Strong-Isospin Violation in the Neutron-Proton Mass Difference from Fully-Dynamical Lattice QCD and PQQCD

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Abstract

We determine the strong-isospin violating component of the neutron-proton mass difference from fully-dynamical lattice QCD and partially-quenched QCD calculations of the nucleon mass, constrained by partially-quenched chiral perturbation theory at one-loop level. The lattice calculations were performed with domain-wall valence quarks on MILC lattices with rooted staggered sea-quarks at a lattice spacing of \( b = 0.125 \) fm, lattice spatial size of \( L = 2.5 \) fm and pion masses ranging from \( m_\pi \sim 290 \) MeV to \( \sim 350 \) MeV. At the physical value of the pion mass, we predict \( M_n - M_p |^{d-u} = 2.26 \pm 0.57 \pm 0.42 \pm 0.10 \) MeV where the first error is statistical, the second error is due to the uncertainty in the ratio of light-quark masses, \( \eta = m_u/m_d \), determined by MILC [1], and the third error is an estimate of the systematic due to chiral extrapolation.
I. INTRODUCTION

It is a basic property of our universe that the neutron is slightly more massive than the proton. The electroweak interactions are responsible for this mass difference, which receives contributions from two sources. The strong isospin breaking contribution (also known as charge-symmetry breaking, for a review see Ref. [2]) is due to the difference in the masses of the up and down quarks, ultimately determined by the values of the Yukawa couplings in the Standard Model of electroweak interactions and the vacuum expectation value of the Higgs field. The other contribution arises from the fact that the proton and neutron carry different electromagnetic charges. The experimental neutron-proton mass difference of $M_n - M_p = 1.2933317 \pm 0.0000005$ MeV [3] receives an estimated electromagnetic contribution of $M_n - M_p |^{\text{em}} = -0.76 \pm 0.30$ MeV, and the remaining mass difference is due to a strong isospin breaking contribution of $M_n - M_p |^{d-u} = 2.05 \pm 0.30$ MeV.

The recent suggestion of a vast landscape of possible universes emerging from string theory [5, 6], and the previously hypothesized multi-universe scenario in general, have led to a resurgence of interest in the anthropic principle, and how it may provide a useful way of constraining fundamental parameters of nature. For this reason and others it is of interest to understand how quantities that affect nuclear physics and the production of elements depend upon the fundamental parameters: the length scale of the strong interactions, $\Lambda_{\text{QCD}}$, the light-quark masses, $m_u$, $m_d$ and $m_s$, and the electromagnetic coupling, $\alpha_e$. For instance, the basic fact that the neutron-proton mass difference is larger than the electron mass is central to the evolution and content of our universe (for a recent detailed discussion of the impact of an unstable proton see Ref. [7].). While a universe with a stable neutron would have a rich periodic table of nuclei, it is far from clear that the organic chemistry required for carbon-based life would exist [7–9].

In this work we have performed lattice calculations of the nucleon mass with domain-wall valence quark masses tuned to the staggered sea-quark masses of the MILC configurations (a mixed-action “QCD” calculation), and with valence quark masses that differ from the sea-quark masses (a mixed-action partially-quenched, “PQ”, calculation). As the computer resources do not presently exist to perform such calculations at the physical values of the light-quark masses, they are performed at QCD pion masses of $m_{\pi}^{\text{latt.}} \sim 290$ MeV and $m_{\pi}^{\text{latt.}} \sim 350$ MeV and a range of partially-quenched pion masses in between. These results are combined with the formal framework of heavy-baryon chiral perturbation theory (HB$\chi$PT [10, 11]) and partially-quenched heavy-baryon chiral perturbation theory (PQHB$\chi$PT [13–15]), and the recent precise lattice extraction of the light-quark mass ratio, $m_u/m_d = 0.43 \pm 0.01 \pm 0.08$ [1] by the MILC collaboration, to calculate the strong isospin-breaking contribution to the neutron-proton mass-difference.

II. THE FORMAL FRAMEWORK

Nucleon observables have a systematic loop expansion about the limit of vanishing quark masses and external momenta defined by HB$\chi$PT [10, 11]. Extensive phenomenology has been performed with HB$\chi$PT, where it is found that some observables appear to converge quite rapidly in the chiral expansion, while others are less convergent. This state of affairs is magnified when dealing with three light flavors rather than two. Recently, the heavy-baryon formalism has been extended to describe the situation where the sea-quark masses differ from the valence quark masses [12–15], as is the case in partially-quenched lattice
calculations.

The mass of the proton, which has valence quark content $uud$, when computed on configurations with sea-quarks, $j$ and $l$, of mass $m_j$ and $m_l$ has the form [15] (we have used the opposite sign convention for the mass counterterms)

$$M_p = M_0 + (m_u + m_d) (\alpha + \beta) + 2\sigma (m_j + m_l) + \frac{1}{3} (2\alpha - \beta) (m_u - m_d)$$

$$- \frac{1}{8\pi f^2} \left( \frac{g_A^2}{3} \left[ m^3_{uu} + m^3_{ud} + 2m^3_{ju} + 2m^3_{lu} + 3G_{\eta_u,\eta_u} \right] \right. + \frac{g_1^2}{12} \left[ m^3_{uu} - 5m^3_{ud} + 3m^3_{jd} + 2m^3_{ju} + 3m^3_{ld} + 2m^3_{lu} + 3G_{\eta_u,\eta_u} + 6G_{\eta_u,\eta_d} + 3G_{\eta_d,\eta_d} \right]$$

$$+ \frac{g_A g_1}{3} \left[ m^3_{ju} + m^3_{lu} - m^3_{ud} + 2m^3_{uu} + 3G_{\eta_u,\eta_d} + 3G_{\eta_d,\eta_d} \right]$$

$$+ \frac{g_A^2 N}{9\pi} \left[ 5F_{ud} + F_{uu} + F_{ju} + F_{lu} + 2F_{jd} + 2F_{ld} + 2E_{\eta_d,\eta_d} + 2E_{\eta_u,\eta_u} - 4E_{\eta_u,\eta_d} \right], \tag{1}$$

where $\alpha, \beta, \sigma$ are the counterterms that enter at ${\cal O}(m_q)$, $g_A$ is the nucleon axial coupling constant, $g_{\Delta N}$ is the $\Delta$-nucleon coupling constant, and $g_1$ is the nucleon coupling to the flavor-singlet meson field, which makes no contribution in the QCD limit where $m_j \to m_u$ and $m_l \to m_d$. The notation is such that the nucleon mass has been computed to one higher order in the partially-quenched chiral expansion, ${\cal O}(m_q^2)$, in Ref. [16], but with the small number of different quark masses available to us in our lattice calculation we will be unable to make use of that work. In the QCD limit, the proton mass computed from eq. (1) becomes the QCD proton mass computed previously with HB$\chi$PT,

$$M_p = M_0 + (\alpha + \beta + 2\sigma) (m_u + m_d) + \frac{1}{3} (2\alpha - \beta) (m_u - m_d)$$

$$- \frac{1}{8\pi f^2} \left[ \frac{3}{2} g_A^2 m^3_{\pi} + \frac{4g_{\Delta N}}{3\pi} F_{\pi} \right], \tag{4}$$

where $m^2_{\pi}$ is the pion mass and $F_{\pi}$ is the pion decay constant.
as required. The expansion of the neutron mass can be recovered from the expansion of the proton mass by interchanging the up and down quark masses, \( u \leftrightarrow d \). At the order to which we are working it is most convenient to replace the explicit quark masses in the expression for the proton mass with the leading order expression for the pion mass to yield

\[
M_p = M_0 + \left( \pi + \beta + 2\sigma \right) m_{\pi}^2 - \frac{1}{3} \left( 2\pi - \beta \right) \frac{1 - \eta}{1 + \eta} m_{\pi}^2 - \frac{1}{8\pi f^2} \left[ \frac{3}{2} g_A^2 m_{\pi}^2 + \frac{4g_N^2}{3\pi} F_{\pi} \right],
\]

where \( \eta = m_u/m_d \). The neutron mass is recovered by making the replacement \( \eta \rightarrow 1/\eta \), and consequently

\[
M_n - M_p |_{d-u} = \frac{2}{3} \left( 2\pi - \beta \right) \frac{1 - \eta}{1 + \eta} m_{\pi}^2.
\]

The one-loop contributions at \( \mathcal{O}(m_q^{3/2}) \) cancel in the mass-difference, as the pions are degenerate up to \( \mathcal{O}(m_q^2) \). The analogous expressions for the partially-quenched proton masses can be found in Appendix A.

III. DETAILS OF THE LATTICE CALCULATION AND ANALYSIS

Our computation uses the mixed-action lattice QCD scheme developed by LHPC [17, 18] using domain-wall valence quarks from a smeared-source on \( N_f = 2+1 \) asqtad-improved [19, 20] MILC configurations generated with rooted \(^1\) staggered sea quarks [26] that are HYP-smeared [27–30]. In the generation of the MILC configurations, the strange-quark mass was fixed near its physical value, \( b_{m_s} = 0.050 \), (where \( b = 0.125 \text{ fm} \) is the lattice spacing) determined by the mass of hadrons containing strange quarks. The two light quarks in the configurations are degenerate (isospin-symmetric). The domain-wall height is \( m = 1.7 \) and the extent of the extra dimension is \( L_5 = 16 \). The MILC lattices were “chopped” using a Dirichlet boundary condition from 64 to 32 time-slices to save time in propagator generation. In order to extract the terms in the mass expansion, we computed a number of sets of propagators corresponding to different valence quark masses, as shown in Table I. On 468 \( b_m = 0.007 \) (denoted by \( V_1 \)) lattices we have computed three sets corresponding to the QCD point with a valence-quark mass of \( b_{m_{\text{dwf}}} = 0.0081 \) (\( V_1 \)), three sets on 367 \( b_m = 0.007 \) lattices with a valence quark mass of \( b_{m_{\text{dwf}}} = 0.0138 \) (denoted by \( V_2 \)), and two sets with a valence quark mass \( b_{m_{\text{dwf}}} = 0.0100 \) (denoted by \( V_3 \)). On 658 of the \( b_m = 0.010 \) (\( V_2 \)) lattices we have computed three sets at the QCD point with a valence-quark mass of \( b_{m_{\text{dwf}}} = 0.0138 \) (\( V_2 \)) and one set with a valence quark mass of \( b_{m_{\text{dwf}}} = 0.0081 \) (\( V_1 \)). The parameters used to generate the QCD-point light-quark propagators have been “matched” to those used to generate the MILC configurations so that the mass of the pion computed with the domain-wall propagators is equal (to few-percent precision) to that of the lightest staggered pion computed with the same parameters as the gauge configurations [26]. The lattice calculations were performed with the Chroma software suite [31, 32] on the high-performance computing systems at the Jefferson Laboratory (JLab).

\(^1\) For recent discussions of the “legality” of the mixed-action and rooting procedures, see Ref. [21–25].
TABLE I: The parameters of the MILC gauge configurations and domain-wall propagators used in this work. For each propagator the extent of the fifth dimension is $L_5 = 16$. The notation of quarks, $V_1,V_2,V_3$, is defined in the text. The last column is the number of propagators generated, and corresponds to the number of lattices times the number of different locations of sources on each lattice.

| Ensemble             | Theory | $b_{m_1}$ | $b_{m_2}$ | $b_{m_{def}}$ | $10^3 \times b_{m_{res}}$ | # props. |
|----------------------|--------|-----------|-----------|---------------|------------------|---------|
| 2064f21b679m007m050 | QCD    | 0.007     | 0.050     | 0.0081        | 1.604 ± 0.038    | 468×3   |
| 2064f21b679m007m050 | PQQCD  | 0.007     | 0.050     | 0.0138        | 1.604 ± 0.038    | 367×3   |
| 2064f21b679m007m050 | PQQCD  | 0.007     | 0.050     | 0.0100        | 1.604 ± 0.038    | 367×2   |
| 2064f21b679m010m050 | QCD    | 0.010     | 0.050     | 0.0138        | 1.552 ± 0.027    | 658×3   |
| 2064f21b679m010m050 | PQQCD  | 0.010     | 0.050     | 0.0081        | 1.552 ± 0.027    | 658×1   |

Various proton and pion correlation functions were constructed from the three (distinct-mass) light-quark propagators that were generated on the $b_{m_1} = 0.007$ lattices, and the two light-quark propagators that were generated on the $b_{m_1} = 0.010$ lattices. Differences between the various proton states were also constructed. It is useful to define the proton mass splitting:

$$
\Delta M_p(V_a, V_b, V_c; V_d) \equiv M_p(V_a, V_b, V_c; V_d) - M_p(V_d, V_d, V_d; V_d),
$$

(7)

where the indices $a,b,c$ range over 1,2,3. Effective mass plots for the ratios of proton correlators that give rise to these mass splittings are displayed in figs. 1, 2 and 3. Results for the extracted proton mass splittings are given in Table II and displayed in fig. 4. The various pion masses relevant to the analysis are also shown in Table II. Using this data in conjunction with the PQHBχPT formulas given above and in the appendix, the coefficients $\bar{\sigma}, \bar{\beta}, g_{\Delta N}$, and $g_1$ that appear in eq. (5) were extracted using various nonlinear fitting techniques.

A tree-level, $O(m_q)$, analysis of the mass differences shown in Table II using the expressions for the partially-quenched proton masses given in the appendix, allows for an extraction of the isospin-breaking coefficient $(2\bar{\sigma} - \bar{\beta})/3$, and the isospin-conserving coefficient $\bar{\sigma} + \bar{\beta}$, as shown in Table III. This leads to a prediction for the strong isospin breaking at the physical quark masses, at $O(m_q)$, of

$$
M_u - M_p \mid_{d-u} = 1.96 \pm 0.92 \pm 0.37 \text{ MeV},
$$

(8)

as shown in Table IV. The first error is statistical and the second error is due to the uncertainty in the determination of the ratio of light quark masses, $\eta = m_u/m_d = 0.43 \pm 0.01 \pm 0.08$ by MILC [1].

The analysis of the partially-quenched data at $O(m_q^{3/2})$ introduces contributions to the various proton masses that vanish in the QCD limit, a characteristic feature of the partially-quenched theory. In this case there is a contribution from loop diagrams involving the flavor-singlet field — due to a mismatch between the ordinary flavor singlet and that of the graded-group — which depends on an axial coupling constant, $g_1$ [15], that must also be determined from the lattice data. Fortunately, with multiple partially-quenched proton states, $g_1$ can be extracted simultaneously with $(2\bar{\sigma} - \bar{\beta})/3$, $\bar{\sigma} + \bar{\beta}$, and $g_{\Delta N}$. However, given that $\bar{\sigma}$ and $\bar{\beta}$ enter at tree-level, while $g_1$ and $g_{\Delta N}$ enter at the one-loop level, the
FIG. 1: Effective mass plots for the ratios of proton correlation functions that give rise to the mass splittings $\Delta M_p(V_a, V_b, V_c; V_1)$ with $a, b, c = 1, 2$.

Fractional uncertainty in $g_1$ and $g_{\Delta N}$ will be parametrically larger than that of $\left(2\pi - \beta\right)/3$ and $\pi + \beta$ (assuming natural sizes).

At this order there are contributions from loops diagrams involving nucleons and diagrams involving $\Delta$’s. The axial coupling between the nucleons and the pions is taken from the chiral perturbation fit to the recent LHPC lattice calculation [33]. We use a value of $g_A$ that is the average of $g_A = 1.25$, corresponding to the QCD point on the $bm_l = 0.007$ lattices, and $g_A = 1.24$, corresponding to the QCD point on the $bm_l = 0.010$ lattices. Similarly, for the pion decay constant, we use a value of $f_\pi = 149.8$, which is the average
of \( f_\pi = 147.8 \) MeV corresponding to the QCD point on the \( bm_l = 0.007 \) lattices, and \( f_\pi = 151.8 \) MeV corresponding to the QCD point on the \( bm_l = 0.010 \) lattices. We fit \( g_{\Delta N} \) to the data, and find \( |g_{\Delta N}^{\text{fit}}| = 0.60 \pm 0.66 \). This value is slightly smaller than the \( SU(6) \) value of \( g_{\Delta N} = -\frac{6}{5}g_A \). The mass difference between the \( \Delta \) and nucleon must be input into the two-parameter fit with \( |g_{\Delta N}| = 1.8 \) (the value obtained at tree-level from \( \Delta \to N\pi \)) yields \( M_n - M_p |_{d-u} = 2.06 \pm 0.99 \pm 0.38 \) MeV while fitting with nucleon loops alone (\( g_{\Delta N} = 0 \)) gives \( M_n - M_p |_{d-u} = 2.78 \pm 0.99 \).
FIG. 3: Effective mass plots for the ratios of proton correlation functions that give rise to the mass splittings $\Delta M_p(V_1, V_1, V_1; V_2)$ with $a, b, c = 1, 2$.

extraction. Ideally, this would also be fit to the data, but we do not have precise enough data to permit such a fit. Instead, we use the experimental value $M_\Delta - M_N = 293$ MeV. At one-loop order, $\mathcal{O}(m_q^{3/2})$, we find

$$M_n - M_p|^{d-u} = 2.26 \pm 0.57 \pm 0.42 \pm 0.10 \text{ MeV},$$

(9)

where the last error is an estimate of the systematic error due to truncation of the chiral

$2.29 \pm 0.53 \pm 0.43$ MeV.
A lattice spacing of $b = 0.125$ fm has been used.

| Quantity | Mass (Difference) (l.u.) | Mass (Difference) (MeV) | Fitting Range |
|----------|--------------------------|-------------------------|---------------|
| $m_{\pi}(V_1, V_1; V_1)$ | $0.1864 \pm 0.0011$ | $294.2 \pm 1.7$ | $5 \rightarrow 15$ |
| $m_{\pi}(V_1, V_1; V_1)$ | $0.2066 \pm 0.0010$ | $326.2 \pm 1.6$ | $5 \rightarrow 15$ |
| $m_{\pi}(V_2, V_2; V_1)$ | $0.22473 \pm 0.00091$ | $354.4 \pm 1.4$ | $5 \rightarrow 15$ |
| $m_{\pi}(V_1, V_3; V_1)$ | $0.1929 \pm 0.0012$ | $304.5 \pm 1.9$ | $5 \rightarrow 15$ |
| $m_{\pi}(V_3, V_3; V_1)$ | $0.1996 \pm 0.0011$ | $315.1 \pm 1.8$ | $5 \rightarrow 15$ |
| $m_{\pi}(V_1, V_1; V_2)$ | $0.1844 \pm 0.0013$ | $291.0 \pm 2.1$ | $5 \rightarrow 15$ |
| $m_{\pi}(V_1, V_2; V_2)$ | $0.2050 \pm 0.0012$ | $323.7 \pm 1.0$ | $5 \rightarrow 15$ |
| $m_{\pi}(V_2, V_2; V_2)$ | $0.2236 \pm 0.0011$ | $352.9 \pm 1.8$ | $5 \rightarrow 15$ |
| $\Delta M_p(V_1, V_1, V_2; V_1)$ | $0.0163 \pm 0.0019$ | $25.7 \pm 3.0$ | $5 \rightarrow 12$ |
| $\Delta M_p(V_2, V_2, V_1; V_1)$ | $0.0209 \pm 0.0029$ | $32.9 \pm 4.7$ | $5 \rightarrow 12$ |
| $\Delta M_p(V_2, V_2, V_2; V_1)$ | $0.0353 \pm 0.0041$ | $55.8 \pm 6.5$ | $5 \rightarrow 12$ |
| $\Delta M_p(V_1, V_1, V_3; V_1)$ | $0.0049 \pm 0.0010$ | $7.7 \pm 1.6$ | $5 \rightarrow 11$ |
| $\Delta M_p(V_3, V_3, V_1; V_1)$ | $0.0061 \pm 0.0016$ | $9.7 \pm 2.5$ | $5 \rightarrow 11$ |
| $\Delta M_p(V_2, V_2, V_3; V_1)$ | $0.0109 \pm 0.0024$ | $17.2 \pm 3.8$ | $5 \rightarrow 11$ |
| $\Delta M_p(V_1, V_1, V_1; V_2)$ | $-0.0309 \pm 0.0038$ | $-48.8 \pm 6.0$ | $4 \rightarrow 11$ |
| $\Delta M_p(V_1, V_1, V_2; V_2)$ | $-0.0161 \pm 0.0022$ | $-25.5 \pm 3.5$ | $4 \rightarrow 11$ |
| $\Delta M_p(V_2, V_2, V_2; V_2)$ | $-0.0137 \pm 0.0016$ | $-21.6 \pm 2.6$ | $5 \rightarrow 12$ |

TABLE II: The pion masses and proton mass differences calculated on the $bm_l = 0.007$ and $bm_l = 0.010$ MILC lattices. The notation of valence and sea quarks, $V_{1,2,3}$, is defined in the text.

| Extraction | $\frac{1}{3} \left( 2\pi - \beta \right)$ (l.u.) | $\bar{\sigma} + \beta$ (l.u.) | $g_1$ | $|g_{\Delta N}|$ | $\chi^2$/dof |
|------------|---------------------------------|-------------------------------|-------|-----------------|-------------|
| LO $\mathcal{O}(m_q)$ | $0.198 \pm 0.093$ | $2.07 \pm 0.08$ | -- | -- | 0.56 |
| NLO $\mathcal{O}(m_q^{1/4})$ | $0.229 \pm 0.058$ | $3.4 \pm 1.1$ | $-0.10 \pm 0.35$ | $0.60 \pm 0.66$ | 0.21 |

TABLE III: Parameter Table. The values of the parameters in the partially-quenched chiral Lagrangian as determined by a $\chi^2$-minimization fit of the theoretical proton mass differences given in Appendix A, to the lattice data given in Table II. The isospin-conserving combination of counterterms, $\bar{\sigma} + \beta$, is renormalization-scale dependent. We have renormalized at $\mu = 1$ GeV.

expansion. It is reassuring that the predicted neutron-proton mass difference is relatively insensitive to the order in the chiral expansion, as shown in Table IV. Both the tree-level and the one-loop extraction of the neutron-proton mass differences are consistent with the “experimental” value of $M_n - M_p |^{d-u} = 2.05 \pm 0.30$ MeV.

An interesting observation can be made by comparing the proton mass differences on the two different lattice sets, as shown in Table II and displayed in fig. 4. Within errors, the magnitude of the mass differences are independent of the value of the sea-quark mass. This is consistent with leading order chiral expansions given eq. (1) and in Appendix A. Higher order contributions to these mass differences in the chiral expansion, which give rise to deviations from these equalities, will become more visible with increased statistics.

There will be finite lattice spacing contributions to the parameters that we have extracted in this work. The recent developments in the inclusion of finite-lattice spacing effects in mixed-action theories in $\chi$PT allow us to determine where such corrections enter and to
FIG. 4: The partially-quenched proton mass differences (in MeV) calculated from the \( b m_l = 0.007 \) and 0.010 MILC lattices plotted vs the pion mass composed of sea quarks. Various data have been displaced horizontally by small amounts for display purposes. A lattice spacing of \( b = 0.125 \) fm has been used.

| Extraction | \( M_n - M_p |^{d-u} \) (MeV) at \( m_\pi^{\text{phys.}} \) |
|------------|-------------------------------------------------|
| LO \( \mathcal{O}(m_q) \)                     | 1.96 ± 0.92 ± 0.37                               |
| NLO \( \mathcal{O}(m_q^{2/2}) \)               | 2.26 ± 0.57 ± 0.42                               |

TABLE IV: The neutron-proton mass-splitting at the physical value of the pion mass, \( m_\pi^{\text{phys.}} = 140 \) MeV, extracted from this partially-quenched lattice calculation, using the parameters shown in Table III. The lattice spacing used to convert between lattice units and physical units is \( b = 0.125 \) fm. The first error is statistical while the second error is due to the uncertainty in the ratio of quark masses, \( m_u/m_d \), in the MILC calculation [1].

estimate how big the corrections should be. The lattice spacing is introduced into the mixed-action theory by extending the \( SU(2)_L \otimes SU(2)_R \) lie-algebra to a graded lie-algebra that makes the distinction between sea and valence quarks explicit. The lattice spacing is incorporated by a spurion field with the appropriate transformation properties under the graded group, e.g. see Ref. [34–37]. There is a leading-order contribution at \( \mathcal{O}(a^2 m_q^3) \) to the nucleon mass (where we are assuming that the exponentially suppressed contribution at \( \mathcal{O}(a m_q^3) \) from the finite \( L_\Delta \) is numerically insignificant). However, such terms do not contribute to the mass differences between the proton states that we have used to extract the parameters. Finite lattice spacing contributions to the nucleon mass that depend upon
the light-quark masses start at $O(a^2 m_q)$. Therefore, we expect the finite lattice spacing corrections to our results to be parametrically suppressed and small. In contrast, the finite lattice spacing contribution to the nucleon mass itself is expected to be roughly the same size as the contribution from the $\sigma$-term, rendering an extraction of the nucleon $\sigma$-term (e.g. see Ref. [38]) somewhat unclean if the physical value of the nucleon mass is used in the extraction. Finite-volume effects in the baryon mass splittings are estimated to be negligible.

IV. CONCLUSIONS

In this work we have performed the first lattice calculation of the neutron-proton mass-difference arising from the difference between the mass of the up and down quarks, and find $M_n - M_p |^{d-u} = 2.26 \pm 0.57 \pm 0.42 \pm 0.10$ MeV. This value is consistent with the number $2.05 \pm 0.30$ MeV based upon the experimentally-measured mass-difference and the best estimate of the electromagnetic contribution. It is clear that further lattice calculations are warranted in order to make a precise prediction for this quantity, which will then enable a precise determination of the electromagnetic contribution to this mass-difference $^3$.

The neutron-proton mass difference is but one of the manifestations of charge-symmetry breaking that has been a focus of both theoretical and experimental investigations for many years [2]. With the recent progress in extracting the nucleon-nucleon scattering amplitudes from fully-dynamical lattice QCD [40], one can imagine using partially-quenched calculations to extract the charge-symmetry breaking contribution to nucleon-nucleon scattering, and other processes, in future investigations.

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$^3$ For an attempt to determine the electromagnetic contribution to the neutron-proton mass difference using quenched lattice QCD, see Ref. [39].
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APPENDIX A: NUCLEON MASS IN PQHB\_PT

In this appendix we give the expression for a proton composed of valence quarks $V_1 V_2 V_1$, $V_1 V_2 V_1$, $V_2 V_1 V_1$ and $V_1 V_2 V_2$ on an isospin-symmetric sea composed of two light quarks $V_1, V_2$. The proton masses are, starting with the QCD point,

$$
M_p(V_1, V_1, V_1; V_1) = M_0 + \left(\frac{\alpha}{\beta} + \frac{\beta}{2\nu} + 2\beta\right) m_{V_1, V_1, V_1}^2
- \frac{3g_\Lambda^2}{16\pi f^2} m_{V_1, V_1, V_1}^2
- \frac{g_\Delta N}{6\pi^2 f^2} F_{V_1, V_1, V_1};
$$

$$
M_p(V_1, V_2, V_1; V_1) = M_0 + \frac{1}{6} \left(\frac{\alpha}{\beta} + \frac{\beta}{2\nu} + 2\beta\right) m_{V_1, V_1, V_1}^2
+ \frac{g_\Lambda^2}{24\pi f^2} \left(\frac{T}{2} m_{V_1, V_2, V_1}^2 - m_{V_1, V_2, V_1}^2\right)
- \frac{g_4 g_1}{24\pi f^2} \left(\frac{5}{2} m_{V_1, V_2, V_1}^2 - m_{V_1, V_2, V_1}^2 - \frac{3}{2} m_{V_2, V_2, V_1}^2\right)
- \frac{g_1^2}{384\pi f^2} \left(14m_{V_1, V_1, V_1}^2 + 4m_{V_1, V_1, V_1}^2 - 27m_{V_2, V_2, V_1}^2 + 9m_{V_1, V_2, V_1}^2 m_{V_2, V_2, V_1}^2\right)
- \frac{g_\Delta N}{72\pi^2 f^2} \left(2F_{V_1, V_1, V_1} + 9F_{V_1, V_2, V_1} + F_{V_2, V_2, V_1} + m_{V_1, V_1, V_1} S_{V_2, V_2, V_1} - m_{V_1, V_1, V_1} S_{V_2, V_2, V_1}\right);
$$

$$
M_p(V_2, V_2, V_1; V_1) = M_0 + \frac{1}{6} \left(\frac{\alpha}{\beta} + \frac{\beta}{2\nu} + 2\beta\right) m_{V_1, V_1, V_1}^2
+ \frac{g_\Lambda^2}{96\pi f^2} \left(20m_{V_1, V_2, V_1}^2 + 9m_{V_1, V_1, V_1}^2 m_{V_2, V_2, V_1}^2 - 11m_{V_2, V_2, V_1}^2\right)
- \frac{g_4 g_1}{96\pi f^2} \left(4m_{V_1, V_2, V_1}^2 + 9m_{V_1, V_1, V_1}^2 m_{V_2, V_2, V_1}^2 - 13m_{V_2, V_2, V_1}^2\right)
- \frac{g_1^2}{384\pi f^2} \left(18m_{V_1, V_1, V_1}^2 - 4m_{V_1, V_1, V_1}^2 - 23m_{V_2, V_2, V_1}^2 + 9m_{V_1, V_1, V_1}^2 m_{V_2, V_2, V_1}^2\right)
- \frac{g_\Delta N}{72\pi^2 f^2} \left(3F_{V_1, V_2, V_1} + 7F_{V_1, V_2, V_1} + 2F_{V_2, V_2, V_1} + m_{V_1, V_1, V_1} S_{V_2, V_2, V_1} - m_{V_1, V_1, V_1} S_{V_2, V_2, V_1}\right);
$$

$$
M_p(V_2, V_2, V_2; V_1) = M_0 + \frac{g_\Lambda^2}{96\pi f^2} \left(16m_{V_1, V_2, V_1}^2 + 9m_{V_1, V_1, V_1}^2 m_{V_2, V_2, V_1}^2 - 7m_{V_2, V_2, V_1}^2\right)
- \frac{g_4 g_1}{48\pi f^2} \left(4m_{V_1, V_2, V_1}^2 + 9m_{V_1, V_1, V_1}^2 m_{V_2, V_2, V_1}^2 - 13m_{V_2, V_2, V_1}^2\right)
- \frac{g_1^2}{96\pi f^2} \left(10m_{V_1, V_2, V_1}^2 + 9m_{V_1, V_1, V_1}^2 m_{V_2, V_2, V_1}^2 - 19m_{V_2, V_2, V_1}^2\right)
- \frac{g_\Delta N}{12\pi^2 f^2} \left(F_{V_1, V_2, V_1} + F_{V_2, V_2, V_1}\right), \quad (A1)
$$
where we have used the leading-order relation between the quark masses, and the function

\[ S(m, \Delta, \mu) = \sqrt{\Delta^2 - m^2} \log \left( \frac{\Delta - \sqrt{\Delta^2 - m^2 + i\epsilon}}{\Delta + \sqrt{\Delta^2 - m^2 + i\epsilon}} \right) - \Delta \left( \log \left( \frac{m^2}{\mu^2} \right) + \frac{1}{3} \right) . \]  

(A2)

The function \( F \) is defined in the text.

The meson masses at leading order in the chiral expansion, starting with the QCD point, are

\[
\begin{align*}
    m_\pi^2(V_1, V_1; V_1) &= m_{V_1,V_1,V_1}^2 = 2 \lambda m_{V_1} \\
    m_\pi^2(V_1, V_2; V_1) &= m_{V_1,V_2,V_1}^2 = \lambda \left( m_{V_1} + m_{V_2} \right) \\
    m_\pi^2(V_2, V_2; V_1) &= m_{V_2,V_2,V_1}^2 = 2 \lambda m_{V_2} ,
\end{align*}
\]

(A3)

where \( \lambda \) is a strong interaction mass-scale, and the semicolon separates valence and sea quarks.