In Search of the Chiral Regime

Silas R. Beane$^{1,2}$

$^1$Department of Physics, University of New Hampshire, Durham, NH 03824-3568.
$^2$Jefferson Laboratory, 12000 Jefferson Avenue, Newport News, VA 23606.

Abstract

A critical appraisal is given of a recent analysis of the quark-mass and finite-size dependence of unquenched lattice QCD data for the nucleon mass. We use this forum to estimate the boundary of the chiral regime for nucleon properties.
How low in quark masses must lattice QCD simulations of baryon properties go in order to reach the regime where chiral perturbation theory (χPT) is an extrapolation tool with controlled errors? In interesting recent work [1, 2] unquenched lattice QCD data for the nucleon mass at large pion masses, $m_\pi > 500$ MeV, has been analyzed using baryon χPT to $O(m_q^2)$ (without including the Δ as an explicit degree of freedom). These papers fit the quark-mass dependence of unquenched lattice QCD data for the nucleon mass (including the physical point) with natural values of the strong-interaction parameters and then successfully predict (in Ref. [2]) the finite-size dependence. These results are quite remarkable. However, little attempt is made in Refs. [1, 2] to gauge the uncertainties associated with the quark-mass extrapolation procedure. Given the provocative results that are found and the rather large quark masses that are simulated, it is essential to perform an error analysis. We will therefore do so in this note. And, in so doing, we will provide an estimate of the quark-mass boundary of the chiral regime for nucleon properties [3].

The nucleon mass at $O(m_q^2)$ in the chiral expansion, evaluated using infrared regularization [4], is given by

$$
M_N = M_0 - 4c_1m_\pi^2 - \frac{3g_A^2}{8\pi^2 f^2}m_\pi^3 \sqrt{1 - \frac{m_\pi^2}{4M_0^2}} \left[ \frac{\pi}{2} + \frac{m_\pi^2}{4M_0^2m_\pi^2 - m_\pi^4} \right]
+ \left[ e_1(\mu) + \frac{3}{32\pi^2 f^2} \left( \frac{g_A^2}{M_0} + c_2 \right) - \frac{3}{16\pi^2 f^2} \left( \frac{g_A^2}{M_0} - 8c_1 + c_2 + 4c_3 \right) \ln \frac{m_\pi}{\mu} \right] m_\pi^4. \tag{1}
$$

Following Refs. [1, 2] we choose the parameter set $g_A = 1.267$, $f = 131$ MeV, $c_2 = 3.2$ GeV$^{-1}$ and $c_3 = -3.4$ GeV$^{-1}$. One then easily fits the remaining low-energy constants to unquenched lattice QCD data [2, 5, 6, 7] over a wide range of pion masses [1, 2]. For instance, in Table I (Fit 1 (IR)) we list a set of parameter values $^1$ which give rise to the solid curve in Fig. II (left panel). While one sees an excellent description of the data with natural values of the strong-interaction parameters (which are consistent with $\pi - N$ phase shift analyses), one must quantify the errors associated with omitted higher-order effects in order to estimate the reliability of perturbation theory over the range of fit pion masses.

There are many ways to estimate the reliability of the chiral expansion and Refs. [1, 2] suggest one robust method. The difference between a matrix element at a given order in the chiral expansion evaluated with the physical values of $g_A$ and $f$ and evaluated with their chiral-limit values $g_A^{(0)}$ and $f^{(0)}$ is a measure of the importance of higher-order effects. Ref. [2] estimate $g_A^{(0)} \sim 1.2$ and $f^{(0)} \sim 124$ MeV and find little variation in the fit curve. However,

---

$^1$ We fit the full expression in eq. (1), while Refs. [1, 2] fit to an expanded form; hence the small differences in the values of the parameters.
this is no surprise as these chiral-limit values leave the ratio $g_A/f$ unchanged. Here we will consider how variation of the chiral-limit parameters affects the chiral expansion.

It is worth considering what is known experimentally about $g_A^{(0)}$ and $f^{(0)}$. At one-loop order in the chiral expansion one has the well-known formulas \[^8, 9\],

$$g_A = g_A^{(0)} \left[ 1 - \frac{(g_A^{(0)})^2 m_\pi^2}{8\pi^2 (f^{(0)})^2} + \frac{4m_\pi^2}{g_A^{(0)} d_{16}} \right], \quad f = f^{(0)} \left[ 1 + \frac{m_\pi^2}{8\pi^2 (f^{(0)})^2} \bar{7}_4 \right], \quad (2)$$

where $\bar{d}_{16}$ and $\bar{7}_4$ are (scale-independent) low-energy constants \[^2\].

The parameter $\bar{7}_4$ is determined from $K_{\ell^3}$ and $K_{\ell^2}$ decays \[^9\] and from a two-loop analysis of $\pi - \pi$ scattering \[^12\]. For simplicity, we will follow Ref. \[^9\] and fix $f^{(0)} = 124$ MeV, keeping in mind that not accounting for variation of $f^{(0)}$ will necessarily lead to an underestimate of the final error. An analysis \[^8, 13\] of the process $\pi N \to \pi \pi N$ at one-loop order in the chiral expansion provides three distinct determinations of $\bar{d}_{16}$: $-0.91 \pm 0.74$, $-1.01 \pm 0.72$ and $-1.76 \pm 0.85$ GeV\(^{-2}\). Taking the $1\sigma$ limits of the three determinations gives $-2.61$ GeV\(^{-2}\) $< \bar{d}_{16} < -0.17$, or $g_A^{(0)} = 1.42 \pm 0.10$. A recent analysis suggests that the $\Delta$ (which is not included as an explicit degree of freedom in Refs. \[^8, 13\]) plays a crucial role in the determination of $\bar{d}_{16}$ and suggests a lower central value: $g_A^{(0)} = 1.20 \pm 0.10$ \[^14\]. Taking

\[^2\] The barred constants contain chiral logarithms and therefore the formulas in eq. (2) are useful only at the physical value of the pion mass. Extrapolation formulas are available in Refs. \[^11, 11\].
\(-2.61 \text{ GeV}^{-2} < \bar{d}_{16} < 2.43 \text{ GeV}^{-2}\) encompasses both analyses, \(i.e. \Delta g_A^{(0)} = 1.10 - 1.52\). As naturalness suggests \(|\bar{d}_{16}| \sim 1\), this range of values does not introduce anomalously large low-energy constants into the chiral expansion. This experimental/theoretical uncertainty therefore provides an estimate of the importance of neglected higher orders in the chiral expansion. In Fig. 1 (left panel), we illustrate (dashed curves) the spread of the fit curve when one replaces \(f\) and \(g_A\) by their chiral limit values, including the range of \(\bar{d}_{16}\) values.

It is important to realize that all curves encompassed by the gray region of Fig. 1 (left panel), between the dashed curves, differ only by terms that are higher order, \(O(m_q^5/2)\), in the chiral expansion. The spread of curves in Fig. 1 (left panel) therefore suggests a 50% error associated with neglected higher orders in the chiral expansion at the lattice point with the lowest pion mass. We also perform a second fit with select chiral-limit values of \(f\) and \(g_A\), see Table I (Fit 2 (IR)), and again considering variation in the chiral limit values. The first and second fit are shown in Fig. 1 (right panel), together with the spread (dashed and dotted curves) of the fit curves when one replaces \(f\) and \(g_A\) by their chiral limit values, including the range of \(\bar{d}_{16}\) values. The spread of curves in Fig. 1 (right panel), suggests an 80% error at the lattice point with the lowest pion mass.

![Figure 2](image-url)

**FIG. 2:** Left panel: The nucleon mass in baryon \(\chi PT\) (computed using dim reg with \(MS\)) at \(O(m_N^2)\) (parameters given in Table I (Fit 1 (DR))) vs. the pion mass squared. Symbols are unquenched lattice QCD data taken from Ref. [2, 5, 6, 7]. The solid curve is the fit curve and the dashed curves give maximal variations due to the spread in chiral limit values of \(f\) and \(g_A\), as explained in the text. The gray region corresponds to the error associated with omitted higher orders. Right panel: Same but with a second fit (parameters given in Table I (Fit 2 (DR))) with corresponding spread in the chiral limit values of \(f\) and \(g_A\).

3 We emphasize that even if \(\bar{d}_{16}\) (and therefore \(g_A^{(0)}\)) were known with high precision, varying \(\bar{d}_{16}\) over a range of natural values would continue to be a legitimate way of estimating errors due to omitted higher-order effects.

4 Notice that although the parameter \(e_1(1 \text{ GeV})\) appears rather large, we have defined \(e_1\) as in Refs. [1, 2] which has absorbed a factor of 4 into its definition as compared to the parameter to which naturalness arguments should be applied. Hence, all values of \(e_1\) in Table I are technically quite natural.
It is interesting to compare the error analysis performed using infrared regularization with the same analysis performed using dimensional regularization (dim reg) with \( \overline{\text{MS}} \); as physics must be independent of the regulator, so must the results of the error analysis. The nucleon mass in dim reg with \( \overline{\text{MS}} \) at \( O(m^2) \) in the chiral expansion is given by \( m_N = M_0 - 4c_1m^2 - \frac{3g_A^2}{16\pi^2 f^2}m^3 + \left[e_1(\mu) + \frac{3}{32\pi^2 f^2}\left(-\frac{g_A^2}{M_0} + \frac{c_2}{2}\right) - \frac{3}{16\pi^2 f^2}\left(\frac{g_A^2}{M_0} - 8c_1 + c_2 + 4c_3\right)\ln\frac{m}{\mu}\right]m^4 \). (3)

 Again one easily finds a fit to unquenched lattice QCD data over a wide range of pion masses. In Table II (Fit 1 (DR)) we list a set of parameter values which give rise to the solid curve in Fig. 2 (left panel). Again we consider variations in the chiral limit values of \( f \) and \( g_A \) (gray region) and perform another fit (see Table II (Fit 2 (DR)) and Fig. 2 (right panel)). We find very little difference in the error analyses for the two regularization schemes.

Our results are summarized in Fig. 3 which plots the errors in the nucleon mass extrapolation curves taken from Figs. 1 and 2; the curves take into account the error associated with the gray regions in Figs. 1 and 2. Clearly the chiral expansion is nicely convergent in the vicinity of the physical pion mass. In our view the dashed curves (right panels of Figs. 1 and 2) give a conservative estimate of the errors. If one is willing to tolerate a 20% error associated with neglected higher-order terms for an \( O(m^2) \) calculation, then the error analysis would indicate that one is in the chiral regime for \( m_{\pi} \lesssim 300 \text{ MeV} \). If one instead takes the errors given by the solid curves (left panels of Figs. 1 and 2), willingness to tolerate a 20% error would indicate that one is in the chiral regime for \( m_{\pi} \lesssim 400 \text{ MeV} \). It may appear odd that our estimate of the boundary of the chiral regime is less than the kaon mass, which governs the convergence of \( SU(3) \) baryon \( \chi \)PT. We stress that the convergence of the chiral expansion is process and flavor dependent; for instance, some observables in \( SU(3) \) baryon \( \chi \)PT converge well and others do not.

The method used here to estimate errors is, of course, only one method among many to quantify the reliability of perturbation theory. For instance, by comparing various orders in the chiral expansion, Ref. \cite{17} finds that one is in the chiral regime for \( m_{\pi} \lesssim 500 \text{ MeV} \). An interesting finding of this work is that the \( O(m^2) \) correction remains a small perturbation on the \( O(m^3/2) \) result for \( m_{\pi} < 600 \text{ MeV} \). It is important to emphasize that error analyses such as that presented in this note and in Ref. \cite{17} are merely indicative. We believe that we have given a conservative estimate of the errors, as they presently stand. Naively, one way of weakening the strength of higher-dimensional operators, and thereby reducing the error, is to include the \( \Delta \) as an explicit degree of freedom in \( \chi \)PT. It may also be possible to reduce the extrapolation error at larger pion masses by computing \( M_N, g_A \) and \( f \) in the same lattice simulation in order to fix the lattice values of \( d_{16} \) and \( l_4 \). It is clear from the results presented here that a definitive determination of the boundary of the chiral regime

---

5 Refs. \cite{1, 2} use the nomenclature “relativistic \( \chi \)PT” to describe infrared regularization; we dislike this appellation as it may be misinterpreted to suggest that there is physics in the regulator.

6 As very-few quantities have been computed including the \( \Delta \) at non-trivial orders in baryon \( \chi \)PT, it is presently unclear whether or not this is the case.

7 This parameter also provides a major source of uncertainty in the quark-mass dependence of the deuteron binding energy \cite{10, 11}.
FIG. 3: Errors in the nucleon mass extrapolation curves vs. the pion mass squared. The solid lines correspond to the errors abstracted from the left panels of Figs. 1 and 2; they each arise from the effect of $\Delta g_A^{(0)}$ and $f^{(0)}$ on a single fit (Fit 1), performed with the physical values of $g_A$ and $f$. The dashed lines correspond to the errors abstracted from the right panels of Figs. 1 and 2; same as above but supplemented with the effect of $\Delta g_A^{(0)}$ and $f^{(0)}$ on a second fit (Fit 2), performed with select chiral-limit values of $g_A$ and $f$. The horizontal dotted lines indicate 10% and 20% errors. The star indicates the physical pion mass.

will not be possible until these strong-interaction parameters are well determined. Finally, it is clear that by imposing various prejudices on our model-independent analysis, one may shrink the gray regions of Figs. 1 and 2 to any desired size.

In this note we have provided evidence that the quark-mass dependence — and by association, the finite-size and lattice-spacing dependence — of currently-extant unquenched lattice QCD data for the nucleon mass are not presently described by a perturbative effective field theory with a controlled error estimate. Hence these lattice data cannot be reliably extrapolated to predict nucleon properties. In our view, a symbiotic relationship between lattice QCD and baryon chiral perturbation theory which will lead to first-principles predictions of baryon properties with meaningful errors must await smaller lattice quark masses.

I would like to thank Maarten Golterman, Thomas Hemmert, Ulf Meißner and Martin Savage for helpful comments/discussions. This work was partly supported by DOE contract DE-AC05-84ER40150, under which the Southeastern Universities Research Association (SURA) operates the Thomas Jefferson National Accelerator Facility.
[1] M. Procura, T.R. Hemmert and W. Weise, *Phys. Rev.* **D69**, 034505 (2004).
[2] A. Ali Khan *et al.* [QCDSF-UKQCD Collaboration], *hep-lat/0312030*.
[3] For a recent discussion, see C. Bernard, S. Hashimoto, D.B. Leinweber, P. Lepage, E. Pallante, S.R. Sharpe and H. Wittig, *Nucl. Phys. Proc. Suppl.* **119**, 170 (2003).
[4] T. Becher and H. Leutwyler, *Eur. Phys. J.* **C9**, 643 (1999).
[5] C.R. Allton *et al.* [UKQCD Collaboration], *Phys. Rev.* **D65**, 054502 (2002).
[6] A. Ali Khan *et al.* [CP-PACS Collaboration], *Phys. Rev.* **D65**, 054505 (2002); [Erratum-ibid. **D67**, 059901 (2003)].
[7] S. Aoki *et al.* [JLQCD Collaboration], *Phys. Rev.* **D68**, 054502 (2003).
[8] N. Fettes, V. Bernard and U.-G. Meißner, *Nucl. Phys.* **A669**, 269 (2000).
[9] J. Gasser and H. Leutwyler, *Annals Phys.* **158**, 142 (1984).
[10] S.R. Beane and M.J. Savage, *Nucl. Phys.* **A717**, 91 (2003).
[11] E. Epelbaum, U.-G. Meißner and W. Glockle, *Nucl. Phys.* **A714**, 535 (2003).
[12] G. Colangelo, J. Gasser and H. Leutwyler, *Nucl. Phys.* **B603**, 125 (2001).
[13] N. Fettes, JUL-3814 (PhD Thesis).
[14] T.R. Hemmert, M. Procura and W. Weise, *Phys. Rev.* **D68**, 075009 (2003).
[15] N. Fettes, U.-G. Meißner, M. Mojzis and S. Steininger, *Annals Phys.* **283**, 273 (2000).
[16] S. Steininger, U.-G. Meißner and N. Fettes, *JHEP* **9809**, 008 (1998).
[17] V. Bernard, T.R. Hemmert and U.-G. Meißner, *Nucl. Phys.* **A732**, 149 (2004).