Physical Nucleon Properties from Lattice QCD

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We investigate various resummations of the chiral expansion and fit to the extremely accurate lattice QCD data for the mass of the nucleon recently obtained by the CP-PACS group. Using a variety of finite-range regulators, we demonstrate a remarkably robust chiral extrapolation of the nucleon mass. The systematic error associated with the chiral extrapolation alone is estimated to be less than 1%.

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Hadronic physics presents fascinating theoretical challenges to the understanding of strongly interacting systems in terms of their fundamental degrees of freedom in QCD, quarks, and gluons. Lattice gauge theory [1] has so far provided the only rigorous method for solving nonperturbative QCD. We will show that recent progress within the field [2] together with advances in effective field theory (EFT) [3] now permit systematically accurate chiral extrapolations of observables, enabling the determination of the physical properties of hadrons from lattice QCD simulations, even though it is not yet feasible to make calculations at the physical quark mass.

It is now possible to make extremely accurate lattice QCD calculations of the masses of hadrons, such as the nucleon, with dynamical fermions. Indeed the CP-PACS group has just reported data with a precision of order 1% [2]. However, such precise evaluations are limited to quark masses an order of magnitude larger than those found in nature. In order to compare with experiment, which is after all one of the main aims in the field, it is therefore necessary to extrapolate in quark mass. Such an extrapolation is complicated by the unavoidable nonanalytic behavior in quark mass, which arises from Goldstone boson loops in QCD with dynamically broken chiral symmetry [4].

Early work motivated by the important role of Goldstone bosons led to the construction of chiral quark models [5], which incorporated this nonanalytic behavior. An alternative, systematic approach, designed to avoid reference to a model, involved the construction of an effective field theory to describe QCD at low energy [6]. The application to baryons has developed to the point where chiral perturbation theory (χPT) is now understood as a rigorous approach near the chiral limit [7,8].

Because it is defined as an expansion in momenta and masses about the chiral limit, χPT provides an attractive approach to the problem of quark mass extrapolation for lattice QCD. The advantages of formulating χPT with a finite-range regulator (FRR), as opposed to the commonly implemented dimensional regularization (DR), have been demonstrated by Donoghue *et al.* [9]. Early implementations of a FRR to evaluate chiral loop integrals in χPT suggested that, in the context of the extrapolation of lattice data from relatively large quark masses, FRR provides a more reliable procedure [10,11]. There has been considerable debate on whether current lattice data are within the scope of dimensionally regularized χPT or whether the form of the FRR chosen introduces significant model dependence [12]. However, this issue has now been addressed in a recent detailed study of numerous regularization schemes in χPT, both dimensional and FRR [3]. This study quantified the applicable range of the EFT and established that all of the FRR considered provided equivalent results over the range $m_\pi^2 \lesssim 0.8$ GeV^2.

Here we demonstrate that by adopting the FRR formulation of χPT one can improve its convergence properties to the point where the chiral extrapolation to the physical quark mass can be carried out with a systematic uncertainty of less than 1%. Given this remarkable result, the current errors on extrapolated quantities are dominated by the statistical errors arising from the large extrapolation distance—the lightest simulated pion mass being typically $m_\pi^2 \simeq 0.27$ GeV^2, in comparison with the physical value, 0.02 GeV^2.

In the usual formulation of effective field theory, the nucleon mass as a function of the pion mass (given that $m_\pi^2 \propto m_q$ [13]) has the formal expansion

$$M_N = a_0 + a_2 m_\pi^2 + a_4 m_\pi^4 + a_6 m_\pi^6 + \cdots + \sigma_{NN}^\pi + \sigma_{N\Delta}^\pi + \sigma_{\rm tad}^\pi. \quad (1)$$

In principle, the coefficients, a_n, can be expressed in terms of the parameters of the underlying effective Lagrangian to a given order of chiral perturbation theory. In practice, for current applications to lattice QCD, the parameters must be determined by fitting to the lattice results themselves. The additional terms, σ_{NN}^π, $\sigma_{N\Delta}^\pi$, and $\sigma_{\rm tad}^\pi$, are loop corrections involving the (Goldstone) pion, which yield the leading (LNA) and next-to-leading nonanalytic (NLNA) behavior of M_N. As these terms involve the coupling constants in the chiral limit, which are essentially model independent [14], the only additional complication they add is that the ultraviolet behavior of the loop integrals must be regulated in some way.

Traditionally, one uses dimensional regularization, which (after infinite renormalization of a_0 and a_2) leaves only the nonanalytic terms, $c_{\rm LNA} m_\pi^3$ and $c_{\rm NLNA} m_\pi^4 \times \ln(m_\pi/\mu)$, respectively. (Note that the coefficient $c_{\rm LNA}$ is the sum of contributions from the $N \to \Delta\pi$ and tadpole diagrams.) Within dimensional regularization, one then arrives at a truncated power series for the chiral expansion,

$$M_N = c_0 + c_2 m_\pi^2 + c_{\rm LNA} m_\pi^3 + c_4 m_\pi^4 + c_{\rm NLNA} m_\pi^4 \ln\frac{m_\pi}{\mu} + c_6 m_\pi^6 + \cdots, \tag{2}$$

where the bare parameters, a_i, have been replaced by the finite, renormalized coefficients, c_i. Through the chiral logarithm, one has an additional mass scale, μ, but the dependence on this is eliminated by matching c_4 to "data" (in this case, lattice QCD). We work to fourth order in the chiral expansion and include the next analytic term to compensate short-distance physics contained in the NLNA loop integrals, as suggested in Ref. [9]. Provided the series expansion in Eq. (2) is convergent over the range of values of m_π where the lattice data exist, one can then use Eq. (2) to evaluate M_N at the physical pion mass. Unfortunately, there is considerable evidence that this series is not sufficiently convergent [3,12,15–17].

In line with the implicit μ dependence of the coefficients in the familiar dimensionally regulated χPT, the systematic FRR expansion of the nucleon mass is

$$M_N = a_0^\Lambda + a_2^\Lambda m_\pi^2 + a_4^\Lambda m_\pi^4 + a_6^\Lambda m_\pi^6 + \sigma_{NN}^\pi(m_\pi, \Lambda) + \sigma_{N\Delta}^\pi(m_\pi, \Lambda) + \sigma_{\rm tad}^\pi(m_\pi, \Lambda), \tag{3}$$

where the dependence on the *shape* of the regulator is implicit. The dependence on the value of Λ and the choice of regulator are eliminated, to the order of the series expansion, by fitting the coefficients, a_n^Λ, to lattice QCD data. The clear indication of success in eliminating model dependence, and hence having found a suitable regularization method, is that the higher order coefficients (a_i^Λ, $i \geq 4$) should be small and that the renormalized coefficients, c_i, and the result of the extrapolation should be insensitive to the choice of ultraviolet regulator.

The key feature of finite-range regularization is the presence of an additional adjustable regulator parameter which provides an opportunity to suppress short-distance physics from the loop integrals of effective field theory. This short-distance physics is otherwise treated incorrectly, as the effective fields are not realized in QCD at short distances. As emphasized in Eq. (3) by the superscripts Λ, the unrenormalized coefficients of the analytic terms of the FRR expansion are regulator-parameter dependent. The large m_π behavior of the loop integrals and the residual expansion (the sum of the a_i^Λ terms) are remarkably different. Whereas the residual expansion will encounter a power divergence, the FRR loop integrals will tend to zero as a power of Λ/m_π as m_π becomes large. Thus, Λ provides an opportunity to govern the convergence properties of the residual expansion and thus the FRR chiral expansion. Since hadron masses are observed to be smooth, almost linear functions of m_π^2 for quark masses near and beyond the strange quark mass [18], it should be possible to find values for the regulator-range parameter, Λ, such that the coefficients a_4^Λ and higher are truly small. In this case, the convergence properties of the residual expansion and the loop expansion are excellent and their truncation benign [19].

In order to investigate the model dependence associated with the truncations of the chiral expansions, several regulators are considered. We evaluate the loop integrals in the heavy baryon limit

$$\sigma_{BB'}^\pi = -\frac{3}{16\pi^2 f_\pi^2} G_{BB'} \int_0^\infty dk \frac{k^4 u^2(k)}{\omega(k)[\omega_{BB'} + \omega(k)]}, \tag{4}$$

$$\sigma_{\rm tad}^\pi = -\frac{3}{16\pi^2 f_\pi^2} c_2 m_\pi^2 \left\{ \int_0^\infty dk \left(\frac{2k^2 u^2(k)}{\sqrt{k^2 + m_\pi^2}} \right) - t_0 \right\}, \tag{5}$$

taking $u(k)$ to be either a sharp cutoff, a dipole, a monopole, or finally a Gaussian. These regulators have very different shapes, with the only common feature being that they suppress the integrand for momenta greater than Λ. In Eq. (4) we have $G_{NN} = g_A^2$ (with $g_A = 1.26$) and $G_{N\Delta} = 16 g_A^2/9$ (to reproduce the empirical width of the Δ resonance). In addition, $\omega(k) = \sqrt{k^2 + m_\pi^2}$, $\omega_{NN} = 0$, and $\omega_{N\Delta} = 292$ MeV, the physical Δ-N mass splitting. In Eq. (5) t_0, defined such that the term in braces vanishes at $m_\pi = 0$, is a local counter term introduced in FRR to ensure a linear relation for the renormalization of c_2.

In addition, we also consider the case where Eq. (2) is modified to maintain the correct branch-point (BP) structure at $m_\pi = \omega_{N\Delta}$ [20], in particular,

$$\sigma_{N\Delta}^\pi = -\frac{3}{16\pi^2 f_\pi^2} G_{N\Delta} \left\{ \frac{1}{4}(2\Delta^3 - 3m^2\Delta) \log\left(\frac{m^2}{\mu^2}\right) - \frac{1}{2}(\Delta^2 - m^2)^{3/2} \times \log\left(\frac{\Delta - \sqrt{\Delta^2 - m^2}}{\Delta + \sqrt{\Delta^2 - m^2}} \right) \right\}. \tag{6}$$

One can now compare the expansion about the chiral limit for these six different regularization schemes in order to assess their rate of convergence. It turns out that all the FRR expansions precisely describe the dimensional regularization expansion over the range $m_\pi^2 \in (0, 0.7)$ GeV^2. Furthermore, the smooth, FRR formulations are consistent with each other, for the renormalized chiral coefficients, $c_{0,2,4}$, to an extraordinarily precise level [3]. This ensures a systematically accurate extrapolation to the regime of physical quark masses.

For this study we use recent precision nucleon mass data obtained in lattice QCD by CP-PACS [2]. Simulations are performed using the mean-field improved clover fermion action with the Iwasaki gluon

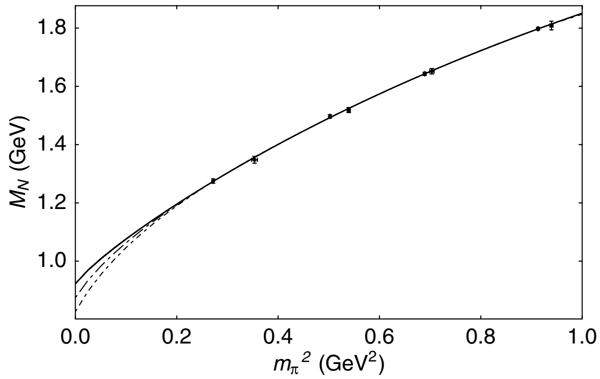

FIG. 1. Fits to lattice data for various ultraviolet regulators. The sharp cutoff, monopole, dipole, and Gaussian cases are depicted by solid lines, *indistinguishable* on this plot. The dimensional regularized forms are illustrated by the dash-dotted curves, with the correct branch point corresponding to the higher curve. Lattice data are from Ref. [2].

action, known to provide small scaling violations. We choose the largest volumes at the two smallest lattice spacings [21] such that the results are good approximations to the continuum theory. These data are used to determine the unknown parameters, a_0–a_6, in Eq. (3) for each choice of regularization. Only in the naive, dimensionally regulated form, i.e., without the $N \to \Delta\pi$ branch structure of Eq. (6), do the a_i coincide with the c_i of Eq. (2). It is only the extreme accuracy of the data which makes the determination of as many as four parameters possible.

Figure 1 shows the resulting fits to the lattice data over the range $m_\pi^2 \in (0, 1.0)\,\mathrm{GeV}^2$, with the corresponding parameters given in Table I. It is remarkable that all four curves based on FRR are indistinguishable on this plot. Furthermore, we see from Table I that the coefficient of m_π^4 in all of those cases is quite small—an order of magnitude smaller than the dimensionally regularized forms. Similarly, the FRR coefficients of m_π^6 are again much smaller than their DR counterparts. This indicates that the residual series, involving a_i, is converging when the chiral loops are evaluated with a FRR.

TABLE I. Bare, unrenormalized, parameters extracted from the fits to lattice data displayed in Fig. 1. All quantities are in units of appropriate powers of GeV and $\mu = 1$ GeV in Eq. (2). Dim. stands for dimensional and BP for the branch-point form defined in Eq. (6).

Regulator	a_0	a_2	a_4	a_6	Λ	χ^2/dof
Dim. regulator	0.827	3.58	3.63	−0.711	···	0.43
Dim. regulator (BP)	0.792	4.15	8.92	0.384	···	0.41
Sharp Cutoff	1.06	1.47	−0.554	0.116	0.4	0.40
Monopole	1.74	1.64	−0.485	0.085	0.5	0.40
Dipole	1.30	1.54	−0.492	0.089	0.8	0.40
Gaussian	1.17	1.48	−0.504	0.095	0.6	0.40

TABLE II. Renormalized expansion coefficients in the chiral limit obtained from various regulator fits to lattice data. (All quantities are in units of appropriate powers of GeV.) Errors are statistical in origin arising from lattice data. Deviations in the central values indicate systematic errors associated with the chiral extrapolation.

Regulator	c_0	c_2	c_4
Dim. regulator	0.827(120)	3.58(50)	3.6(15)
Dim. regulator (BP)	0.875(120)	3.14(50)	7.2(15)
Sharp cutoff	0.923(130)	2.61(66)	15.3(16)
Monopole	0.923(130)	2.45(67)	20.5(30)
Dipole	0.922(130)	2.49(67)	18.9(29)
Gaussian	0.923(130)	2.48(67)	18.3(29)

As explained by Donoghue *et al.* [9], one can combine the order $m_\pi^{0,2,4\ldots}$ terms from the self-energies with the "bare" expansion parameters, $a_{0,2,4\ldots}$, to obtain physically meaningful renormalized coefficients. These are shown in Table II, in comparison with the corresponding DR coefficients found using Eq. (2). Details of this renormalization procedure are given in Ref. [3]. The degree of consistency between the best-fit values found using all choices of FRR is remarkably good. On the other hand, DR significantly underestimates c_4. We can understand the problem very simply; it is not possible to accurately reproduce the necessary $1/m_\pi^2$ behavior of the chiral loops (for $m_\pi > \Lambda$) with a third order polynomial in m_π^2.

It is clear that the use of an EFT with a FRR enables one to make an accurate extrapolation of the nucleon mass as a function of the quark mass. Although minimal deviation is seen between the best-fit curves, we need to determine how well these curves are in fact constrained by the statistical uncertainties of the lattice data. As all data points are statistically independent, the one-sigma deviation from the best-fit curve is defined by the region for $(\chi^2 - \chi^2_{\rm min})/\mathrm{dof} < 1$. We use a standard χ^2 measure, weighted by the squared error of the simulated data point, and $\chi^2_{\rm min}$ corresponds to the optimum fit to the data.

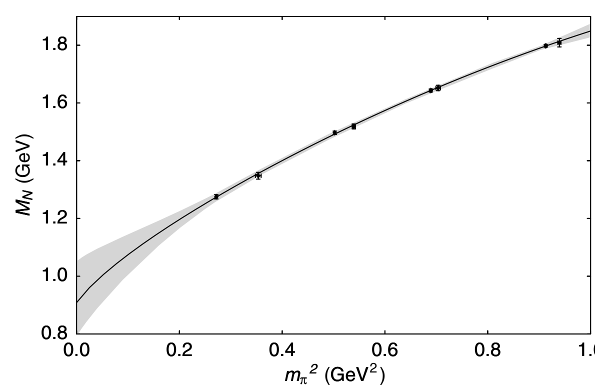

FIG. 2. Error analysis for the extraction of the nucleon mass using a dipole regulator. The shaded region corresponds to the region allowed within the present statistical errors.

TABLE III. The nucleon mass, m_N (GeV), and the sigma commutator, σ_N (MeV), extrapolated to the physical pion mass obtained in a NLNA (fourth order) chiral expansion. Convergence of the expansion is indicated by the nucleon mass obtained in an analysis where we retain only the LNA (third order) behavior.

Regulator	LNA m_N	NLNA m_N	NLNA σ_N
Dim. regulator	0.784	0.884 ± 0.103	50.3 ± 10.0
Dim. regulator (BP)	0.784	0.923 ± 0.103	42.7 ± 10.0
Sharp cutoff	0.968	0.961 ± 0.116	34.0 ± 13.0
Monopole	0.964	0.960 ± 0.116	33.0 ± 13.0
Dipole	0.963	0.959 ± 0.116	33.3 ± 13.0
Gaussian	0.966	0.960 ± 0.116	33.2 ± 13.0

We show the one-sigma variation from the best-fit dipole curve by the shaded region in Fig. 2. The primary source of the large error band is the large extrapolation distance. It is clear that a simulated point at a pion mass, $m_\pi^2 \sim 0.1$ GeV^2, would greatly reduce the statistical error in the extrapolation. The extrapolated values for the nucleon mass are shown in Table III [25]. It is especially interesting to observe the very small difference between the physical nucleon masses obtained with each FRR when we go from LNA to NLNA, i.e., when the effect of the Δ is included. (The change is typically a few MeV for a FRR but more than 100 MeV for DR.) Once again the convergence properties of the FRR expansion are remarkable.

To summarize, we have shown that the extremely precise dynamical simulation data from CP-PACS permit one to determine four parameters in the chiral extrapolation formulas, Eqs. (2) and (3). Whereas the former (involving dimensional regularization) does not appear to be convergent over the required mass range, the improved convergence properties of the finite-range regularized expansion yield an excellent description of the data over the full mass range, regardless of the functional form chosen for the vertex regulator. Table III summarizes the resulting values of the physical nucleon mass and sigma commutator. The systematic error in the chiral extrapolation, based upon a smooth FRR, is less than 1% for the nucleon mass and within 2% for the sigma commutator. We note also that the systematic uncertainty in the determination of the low energy constant, c_0, is less than 1%, while for c_2 it is at the level of a few percent. With the issue of chiral extrapolation addressed, there is an urgent need for high precision lattice QCD simulations at $m_\pi^2 \sim 0.1$ GeV^2 in order to reduce the present statistical error on the extrapolation. Such simulations should be feasible with the new generation of computers dedicated to lattice QCD currently under construction.

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