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Octet baryon masses and sigma terms from an SU(3) chiral extrapolation

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We report an analysis of the impressive new lattice simulation results for octet baryon masses in 2 + 1-flavor QCD. The analysis is based on a low-order expansion about the chiral SU(3) limit in which the symmetry breaking arises from terms linear in the quark masses plus the variation of the Goldstone boson masses in the leading chiral loops. The baryon masses evaluated at the physical light-quark masses are in remarkable agreement with the experimental values, with a model dependence considerably smaller than the rather small statistical uncertainty. From the mass formulas one can evaluate the sigma commutators for all octet baryons. This yields an accurate value for the pion-nucleon sigma commutator. It also yields the first determination of the strangeness sigma term based on 2 + 1-flavor lattice QCD and, in general, the sigma commutators provide a resolution to the difficult issue of fine-tuning the strange-quark mass.

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In recent years lattice QCD has matured to a level where it can be used as a precision tool to confront experimental aspects of nonperturbative QCD. This advance has occurred primarily in the heavy-meson sector [1], while for light quarks, and especially for light-quark baryons, progress has been more steady. However, new high-precision studies of the baryon spectrum in 2 + 1-flavor dynamical simulations have recently been reported by LHPC [2], PACS-CS [3], HSC [4], and Dürr *et al.* [5]. In this paper, we demonstrate that these results are sufficiently close to the chiral regime that they permit a reliable determination of the octet baryon masses at the physical point, as well the associated sigma terms.

Our analysis focusses (chronologically) on the first two of the above cited studies, those of LHPC and PACS-CS. The smallest pion masses are of order 0.29 and 0.30 GeV, respectively. The lattice spacing for the MILC configurations, used by LHPC, has been carefully determined in heavy-quark systems [6]. That same analysis also produced a physical determination of the Sommer scale, $r_0 = 0.465 \pm 0.012$ fm, which we use to set the scale in the PACS-CS simulations.

Our working hypothesis is that the (different) improved actions employed by the two groups yield a very good approximation to the continuum theory, so that discretization artifacts are small. A unified treatment of the continuum extrapolation is only possible once there are results available at multiple lattice spacings, such as the study of Ref. [5]. On the other hand, a comparison of the absolute values of the baryon masses extracted from the analysis of the separate LHPC and PACS-CS data sets provides a test, *a posteriori*, of the validity of this hypothesis. We shall see that it appears to be a very good approximation.

The first step in our analysis is to calculate the finite-volume corrections within the low-energy effective field theory (EFT), at each combination of quark masses. We can then focus our attention on the extrapolation within an infinite-volume, continuum effective field theory framework. A detailed volume dependence analysis of the nucleon mass in 2-flavor simulations has observed that the finite-volume corrections are well described by the leading one-loop results of chiral effective field theory [7]. We extend this approach to the SU(3) case in order to estimate the infinite-volume limit of the present lattice results. While the leading infrared effects of the loop integral are independent of the ultraviolet regularization, to be conservative we include an uncertainty in this correction which amounts to the difference between the finite-volume correction determined without a regulator [8] and that evaluated with a dipole of mass of 0.8 GeV [9]. The largest shift we use in our analysis is for the nucleon at the lightest pion mass (where $m_\pi L = 3.7$), giving a correction of -0.019 ± 0.005 GeV. We choose to neglect the lightest simulation ensemble of the PACS-CS calculation [3], where finite-volume corrections may not be well estimated by these leading one-loop graphs, given that $m_\pi L = 2.3$.

The chiral expansion of the octet baryons has been presented on numerous occasions in the literature—e.g., Refs. [10–13]. It may be expressed as

$$M_B = M^{(0)} + \delta M_B^{(1)} + \delta M_B^{(3/2)} + \ldots, \qquad (1)$$

where the superscript denotes the order of the expansion in powers of the quark mass—the *explicit* chiral symmetry breaking parameter of QCD. Here, $M^{(0)}$ denotes the baryon mass in the SU(3) chiral limit.

The $\delta M_B^{(1)}$ term is linear in the scale-dependent, running quark masses, m_l and m_s; we refer to Ref. [13] for explicit expressions. In this analysis, we replace the quark masses by the corresponding meson masses squared, as also done in Ref. [2]. To the order that we work in this manuscript, the use of either quark masses or meson masses squared is equivalent.

The next higher-order term, $\delta M_B^{(3/2)}$, involves the leading one-loop corrections arising from the baryons coupling to the pseudo-Goldstone bosons, $\phi \equiv \pi$, K, η. For the baryons, we include both the octet and decuplet. Certainly, in the limit $m_\phi \ll \delta$ (the octet-decuplet mass splitting in the chiral limit), the decuplet contributions are formally of higher order. However, with a physical kaon mass $\sim$0.7 GeV, it is clear that $\delta \sim 0.3$ GeV cannot be treated as a heavy energy scale. For this reason our formal assessment of the order of a given diagram treats the octet and decuplet baryons as degenerate. However, in order to more accurately represent the branch structure in the transition region $m_\phi \sim \delta$, in the numerical evaluation of the loop integrals we maintain the octet-decuplet mass splitting. Further, the renormalization is performed such that the decuplet is formally integrated out in the limit $m_\phi \ll \delta$.

For the explicit forms of the loop integrals, we refer the reader to Ref. [14]. The coefficients of these loop contributions [13] are expressed in terms of the pseudoscalar decay constant and the relevant baryon axial charges. The nucleon axial charge, $g_A = D + F = 1.27$ is fixed by experiment, while all other couplings are determined by SU(6) relations ($F = \frac{2}{3}D$ and $\mathcal{C} = -2D$). We note that $\mathcal{C}$ is also related to the decay width of the Δ, from which a similar value can be inferred. We also adopt the chiral perturbation theory estimate for the meson decay constant in the SU(3) chiral limit, $f = 0.0871$ GeV [15]. The octet-decuplet splitting is chosen phenomenologically to be the physical N-Δ splitting, $\delta = 0.292$ GeV. In principle, all of these input parameters could be constrained by actual lattice simulation results, at least in the near future—we refer to recent progress in the computation of the axial charges [16]. For this study we take these parameters from phenomenology, we incorporate generous uncertainties in these inputs into our systematic error analysis, allowing f to vary by $\pm 5\%$, and D, F, $\mathcal{C}$, and δ to vary by $\pm 15\%$. We leave a global analysis that determines all of these inputs simultaneously from the same lattice calculation to future work.

In fitting the lattice results, we wish to minimize the uncertainty from higher-order terms in the chiral expansion. We therefore limit ourselves to the smallest domain of the light quarks possible with these latest lattice results. For both the LHPC and PACS-CS results, we include *only* the results of the simulations for $m_\pi^2 < 0.2$ GeV^2.

We first fit the baryon masses to leading order, keeping only $\delta M_B^{(1)}$ in the expansion (1). This gives a reasonable description of the (finite-volume corrected) lattice results, with a reduced χ^2 ($\chi^2_{\rm dof}$) of 0.9 and 0.3 for the LHPC and PACS-CS results, respectively. We caution reading too much into the absolute value of this naive χ^2, as there are certainly strong correlations among the points on the same gauge configurations, as mentioned in Ref. [2]. In particular, the mass splittings among the baryons will typically be known better than one would estimate from naively adding the uncertainties in the absolute masses. Without further information on these correlations, our χ^2 will typically underestimate the total χ^2 constructed from the full information contained in the lattice simulation.

We now investigate the inclusion of the loop corrections. We perform fits where the regularization scale dependence has been removed to *all* orders and just the leading term of the loop integration is retained. Using the phenomenological coefficients, the best-fit produces a (naive) $\chi^2_{\rm dof}$ of order the order 40 (36) for the LHPC (PACS-CS) results. Alternatively, a similar fit was also done by the LHPC [2], where a suitable $\chi^2_{\rm dof}$ was achieved by allowing the chiral coefficients to be fit. While this produced a reasonable description of the data, the determined coefficients (such as g_A^2 or $\mathcal{C}^2$) were found to be an order of magnitude smaller than phenomenological estimates. The most natural conclusion of these observations (as also noted in [2]) is that the meson masses lie beyond the model independent or ''power counting'' region (PCR) of the expansion at this order. It is therefore a challenge to maintain the constraints of both the EFT and the lattice results (without abandoning one of them).

The breakdown of the expansion at this order should come as no surprise, as it has long been known that the SU(3) chiral expansion in the baryon sector is quite poor—even at the physical quark masses (see, e.g., [10,11]). Donoghue *et al.* formulated a solution to this problem through long-distance regularization [11]. Concurrently, the same techniques were being developed to alleviate the problem of chiral extrapolation at moderate quark masses in lattice QCD with the development of finite-range regularization (FRR) [17]. While this has largely been developed for applications in SU(2) chiral extrapolations [18], here we utilize the features of the long-distance regularization/FRR formalism to perform extrapolations in the framework of chiral SU(3).

For the relevant formulas describing the renormalization of the loop integrals, we direct the interested reader to Ref. [14]. Upon renormalization, and to the order we are working, the FRR forms produce exactly the same expansion as we have described above. The difference lies in a resummation of higher-order terms, which are suppressed by inverse powers of the regularization scale. At this order, the lowest-order addition to the renormalized expansion will explicitly appear in the form m_ϕ^4/Λ, with Λ the regulator mass.

In working towards *ab initio* studies of QCD, where no external, phenomenological input is used, we do not wish

to impose any external constraints on the regularization scale. Based on the success of FRR, we should like to utilize the observation that the induced resummation of higher-order terms provides an improved description of a range of lattice observables. Here we use the lattice results themselves to determine the regularization scale by minimizing the χ^2.

Some significant features of using the χ^2 measure, with the regularization scale treated as a free parameter, are

(i) no bias of a preferred scale is dictated by phenomenology;
(ii) if one is working with results that genuinely lie within the PCR, then the χ^2 function will be essentially independent of Λ;
(iii) this method provides a quantitative assessment of the potential size of the higher-order terms. Furthermore, an uncertainty arising from the truncation of the expansion is automatically incorporated into the uncertainties of the fit;
(iv) if lattice results are included from outside the PCR, then through the χ^2, Λ is optimized so as to give a best estimate of a resummation of a subset of higher-order terms from beyond the working order of the chiral expansion.

To begin, we introduce a single new parameter through the regularization scale. The best fit to the LHPC (PACS-CS) results, with 5 fit parameters, is shown in the upper (lower) panel of Fig. 1, where the dipole form is shown as an example. As explained above, the fits include only those simulation points for $m_\pi^2 < 0.2$ GeV^2 (the largest kaon mass is $m_K^2 \simeq 0.40$ GeV^2). Nevertheless, we see that the level of agreement with the lattice simulations at higher m_π^2 is remarkably good. Further, the low-energy constants obtained in the two data sets are in agreement to better than half the statistical precision of their determination, where, for example, the renormalized value, $M^{(0)}$, in the SU(3) chiral limit is found to be 0.82 ± 0.06 and 0.83 ± 0.08 GeV for the LHPC and PACS-CS results, respectively.

The fits are determined by evaluating the baryon mass function at each of the lattice kaon and pion masses. The curves in Fig. 1 are shown for illustrative purposes, where the kaon mass at any point on the curve is determined by fitting m_K^2 as a linear function in m_π^2 for the corresponding lattice ensemble. The physical masses are determined by evaluating the fit function at the physical pion and kaon masses (which has no bearing on the linear form used for the figure). To illustrate how this extrapolation in the strange-quark mass works, the lower panel of Fig. 1 shows a fit to just the two PACS-CS results at fixed κ_s. Using that fit, the results of the simulation at the different κ_s are shown as a *prediction*—by evaluating the fit function at the lattice kaon mass of this ensemble. The agreement between the results of the simulation and the predicted values is illustrative of the reliability of the fit in estimating

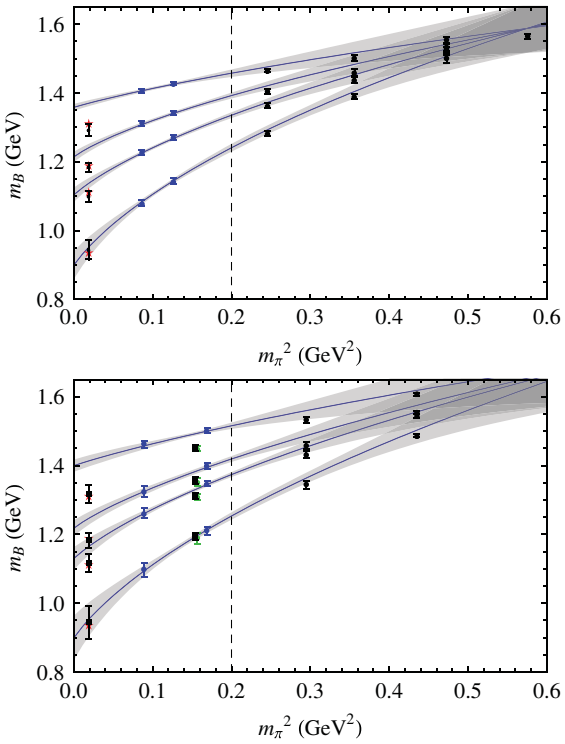

FIG. 1 (color). The upper and lower panels show, respectively, the dipole fits (lines) to the LHPC and PACS-CS lattice simulation results (circles) of the octet baryon masses (curves top to bottom show Ξ, Σ, Λ, and N). The squares at the physical pion mass display the extrapolation to the physical quark masses. The stars denote the physical baryon masses. The errors indicated by the bands represent the total statistical errors, including the variation of Λ. The third lightest pion mass of the PACS-CS results, which involved a lower strange-quark mass, is *not* included in the displayed fit. This allows a prediction (squares) based on the other points (see text).

the dependence of the octet masses on the strange-quark mass. In our final results, the lattice points at this extra strange-quark mass *are* also included.

For the LHPC (PACS-CS) results the optimal dipole regularization scale is found to be $\Lambda = 1.1 \pm 0.4$ GeV (0.91 ± 0.34 GeV). The minimum $\chi^2_{\rm dof}$ is 0.25 (0.05), where the improvement over the above linear forms is evident. As discussed, the existence of a preferred regularization scheme is a direct signature that the results lie outside the PCR. Nevertheless, the extrapolated precision obtained is rather encouraging, considering that the uncertainties incorporate the effect of the relatively large range permitted for the regularization scale, as much as $\sim$0.7–1.5 GeV.

Given that our results do demonstrate that we are outside the PCR, we also investigate the model dependence in the choice of regulator. Smooth forms, such as a dipole, monopole, and a Gaussian give indistinguishable results, with the most significant difference to these seen in a sharp cutoff, as was seen in Ref. [18]. Our estimate of the

model-dependent uncertainties incorporates the full variation over these different functional forms, in addition to all the uncertainties in the phenomenological input parameters, as described above.

In Table I we report best estimates of the physical masses by combining the different lattice simulations assuming they are each good approximations of the continuum limit. We treat the difference between the simulations as an estimate of the discretization uncertainty. The size of these discretization uncertainties are perhaps surprisingly small, appearing at the $\sim 1\%$ level. Indeed before this work, one may have anticipated the discretization errors to be of the order of 10%. To investigate this surprise agreement, we have tested how well one simulation can predict the other. In Fig. 2 we show the predictions of the PACS-CS results based on the fits to just the lightest two ensembles of the LHPC. The fits to the two light-quark mass points, and fixed strange-quark mass, reproduce the PACS-CS results well within the anticipated 10% bounds. Further, the dependence on both the light- and strange-quark mass dependence is well described. For statistical comparison, the LHPC fit recovers the complete set of PACS-CS points at a $\chi^2/\mathrm{dof} \sim 2.2$. Including a uniform offset parameter of just 10 MeV reduces the χ^2 to order unity.

We also report the dimensionless baryon sigma terms, $\bar{\sigma}_{Bq} \equiv (m_q/M_B)\partial M_B/\partial m_q$. We note that the model dependence, is relatively small compared with the present statistical precision. This model dependence will not decrease with increased statistics and therefore the present analysis, at this order and at these quark masses, is precision limited. Improvements beyond this will certainly require increased efforts in the EFT and numerical computations deeper in the chiral regime.

Our results show agreement between the absolute values of the baryon masses and the corresponding experimental values. This is an important independent confirmation of the absolute scale determination reported by Aubin *et al.* [6]. Further, the sigma terms extracted by differentiating the fitting formulas, have some quite interesting features. The pion-nucleon sigma commutator is, within uncertainties, compatible with phenomenological estimates [19]. The strangeness sigma commutator is consistent with best EFT estimates [10], yet an order of magnitude more precise. This small value is observed to be consistent with ''unquenching'' estimates [20], as well as a recent 2-flavor lattice QCD estimate [21].

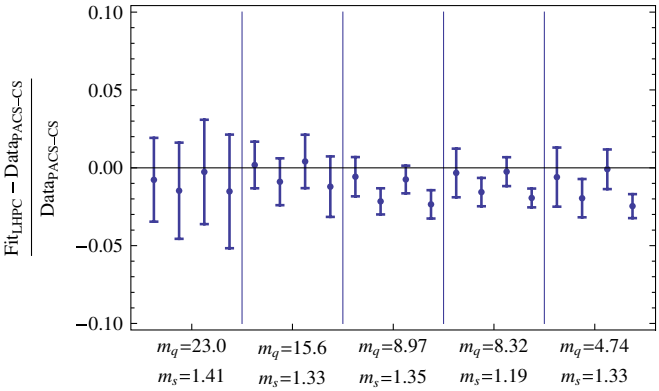

FIG. 2 (color online). Comparison of the PACS-CS results with the predicted values from the fit to the LHPC results. The light- and strange-quark masses are shown in units of their physical values (as inferred from the Gell-Mann–Oakes–Renner relation). Each grouping of four is ordered, from left to right, by N, Λ, Σ, and Ξ.

In line with quark-model expectations, we note that the Ξ is most sensitive to the strange-quark mass. The linear projections of kaon masses of the LHPC and PACS-CS results, used in Fig. 1, give strange-quark masses (or $m_K^2 - m_\pi^2/2$) that are $\sim 30\%$ too high. With the definition of the sigma term giving $\frac{\delta M_B}{M_B} = \bar{\sigma}_{Bq}\frac{\delta m_q}{m_q}$, and $\bar{\sigma}_{\Xi s} \sim 0.24$ from Table I, this indicates that the Ξ mass on each curve should lie high by roughly $0.24 \times 0.30 \sim 7\%$.

In summary, we have demonstrated an excellent description of current 2 + 1-flavor lattice QCD results based on a low-order SU(3) chiral expansion. While the expansion to this order is not sufficiently convergent to ensure that the fits are model independent, we find that the model dependence is actually small compared with the current statistical precision. In the future, as more simulations and statistics accumulate, the significance of the model-dependent component of the error will increase and will necessitate an increased effort in the EFT. We also anticipate that future studies will strengthen the numerical con-

TABLE I. Extracted masses and sigma terms for the physical baryons. The first error is statistical; the second estimates the discretization artifacts by the difference between the results for the LHPC and PACS-CS results; the third error represents a model-dependence estimate as described in the text. A further $\sim 2\%$ uncertainty in the absolute scale [6] is understood. The experimental masses are shown for comparison.

B	Mass (GeV)	Experimental	$\bar{\sigma}_{Bl}$	$\bar{\sigma}_{Bs}$
N	0.945(24)(4)(3)	0.939	0.050(9)(1)(3)	0.033(16)(4)(2)
Λ	1.103(13)(9)(3)	1.116	0.028(4)(1)(2)	0.144(15)(10)(2)
Σ	1.182(11)(2)(6)	1.193	0.0212(27)(1)(17)	0.187(15)(3)(4)
Ξ	1.301(12)(9)(1)	1.318	0.0100(10)(0)(4)	0.244(15)(12)(2)

straints on both the continuum and infinite-volume extrapolations, such as the work of Ref. [5].

Within the caveats of the present study, we have demonstrated a robust and precise determination of the absolute values of the octet bayon masses. The controlled extrapolations have also permitted a reliable determination of the baryon sigma terms, where we have been able to extract an accurate determination of the σ commutator as well as showing that the strange-quark sigma term of the nucleon is considerably smaller than phenomenological estimates. As just one example of the importance of these results, we note the significance for dark matter searches explained in Ref. [22].

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