13], whereas the second error is the difference between five- and four-loop running. Using the scale-independence of $m\Sigma_0$ and taking the third root, we obtain

$$\Sigma_0^{1/3}(\overline{\text{MS}}, 2 \text{ GeV}) = 236_{(6)}^{(7)} \text{ MeV}. \quad (29)$$

Fig. 10 shows a comparison of our results for F_0 and Σ_0 with the most recent determinations from SU(3) ChPT analyses of other groups, also see the present FLAG report [1] for a detailed discussion. One issue with $N_f = 2 + 1(+1)$ simulations is that the strange quark mass is usually kept close to its physical value, which limits the sensitivity of observables to the deviation of F_0 and B_0 from their SU(2) ChPT counter parts and necessitates partially quenched analyses. The only other simulation with $N_f = 3$ mass-degenerate quarks was carried out over a decade ago by JLQCD/TWQCD [55].

From an analysis of several lattice datasets Guo *et al.* [56] estimated $F_0 = 71(3)$ MeV. Hernández *et al.* [57] find from a large N_c scaling analysis of $N_f = 4$ and $N_c = 3-6$ lattice data $F_0 = 71(3)$ MeV and $\Sigma_0^{1/3} = 223(4)(8)$ MeV for $N_f = N_c = 3$. Simulating $N_f = 3$ flavors, JLQCD/TWCQD [55] determine $F_0 = 71(3)(8)$ MeV and $\Sigma_0 = 214(6)(24)$ MeV. Employing $N_f = 2 + 1$ flavor simulations, the most recent determinations of F_0 are 68(1)(3) MeV by χ QCD [8], 80.3(2.5)(5.4) MeV by MILC [58], 66.1(5.2) MeV by RBC/UKQCD [59] and 83.8(6.4) MeV by PACS-CS [60]. For $\Sigma_0^{1/3}$ in the $\overline{\text{MS}}$ scheme at 2 GeV, χ QCD [8] find 233(1)(2) MeV, MILC [61] quote 245(5)(4)(4) MeV, while PACS-CS [60] report 290(16) MeV. In summary, all the results for the mesonic LECs agree within their errors, with the exception of PACS-CS [60], in particular regarding the chiral condensate.

³The normalization of the RGI mass used in RUNDEC3 differs from the one we employ. References [1,48,49] share our convention.

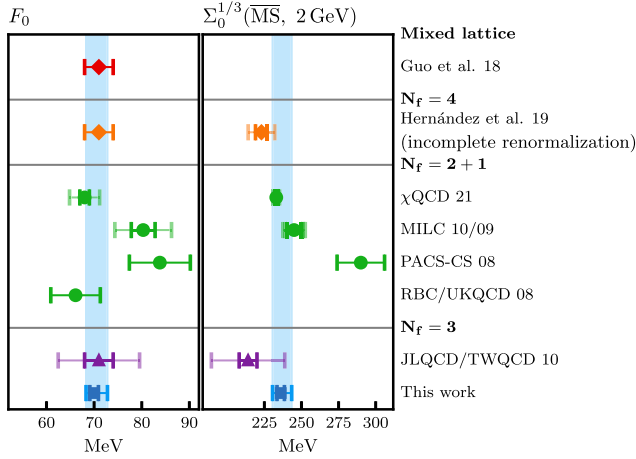


FIG. 10. Comparison with the most recent SU(3) ChPT determinations of F_0 and $\Sigma_0 = B_0 F_0^2$ from other groups. The latter is in the $\overline{\text{MS}}$ scheme at the scale 2 GeV with three active flavors. Note that the result labeled “ $N_f = 4$ ” is for the $N_f = 3$ LECs, however, extrapolated from $N_f = 4$ simulations at different numbers of colors. Dark error bars correspond to the statistical error only, whereas the lighter error bars include a systematic error estimate, added in quadrature.

A compilation of the most recent results for the octet baryon mass in the SU(3) chiral limit is shown in Fig. 11. Our result, including the systematic uncertainties and converted into physical units, reads

$$m_0 = 736_{(32)}^{(25)} \text{ MeV}. \quad (30)$$

Carrying out SU(3) HBChPT or BChPT analyses of data from $N_f = 2 + 1$ flavor simulations for m_0 , Walker-Loud [6] predicts 899(40) MeV, BMW [62] find 750(150) MeV and Martin Camalich *et al.* [63] obtain 756(32) MeV.

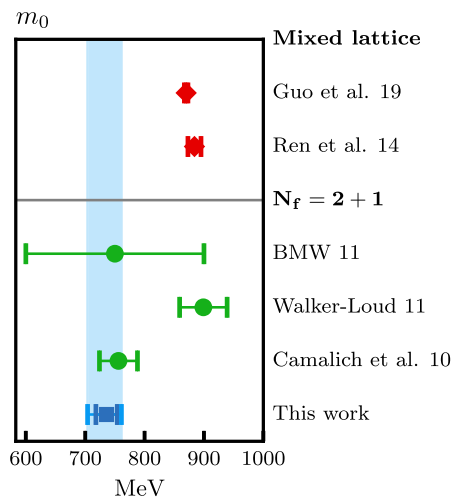


FIG. 11. Comparison with the most recent determinations of the octet baryon mass in the $N_f = 3$ chiral limit m_0 , obtained from fits to Lattice QCD results.

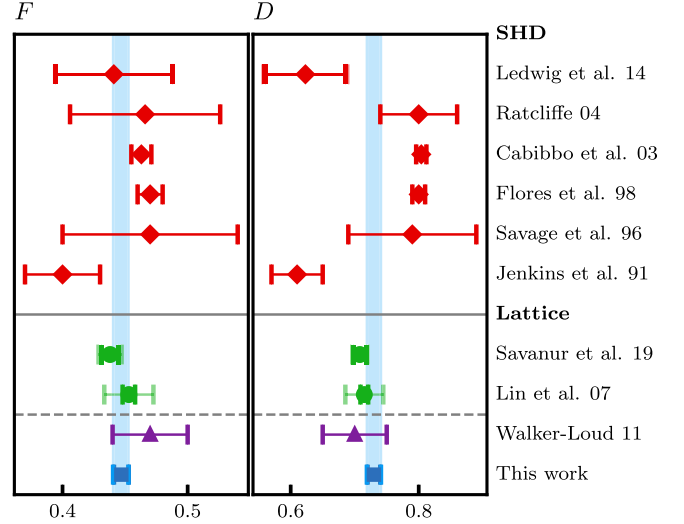


FIG. 12. Comparison of our results for the LECs F and D with results obtained from lattice QCD calculations of the hyperon axial charges (green points)—albeit for physical quark masses, rather than in the chiral limit—and the baryon mass (purple point). In addition, we show selected results obtained from measurements of semileptonic hyperon decays.

Investigating multiple lattice datasets, Guo *et al.* [64,65] obtain 870(3) MeV (mean and error estimated from the two fit results quoted in Ref. [65]) and Ren *et al.* [66] 884(11) MeV. A number of earlier results exists [23,67–70], which are not displayed in the figure. While it is difficult to estimate realistic errors for the two very global fits to lattice data [64,66], there is disagreement between our results and Walker-Loud [6] who obtains a much larger value.

In Fig. 12 we compare our results (27) for the baryonic LECs F and D with results obtained from lattice as well as phenomenological determinations. From a lattice QCD calculation of the axial charges, Lin and Orginos [71] determine $F = 0.453(5)(19)$ and $D = 0.715(6)(29)$ with $N_f = 2 + 1$ flavors. Later Savanur and Lin [72] find $F = 0.438(7)(6)$ and $D = 0.708(1)(6)$, this time with $N_f = 2 + 1 + 1$ flavors. Both values, however, refer to the physical quark mass point, where the definition of F and D is ambiguous, rather than to the chiral limit. From the baryon masses, Walker-Loud [6] finds $F = 0.47(3)$ and $D = 0.70(5)$. Most phenomenological predictions are inferred from semileptonic hyperon decays. A selection of such analyses contains Jenkins *et al.* [27], Savage *et al.* [73], Flores *et al.* [74], Cabibbo *et al.* [75], Ratcliffe [76] and Ledwig *et al.* [26]. Regarding F , there is no clear contradiction when comparing any pair of results within the stated errors. With respect to D , however, Flores *et al.* [74] and Cabibbo *et al.* [75]—while obtaining central values very similar to those of Savage *et al.* [73] and Ratcliffe [76]—are at variance with the lattice determinations, within their errors. Note that the lattice results agree with each other,

however, this should change if the precision was increased since two of the studies give numbers that correspond to the physical strange quark mass, rather than to the $N_f = 3$ chiral limit.

V. SUMMARY AND OUTLOOK

We carried out a simultaneous determination of all LO mesonic (B_0 , F_0) and octet baryonic (m_0 , D , F) SU(3) ChPT LECs, using $N_f = 3$ lattice QCD simulations. The analysis is based on fifteen gauge ensembles, spanning a range of pion masses from 430 MeV down to 240 MeV across six different lattice spacings between $a \approx 0.039$ fm and $a \approx 0.098$ fm and spatial lattice sizes between $3.3 \leq LM_\pi \leq 6.4$. We found that a consistent description of the pion mass and volume dependence of the axial charges and the octet baryon mass was possible with the same set of LECs. Systematic errors were assessed and included by imposing cuts on the pion mass, the lattice spacing and the volume. For the baryon mass both covariant BChPT and HBChPT were employed. The resulting LECs are as follows ($\Sigma_0 = F_0^2 B_0$):

$$\begin{aligned} F_0 &= 70_{(2)}^{(3)} \text{ MeV}, \\ \Sigma_0^{1/3} &= 214_{(5)}^{(7)} \text{ MeV(RGI)}, \\ &= 236_{(6)}^{(7)} \text{ MeV}(\overline{\text{MS}}, 2 \text{ GeV}), \\ B_0 &= 1.98_{(8)}^{(7)} \text{ GeV(RGI)}, \\ &= 2.63_{(10)}^{(10)} \text{ GeV}(\overline{\text{MS}}, 2 \text{ GeV}), \\ m_0 &= 736_{(32)}^{(25)} \text{ MeV}, \\ F &= 0.447_{(7)}^{(6)}, \\ D &= 0.730_{(11)}^{(11)}, \\ \frac{F}{D} &= 0.612_{(12)}^{(14)}, \end{aligned}$$

where the uncertainties of the continuum, chiral and infinite volume extrapolation as well as of the conversion into physical units are included in the error. The RGI and $\overline{\text{MS}}$ results above refer to the three-flavor scheme. We compare the mesonic SU(3) LECs $X_0 \in \{F_0, \Sigma_0, B_0\}$ with their SU(2) ChPT counterparts X , where the strange quark mass is fixed at its physical value, in the $\overline{\text{MS}}$ scheme with three active flavors at 2 GeV: the decay constant $F_0 < F \approx 86$ MeV [1,77] and the chiral condensate $\Sigma_0 < \Sigma \approx (270 \text{ MeV})^3$ [1] decrease significantly as we send the strange quark mass to zero, whereas the GMOR parameter $B_0 \approx B \approx 2.66$ GeV remains unaffected within its present uncertainty.

Further constraining the mass-dependence by including ensembles with lighter pion masses would be very interesting, in particular regarding the axial couplings. In

addition to this, in the near future we plan to extend the analysis to the $N_f = 2 + 1$ case in order to further improve the accuracy, to test the applicability range of SU(3) ChPT and also to determine higher order LECs.

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APPENDIX A: FURTHER ChPT EXPRESSIONS

We collect ChPT expressions that were not used in the final analysis. In particular, these are expressions that include decuplet loops (and therefore additional LECs that we were unable to resolve) and the finite volume effects for the axial charges. Regarding the latter, these have been computed using SU(2) HBChPT [87] and confirmed in SU(2) BChPT [88]. We define the function

$$h_1(\lambda_\pi) = \sum_{\mathbf{n} \neq \mathbf{0}} \left[K_0(\lambda_\pi | \mathbf{n}) - \frac{K_1(\lambda_\pi | \mathbf{n})}{\lambda_\pi | \mathbf{n}|} \right], \quad (\text{A1})$$

that corresponds to \mathbf{F}_1 of Ref. [87] while for $h(\lambda_\pi)$, defined in Eq. (14): $h(\lambda_\pi) = -(8/3)\mathbf{F}_3(M_\pi, L)$. Again $\lambda_\pi = LM_\pi$. The SU(3) finite size effects in the flavor symmetric limit [utilizing the couplings that are tabulated in Ref. [26] and truncating at $\mathcal{O}(p^3)$] read:

$$\begin{aligned} g_A^N(L) &= g_A^N - \frac{3}{2}(D+F)\xi h(\lambda_\pi) \\ &+ \frac{2}{9}(27D^3 + 25D^2F + 45DF^2 + 63F^3) \\ &\times \xi h_1(\lambda_\pi), \end{aligned} \quad (\text{A2})$$

$$g_A^\Sigma(L) = g_A^\Sigma - 3F\xi h(\lambda_\pi) + \frac{4}{9}F(25D^2 + 63F^2)\xi h_1(\lambda_\pi). \quad (\text{A3})$$

The gap between the decuplet and octet baryon mass in the chiral limit $\Delta = m_{D0} - m_0$ is within the range covered by our pion masses. Therefore, decuplet loop effects may in principle be relevant. Indeed, neglecting such terms, the finite volume effects of g_A^B have a sign opposite to what we

see in the data. Already in Ref. [27] corrections due to transitions to decuplet baryons were considered. The full SU(3) result [63] for the octet baryon mass for the case $m_s = m_\ell$, to be added to Eq. (6), reads⁴:

$$\begin{aligned} m_B \mapsto m_B - \frac{\Delta^3}{(4\pi F_0)^2} \frac{5}{3} \mathcal{C}^2 \left[\left(2 - 3 \frac{M_\pi^2}{\Delta^2} \right) \log \left(\frac{M_\pi}{2\Delta} \right) \right. \\ \left. + \frac{M_\pi^2}{2\Delta^2} + 2 \left(1 - \frac{M_\pi^2}{\Delta^2} \right) w \left(\frac{M_\pi}{\Delta} \right) \right], \end{aligned} \quad (\text{A4})$$

$$w(r) = \begin{cases} -(r^2 - 1)^{1/2} \arccos(r^{-1}), & r \geq 1 \\ (1 - r^2)^{1/2} \log(r^{-1} + \sqrt{r^2 - 1}), & r < 1 \end{cases} \quad (\text{A5})$$

with the additional LECs \mathcal{C} and Δ . Regarding the above decuplet baryon effects, we restrict ourselves to the heavy baryon approximation. The full EOMS BChPT result can be found in Ref. [63]. Note that the decuplet decouples as $M_\pi \rightarrow 0$ as it should since in this case the extra term is proportional to $[3 - 4 \log(M_\pi/(2\Delta))]M_\pi^4/(\Delta F_0^2)$, which is of a higher order in the chiral expansion. The associated finite volume corrections to Eq. (15) read [36,91]

$$m_B(L) \mapsto m_B(L) + \frac{5}{3} \mathcal{C}^2 \xi \frac{m_0^3}{(m_0 + \Delta)^2} \int_0^\infty dy \left\{ \left(2 - y + \frac{\Delta}{m_0} \right) f(y) \sum_{\mathbf{n} \neq \mathbf{0}} \left[f(y) K_0(\lambda_\pi | \mathbf{n} | f(y)) - \frac{K_1(\lambda_\pi | \mathbf{n} | f(y))}{\lambda_\pi | \mathbf{n}|} \right] \right\}, \quad (\text{A6})$$

where

$$f(y) = \sqrt{1 + M_\pi^{-2} [(\Delta^2 + 2m_0\Delta - M_\pi^2)y + m_0^2 y^2]}. \quad (\text{A7})$$

We refer to Ref. [63] for the full SU(3) result and to Refs. [36,91] for the corresponding finite volume corrections.

For the axial charges, we start from Ref. [87] and implement the decoupling constraints [92,93] at $\mathcal{O}(p^3)$. We obtain for the special $N_f = 3$ case $m_s = m_\ell$:

$$\begin{aligned} g_A^B \mapsto g_A^B - j_B \frac{\Delta^2}{16\pi^2 F_0^2} J(M_\pi/\Delta) \\ - n_B \frac{\Delta^2}{16\pi^2 F_0^2} N(M_\pi/\Delta), \end{aligned} \quad (\text{A8})$$

where

$$J(r) = -r^2 - (2 - r^2) \log \left(\frac{r}{2} \right) - 2w(r), \quad (\text{A9})$$

⁴For the LEC \mathcal{C} we use the normalization of Refs. [7,27,89], where $\mathcal{C}^2 = g_{\Delta N\pi}^2$ [90].

$$\begin{aligned} N(r) &= -\frac{r^2}{3} + \frac{\pi r^3}{3} - \left(\frac{2}{3} - r^2 \right) \log \left(\frac{r}{2} \right) \\ &- \frac{2}{3} (1 - r^2) w(r) \end{aligned} \quad (\text{A10})$$

and the coefficients are given as

$$j_N = 5 \left(F + D + \frac{8}{27} \mathcal{H} \right) \mathcal{C}^2, \quad (\text{A11})$$

$$n_N = -4 \left(\frac{11}{9} D + F \right) \mathcal{C}^2, \quad (\text{A12})$$

$$j_\Sigma = 10 \left(F + \frac{5}{27} \mathcal{H} \right) \mathcal{C}^2, \quad (\text{A13})$$

$$n_\Sigma = -\frac{40}{9} D \mathcal{C}^2. \quad (\text{A14})$$

We remind the reader that the term $d_B \xi^{3/2}$ within Eqs. (8) and (9) does not appear at $\mathcal{O}(p^3)$ in the chiral expansion but is purely phenomenological. However, the function $\Delta^2 N(M_\pi/\Delta)$ contains a genuine term $\propto \xi^{3/2} (4\pi F_0)/\Delta$, justifying the inclusion of that parameter.

Regarding finite volume effects, we infer from Ref. [87] (see also Ref. [88]) that the following terms need to be added to Eqs. (A2)–(A3)

$$g_A^B(L) \mapsto g_A^B(L) + \frac{4}{3}\xi \left[j_N \mathbf{F}_2(LM_\pi, M_\pi/\Delta) - \frac{9}{8}n_N \mathbf{F}_4(LM_\pi, M_\pi/\Delta) \right], \quad (\text{A15})$$

where \mathbf{F}_2 and \mathbf{F}_4 are defined in Ref. [87].

APPENDIX B: MODEL AVERAGING

To address systematic effects we carry out fits varying the fit function (e.g., BChPT vs. HBChPT) as well as the number of data points included. This gives us a set of N_M different results, one for each model j , from which we compute an average and its uncertainty that includes the statistical error and the systematic uncertainty due to the model variation.

One widely used approach is to assign a weight w_j given by the Akaike information criterion (AIC) [94] to each model j in the model averaging procedure. Here we employ the weights

$$w_j = A \exp \left\{ -\frac{1}{2} [\max(\chi_j^2, N_{\text{dof},j}) - N_{\text{dof},j} + k_j] \right\}, \quad (\text{B1})$$

see, e.g., Eq. (161) of the e-print version of Ref. [95] and references therein.⁵ The normalization A is such that

⁵Recently, instead of subtracting $N_{\text{dof}} - k$ from χ^2 in the exponent, in Ref. [96] it has been suggested to subtract $-2n_{\text{cut}} - 2k = \text{const} + 2N_{\text{dof}}$, where n_{cut} is the number of removed data points. This seems counterintuitive: since for a good fit $\chi^2 \sim N_{\text{dof}}$, this change would result in a very strong preference for fits that include as many data points as possible, even if the corresponding χ^2/N_{dof} -values were significantly larger.

$\sum_i^{N_M} w_i = 1$. χ_j^2 denotes the χ^2 -value of the fit to model j , k_j the number of fit parameters and $N_{\text{dof},j} = n_j - k_j$ the number of degrees of freedom. By replacing $\chi^2 \mapsto \max(\chi^2, N_{\text{dof}})$, we deviate somewhat from Ref. [95] in so far as reducing the χ^2 -value below N_{dof} will not further increase the weight. The rationale for this choice is that if the fit function perfectly described the data then a value $\chi^2 < N_{\text{dof}}$ should not be more likely than the expected value $\chi^2 = N_{\text{dof}}$. The above equation extends the AIC to also varying the number of data points n_j and not only the fit function. It is valid as long as there are no correlations between the removed and the remaining data points, the fit function is smooth and the parametrization does not depend on the data space. This applies to our case where we reduce the number of data points by removing entire ensembles and carry out the same set of fits for every dataset.

For each parameter a that we are interested in, we generate for each model j a bootstrap distribution $a_j(b)$ with $N_b = 500$ bootstrap samples b . The (normalized) bootstrap histograms are usually normal distributed,

$$f_j(a) = \frac{1}{\sqrt{2\pi}\sigma_j} \exp \left\{ -\frac{1}{2} \left(\frac{a - a_j}{\sigma_j} \right)^2 \right\}, \quad (\text{B2})$$

with a mean a_j and a standard deviation σ_j . From the (discrete) histograms, we obtain the model averaged distribution

$$f(a) = \sum_j w_j f_j(a), \quad (\text{B3})$$

from which we take the median and the 1σ confidence interval determined by the 15.9% and 84.1% percentiles as the model average \bar{a} and its upper and lower confidence limits $\bar{a} + \Delta a_+$ and $\bar{a} - \Delta a_-$. We then quote the average and its total error as $\bar{a}_{\Delta a_{\pm}}$. This procedure is illustrated in Figs. 6 and 9, where the histograms are coarsely binned for a better visualization.

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