Physical Nucleon Properties from Lattice QCD

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We demonstrate that the extremely accurate lattice QCD data for the mass of the nucleon recently obtained by CP-PACS, combined with modern chiral extrapolation techniques, leads to a value for the mass of the physical nucleon which has a systematic error of less than one percent.

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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. Traditional perturbative methods in quantum field theory cannot account for the highly non-trivial structure of the QCD vacuum – which is dominated by large scale quark and gluon correlations. Lattice gauge theory has so far provided the only rigorous method of solving non-perturbative QCD. We will show that recent progress within the field, together with advances in effectively field theory (EFT), now permit the accurate, model-independent extraction 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 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 necessary to extrapolate in quark mass. It is well known that such an extrapolation is complicated by the unavoidable non-analytic behaviour 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 [3], which incorporated this non-analytic behavior. An alternative, systematic approach, designed to avoid reference to a model, involved the construction of an effective field theory (EFT) to describe QCD at low energy [4]. The application to baryons has developed to the point where chiral perturbation theory ($\chi$PT) is now understood as a rigorous approach near the chiral limit [4,8].

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

Here we demonstrate that by adopting the FRR formulation of $\chi$PT one can improve its convergence properties to the point where the chiral extrapolation to the physical quark mass can be carried out in a model-independent way with a systematic uncertainty of less than one percent. 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 $m^2_{\pi,0} \approx 27$ 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 $m^2_{\pi} \propto m_q$ [12]) has the formal expansion:

$$ M_N = a_0 + a_2 m^2_{\pi} + a_4 m^4_{\pi} + a_6 m^6_{\pi} + \ldots + \sigma_{N\pi} + \sigma_{\Delta\pi}. \quad (1) $$

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, $\sigma_{N\pi}$ and $\sigma_{\Delta\pi}$, are the two self-energy terms involving the (Goldstone) pion which yield the leading and next-to-leading non-analytic behaviour of $M_N$. As these terms involve the coupling constants in the chiral limit, which are essentially model-
independent \textsuperscript{13}, the only additional complication they add is that the ultra-violet behaviour of the loop integrals must be regulated in some way.

Traditionally, one uses dimensional regularisation which (after infinite renormalisation of all even powers of $m_\pi$) leaves only the non-analytic terms $-c_{\text{LNA}}m_\pi^3$ and $c_{\text{NLNA}}m_\pi^4 \ln(m_\pi/\mu)$, respectively. Within dimensional regularisation one then arrives at a truncated power series for the chiral expansion,

$$M_N = c_0 + c_2 m_\pi^2 + c_{\text{LNA}} m_\pi^3 + c_{\text{NLNA}} m_\pi^4$$

$$+ c_{\text{NLNA}} m_\pi^4 \ln(m_\pi/\mu) + c_6 m_\pi^6 + \ldots ,$$

where the bare parameters, $a_i$, have been replaced by the finite, renormalised coefficients, $c_i$. Through the chiral logarithm one has an additional mass scale, $\mu$, but the dependence on this is eliminated by matching $c_\mu$ to “data” (in this case lattice QCD). Provided the series expansion in Eq. (2) is convergent over the range of values of $m_\pi$ where the lattice data exists, 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 \textsuperscript{8,11,13,15,16}.

The physical reason for the lack of convergence seems to be that, apart from the usual symmetry breaking scale in $\chi$PT, $\Lambda_{\chi\text{SB}} \sim 4\pi f_\pi \sim 1$ GeV, there is another mass scale in the problem which does not appear explicitly in a dimensionally regularised theory. This additional scale, $\Lambda$, is the inverse of the size of the nucleon, the source of the pion cloud \textsuperscript{17}. Of course, this scale must appear implicitly in the correct effective field theory as a correlation between the coefficients $c_n$. However, since we want to access pion masses above 0.5 GeV and the nucleon size of 0.5–1.0 fm suggests $\Lambda \sim 0.4$ GeV, it is clear that $m_\pi/\Lambda > 1$ and the naive series should not be expected to converge over the range of pion masses of interest. This problem can be overcome through the use of a FRR \textsuperscript{8,13,14}.

Clearly, in extracting information from lattice data for physical hadrons one must avoid model dependence. In line with the implicit $\mu$-dependence of the coefficients in the familiar dimensionally regulated $\chi$PT, in the case of a FRR the systematic expansion of the nucleon mass is:

$$M_N = a_0^N + a_2^N m_\pi^2 + a_4^N m_\pi^4$$

$$+ a_6^N m_\pi^6 + \sigma_{\pi N}(m_\pi, \Lambda) + \sigma_{\Delta N}(m_\pi, \Lambda),$$

where the dependence on the shape of the regulator is implicit. As for the mass scale, $\mu$, entering the usual chiral logarithms, the dependence on the value of $\Lambda$ and the choice of regulator is once again eliminated, to the order of the series expansion, by fitting the coefficients, $a_i^N$, to lattice data. The clear indication of success in eliminating model dependence and hence having found a suitable regularisation method, is that the higher order coefficients (for the best fit value of $\Lambda$) should be small and that the result of the extrapolation should be insensitive to the shape of the ultraviolet regulator.

In order to investigate the model dependence associated with the self-energies, several regulators are considered. We evaluate the loop integrals in the heavy baryon limit

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

taking $u(k)$ to be either a sharp cut-off, $\theta(\Lambda - k)$, a dipole, $(1 + k^2/\Lambda^2)^{-2}$, a monopole, $(1 + k^2/\Lambda^2)^{-1}$ or finally a Gaussian, $\exp(-k^2/\Lambda^2)$. We note that the dipole is the most physical, in that the observed axial form factor of the nucleon has this shape \textsuperscript{13}. In Eq. (4) for $B = B'$ we have $G_{NN} = g_A^2$ (with $g_A = 1.26$), while $G_{N\Delta} = 32g_A^2/25$, the SU(6) value. In addition, $\omega(k) = \sqrt{k^2 + m_\pi^2}, \omega_{BB'} = 0$ and $\omega_{N\Delta} = 292$ MeV, the physical $\Delta$-N mass splitting. Clearly the four choices of regulator have very different shapes, with the only common feature being that they suppress the integrand for momenta greater than $\Lambda$.

In addition to the FRR expansions of Eq. (5) and the standard dimensionally regulated expansion of Eq. (2), we also consider the case where Eq. (2) is modified to maintain the square-root branch-cut at $m_\pi = \omega_{N\Delta}$ \textsuperscript{3}. One can now compare the expansion about the chiral limit for these six different regularisation 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\textsuperscript{2}. Furthermore, the smooth, FRR formulations are consistent with each other, for the renormalized chiral coefficients, $a_{0,2,4}$, to an extraordinarily precise level \textsuperscript{8}. This ensures a reliable extrapolation to the regime of physical quark masses.

We now exploit the accuracy of the most recent CP-PACS data \textsuperscript{2} by using it to determine either the first four unknown parameters, $c_0 - c_6$, appearing in Eq. (2) (i.e. using dimensional regularisation, with and without the $\Delta \to N\pi$ branch point) or the four parameters $a_0, a_2, a_4$ and $\Lambda$ in Eq. (3), for each choice of ultra-violet regulator \textsuperscript{13}. It is only the extreme accuracy of the data which makes the determination of as many as four parameters possible. Figure 1 shows the result of fits to the lattice data over the range $m_\pi^2 \in (0, 1.0)$ GeV\textsuperscript{2}, with the corresponding parameters given in Table I. It is remarkable that three of the four curves based on Eq. (3), the dipole, monopole and Gaussian cases, are indistinguishable on this plot. Furthermore, we see from Table I that the coefficient of $m_\pi^4$ in all of those cases is quite small – an order of magnitude smaller than the higher order coefficients obtained using Eq. (2), which also oscillate in sign. This indicates that the residual series, involving $a_{0,2,4}$, is converging when the chiral non-analytic behaviour is evaluated with a FRR.
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The monopole, dipole and Gaussian cases are depicted by
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the fits to lattice data displayed in Figure 1. (All quantities
TABLE I: Bare, unrenormalised, parameters extracted from
FIG. 1: Fits to lattice data for various ultra-violet regulators.
The monopole, dipole and Gaussian cases are depicted by
solid lines, indistinguishable on this plot, the sharp cutoff
is shown by the dashed curve. The dimensional regularised
forms are illustrated by the dash-dot curves, with the correct
branch point corresponding to the higher curve. Lattice data
is from Ref. [2].

| Regulator       | $a_0$ | $a_2$ | $a_4$ | $a_6$ | $\Lambda$ |
|-----------------|-------|-------|-------|-------|---------|
| Dim. Reg.       | 0.700 | 5.10  | 3.87  | −2.35 | −       |
| Dim. Reg. (BP)  | 0.691 | 5.32  | 7.65  | −1.36 | −       |
| Sharp Cutoff    | 1.06  | 0.06  | −0.249| −     | 0.440   |
| Monopole        | 1.38  | 0.950 | −0.217| −     | 0.443   |
| Dipole          | 1.15  | 0.998 | −0.227| −     | 0.732   |
| Gaussian        | 1.11  | 1.02  | −0.234| −     | 0.593   |

TABLE I: Bare, unrenormalised, parameters extracted from
the fits to lattice data displayed in Figure 1. (All quantities
are in units of appropriate powers of GeV and $\mu = 1$ GeV in
Eq. (2).)

As explained by Donoghue et al. [2], one can combine
the order $m_{\pi}^{2,4}$ terms from the self-energies with the
“bare” expansion parameters, $a_{0,2,4}$, to obtain physically
meaningful renormalized coefficients. These are shown
in Table III in comparison with the corresponding 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 three smooth
choices of FRR is remarkably good, whereas the large numerical
values and the change of sign in the coefficients
found from the fit using Eq. (2) suggest that the latter
is nowhere near convergence. We can understand the problem very simply; it is not possible to accurately re-
produce the necessary $1/m_{\pi}^2$ behaviour of the chiral loops
(for $m_{\pi} > \Lambda$) with a 3rd order polynomial in $m_{\pi}^2$. The
final point to notice about the finite range regulators is
that all but the sharp cutoff naturally yield a correction
to the Goldberger-Treiman relation of approximately the
right size. As shown by Birse and McGovern [20], this
correction dominates the non-analytic term of order $m_{\pi}^5$
which only arises at two loops in dimensionally regulated
$\chi$PT. The absence of the correct $m_{\pi}^2$ term in the case
of the sharp cutoff explains its slight deviation from the
results of the other FRR.

It is clear that the use of an EFT with FRR enables
one to make a model-independent 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 ($\chi^2 - \chi_{\text{min}}^2$)/dof < 1. We use a standard $\chi^2$
measure, weighted by the squared error of the simulated
data point and $\chi_{\text{min}}^2$ corresponds to the optimum fit to the
data. To preserve the infrared physics of EFT, we
put a lower bound of 300 MeV (just above the $N - \Delta$
mass splitting) on the regulator parameter, $\Lambda$.

We show the one-sigma variation from the best-fit
dipole curve by the shaded region in Figure 2. The
extrapolated values for the nucleon mass are shown in Table III. It is clear that the large lower-deviation on the extrapolated values are a result of the regulator mass not being constrained from above. Alternatively, for the
FRR cases, one could fix $\Lambda$ and vary an additional parameter, $a_6$, in the spirit of dimensional regularisation.
In that case the error bounds are symmetric and similar
in magnitude to those found for the dimensionally regulated
cases reported in Table III. The primary source of the large error band is the large extrapolation distance.

We also quote the $\sigma$-commutator in Table III — cal-
culated as $m_{\pi}^2 \partial M_N / \partial m_{\pi}^2$ at the physical pion mass [21].
Again the statistical errors are large. In this case, as well as
for the nucleon mass itself, it is clear that a simulated point at a pion mass $m_{\pi}^2 \sim 0.1 \text{ GeV}^2$ would greatly re-
duce the statistical error in the extrapolation. We note that our study has focused on the systematic errors asso-
ciated with chiral extrapolation, while those arising from
finite lattice spacing and volume [15, 22] remain to be quantified.

| Regulator       | $c_2$ | $c_4$ | $c_6$ |
|-----------------|-------|-------|-------|
| Dim. Reg.       | 0.700 | 5.10  | 3.87  |
| Dim. Reg. (BP)  | 0.750 | 4.59  | 6.43  |
| Sharp cutoff    | 0.892 | 3.16  | 12.9  |
| Monopole        | 0.914 | 2.63  | 26.1  |
| Dipole          | 0.910 | 2.72  | 23.4  |
| Gaussian        | 0.906 | 2.79  | 21.4  |

TABLE II: Renormalised expansion coefficients in the chiral
limit obtained from various regulator fits to lattice data. (All quantities
are in units of appropriate powers of GeV.)
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.

| Regulator | $m_N$ (GeV) | $\sigma_N$ (MeV) |
|-----------|-------------|-----------------|
| Dim. Reg. | $0.782^{+0.122}_{-0.122}$ | $73^{+15}_{-15}$ |
| Dim. Reg. (BP) | $0.823^{+0.122}_{-0.122}$ | $65^{+15}_{-15}$ |
| Sharp cutoff | $0.939^{+0.076}_{-0.219}$ | $41^{+35}_{-12}$ |
| Monopole | $0.955^{+0.063}_{-0.219}$ | $35^{+36}_{-8}$ |
| Dipole | $0.951^{+0.081}_{-0.217}$ | $36^{+33}_{-13}$ |
| Gaussian | $0.948^{+0.080}_{-0.216}$ | $37^{+35}_{-13}$ |

TABLE III: Here we show the nucleon mass, $m_N$ (GeV), and the sigma commutator, $\sigma_N$ (MeV), extrapolated to the physical pion mass.

To summarize, we have shown that the extremely precise dynamical simulation data from CP-PACS permits us 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 a finite range regulator yield an excellent description of the data over the full mass range, regardless of the functional form chosen for the vertex regulator. Table III summarises the resulting values of the nucleon mass and the $\sigma$-commutator evaluated at the physical pion mass. The nucleon mass is constrained by the chiral extrapolation technique based upon a FRR procedure to a systematic error less than 1%. The $\sigma$-commutator is similarly constrained to within a systematic error of 3%. The values obtained are both consistent with earlier extractions from lattice data using a similar technique and, within the relatively large statistical errors, in agreement with the experimental values. We note also that the systematic uncertainty in the extraction 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 model independence resolved, there is an urgent need for high precision lattice QCD simulations at $m^2 \sim 0.1 \text{ GeV}^2$ in order to reduce the present statistical error on the extrapolation. Such simulations should be feasible with the new generation of lattice QCD computers currently under construction.

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