

Strong-isospin breaking in the neutron-proton mass difference

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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 $b \sim 0.125$ fm, lattice spatial size of $L \sim 2.5$ fm and pion masses ranging from $m_\pi \sim 290$ MeV to ~ 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.

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1. 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. With the down-quark more massive than the up-quark, the neutron would be more massive than the proton in the absence of electromagnetism. The experimental neutron-proton mass difference of $M_n - M_p = 1.2933317 \pm 0.0000005$ MeV [3] receives an estimated electromagnetic contribution of [4] $M_n - M_p|^{em} = -0.76 \pm 0.30$ MeV (estimated using the Cottingham sum-rule saturated by the Born diagrams), and the remaining mass difference of $M_n - M_p|^{d-u} = 2.05 \mp 0.30$ MeV is due to strong-isospin breaking. The uncertainty is estimated from the Born contribution of baryon-resonances to the Cottingham sum-rule.

Before delving into the details of the lattice calculation we have performed, it is useful to remind ourselves why we should care about this mass-splitting in the first place. If we were in a situation where $M_n < M_p + M_e - M_\nu$, hydrogen would not be stable. It would decay weakly via $p + e \rightarrow n + \nu$ and chemistry of our universe would be quite different from what we are familiar with. Therefore, in the limit of strong-isospin symmetry, hydrogen would not be stable, and from our present calculation we find that for hydrogen to be stable, $m_u/m_d \lesssim 0.77$ (taken from the central values of our determination and the electromagnetic contribution). Of course, one would still have some form of nuclear physics, but it might look quite different from what we are familiar with. In order to determine just how similar, or different, nuclear physics would be, we need to perform further calculations.

2. The chiral expansion of the Nucleon Mass

In order to extract isospin breaking quantities from lattice calculations on isospin symmetric lattices, one must perform partially-quenched calculations, and then determine coefficients in the chiral theory describing QCD quantities. In QCD the proton mass has a chiral expansion of the form

$$M_p = M_0 + (\bar{\alpha} + \bar{\beta} + 2\bar{\sigma}) m_\pi^2 - \frac{1}{3} (2\bar{\alpha} - \bar{\beta}) \left(\frac{1-\eta}{1+\eta} \right) m_\pi^2 - \frac{1}{8\pi f^2} \left[\frac{3}{2} g_A^2 m_\pi^3 + \frac{4g_{\Delta N}^2}{3\pi} F_\pi \right], \quad (2.1)$$

where $\eta = m_u/m_d$ is the ratio of the mass of the up-quark and down-quark. The function F_π is given by $F_\pi = F(m_\pi, \Delta, \mu)$, with

$$F(m, \Delta, \mu) = (m^2 - \Delta^2) \left(\sqrt{\Delta^2 - m^2} \log \left(\frac{\Delta - \sqrt{\Delta^2 - m^2 + i\epsilon}}{\Delta + \sqrt{\Delta^2 - m^2 + i\epsilon}} \right) - \Delta \log \left(\frac{m^2}{\mu^2} \right) \right) - \frac{1}{2} m^2 \Delta \log \left(\frac{m^2}{\mu^2} \right), \quad (2.2)$$

and arises from Δ -resonance intermediate states in one-loop diagrams. Δ is the mass difference between the Δ -resonance and the nucleon. The mass-splitting between the neutron and proton due to the quark mass differences is therefore,

$$M_n - M_p|^{d-u} = \frac{2}{3} (2\bar{\alpha} - \bar{\beta}) \left(\frac{1-\eta}{1+\eta} \right) m_\pi^2 . \quad (2.3)$$

The one-loop contributions at $\mathcal{O}(m_q^{3/2})$ cancel in the mass-difference, as the pions are degenerate up to $\mathcal{O}(m_q^2)$. Consequently, at leading order, it is the combination of parameters $2\bar{\alpha} - \bar{\beta}$ that needs to be extracted from lattice calculations.

The nucleon mass was computed in $SU(2)_L \otimes SU(2)_R$ partially-quenched chiral perturbation theory (PQ χ PT) in Ref. [5], and involves quite lengthy expressions. In the case of an isospin-symmetric set of lattice configurations, the proton masses for different combinations of valence quarks can be found in Ref. [6]. As an example, the mass of a proton with valence quantum numbers V_1, V_1, V_2 on a sea of V_1 quarks has the form

$$\begin{aligned} M_p(V_1, V_1, V_2; V_1) &= M_0 + 2\bar{\sigma} m_{V_1, V_1; V_1}^2 + \frac{1}{6} (5\bar{\alpha} + 2\bar{\beta}) m_{V_1, V_1; V_1}^2 \\ &+ \frac{1}{6} (\bar{\alpha} + 4\bar{\beta}) m_{V_2, V_2; V_1}^2 \\ &- \frac{g_A^2}{24\pi f^2} \left(\frac{7}{2} m_{V_1, V_1; V_1}^3 + m_{V_1, V_2; V_1}^3 \right) \\ &- \frac{g_A g_1}{24\pi f^2} \left(\frac{5}{2} m_{V_1, V_1; V_1}^3 - m_{V_1, V_2; V_1}^3 - \frac{3}{2} m_{V_2, V_2; V_1}^3 \right) \\ &- \frac{g_1^2}{384\pi f^2} (14m_{V_1, V_1; V_1}^3 + 4m_{V_1, V_2; V_1}^3 - 27m_{V_2, V_2; V_1}^3 + 9m_{V_1, V_1; V_1}^2 m_{V_2, V_2; V_1}) \\ &- \frac{g_{\Delta N}^2}{72\pi^2 f^2} (2F_{V_1, V_1; V_1} + 9F_{V_1, V_2; V_1} + F_{V_2, V_2; V_1} + m_{V_1, V_1; V_1}^2 S_{V_2, V_2; V_1} - m_{V_2, V_2; V_1}^2 S_{V_2, V_2; V_1}) ; \end{aligned} \quad (2.4)$$

where the function S is given by $S_\pi = S(m_\pi, \Delta, \mu)$ with

$$S(m, \Delta, \mu) = \sqrt{\Delta^2 - m^2} \log \left(\frac{\Delta - \sqrt{\Delta^2 - m^2 + i\epsilon}}{\Delta + \sqrt{\Delta^2 - m^2 + i\epsilon}} \right) - \Delta \left(\log \left(\frac{m^2}{\mu^2} \right) + \frac{1}{3} \right) . \quad (2.5)$$

$m_{V_a, V_b; V_c}$ is the mass of a pion composed of valence quarks V_a, V_b on configurations with quarks V_c . In partially-quenched proton masses, there are contributions that depend upon the axial-isosinglet coupling, g_1 . This coupling is one of the fit parameters in our extraction.

3. The Lattice QCD Calculation

Our computation [6] uses the mixed-action lattice QCD scheme developed by LHPC [7, 8] using domain-wall valence quarks from a smeared-source on $N_f = 2 + 1$ asqtad-improved [9, 10] MILC configurations generated with rooted¹ staggered sea quarks [18] that are hypercubic-smeared

¹For recent discussions of the ‘‘legality’’ of the mixed-action and rooting procedures, see Ref. [11, 12, 13, 14, 15, 16, 17]. While it still could be the case that staggered fermions do not reproduce QCD in the continuum limit, recent work by Shamir [17] on this issue, relying heavily on the renormalization group evolution of the staggered theory, has concluded that under certain plausible assumptions that can be tested, the continuum limit of the staggered theory is QCD.

Ensemble	Theory	bm_l	bm_{dwf}	$10^3 \times bm_{res}$	# props.
2064f21b679m007m050	QCD	0.007 (V_1)	0.0081 (V_1)	1.604 ± 0.038	468×3
2064f21b679m007m050	PQ	0.007 (V_1)	0.0138 (V_2)	1.604 ± 0.038	367×3
2064f21b679m007m050	PQ	0.007 (V_1)	0.0100 (V_3)	1.604 ± 0.038	367×2
2064f21b679m010m050	QCD	0.010 (V_2)	0.0138 (V_2)	1.552 ± 0.027	658×3
2064f21b679m010m050	PQ	0.010 (V_2)	0.0081 (V_1)	1.552 ± 0.027	658×1

Table 1: 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. We have worked at one lattice-spacing only, $b \sim 0.125$ fm. PQ denotes partially-quenched QCD. For each set of configurations $bm_s = 0.050$.

(HYP-smear) [19, 20, 21, 22]. In the generation of the MILC configurations, the strange-quark mass was fixed near its physical value, $bm_s = 0.050$, (where $b \sim 0.125$ 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 $bm_l = 0.007$ (denoted by V_1) lattices we have computed three sets corresponding to the QCD point with a valence-quark mass of $bm_{dwf} = 0.0081$ (V_1), three sets on 367 $bm_l = 0.007$ lattices with a valence quark mass of $bm_{dwf} = 0.0138$ (denoted by V_2), and two sets with a valence quark mass $bm_{dwf} = 0.0100$ (denoted by V_3). On 658 of the $bm_l = 0.010$ (V_2) lattices we have computed three sets at the QCD point with a valence-quark mass of $bm_{dwf} = 0.0138$ (V_2) and one set with a valence quark mass of $bm_{dwf} = 0.0081$ (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 [18]. The lattice calculations were performed with the *Chroma* software suite [23, 24] on the high-performance computing systems at the Jefferson Laboratory (JLab). To extract the isospin-breaking terms it is sufficient to look at mass-differences between proton states. The ratio of correlation functions is formed so that a mass-difference can be extracted from its large-time behavior. An example of the ratio of correlation functions found in our work is shown in fig. 1. We define the mass difference to be

$$\Delta M_p(V_a, V_b, V_c; V_d) = M_p(V_a, V_b, V_c; V_d) - M_p(V_d, V_d, V_d; V_d) \quad . \quad (3.1)$$

Each pair of partially-quenched propagators generated four different proton states and hence three different mass-splittings from the isospin symmetric QCD proton state. The results of our calculations are shown in fig. 2. By fitting four parameters, $\bar{\alpha}, \bar{\beta}, g_1$ and $g_{\Delta N}$ to the six mass-splitting we are able to extract the combination of constants in eq. 2.3. Further, using the ratio of light-quark masses determined by the MILC collaboration, $m_u/m_d = 0.43 \pm 0.01 \pm 0.08$ [1], we can

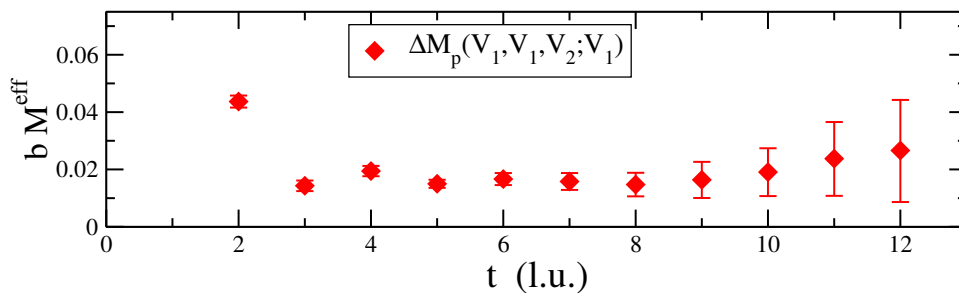


Figure 1: The effective mass plot for the mass splitting $\Delta M_p(V_1, V_1, V_2; V_1)$.

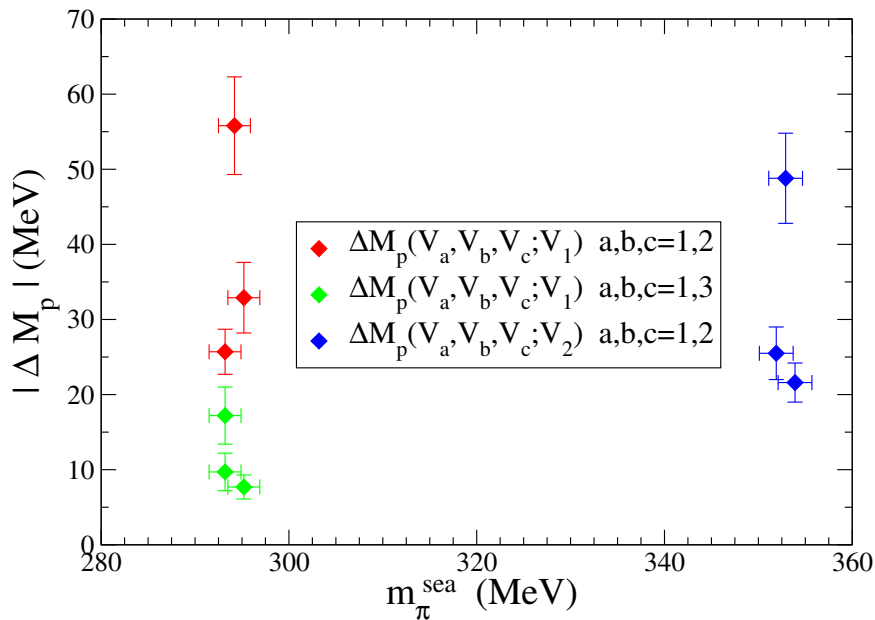


Figure 2: The partially-quenched proton mass differences (in MeV) calculated from the $bm_l = 0.007$ and 0.010 MILC lattices plotted vs the pion mass composed of sea quarks. Various data have been displaced horizontally by small amounts for display purposes. A lattice spacing of $b = 0.125$ fm has been used to set the scale.

make a prediction for the strong-isospin breaking contribution to the neutron-proton mass-splitting of

$$M_n - M_p \Big|^{d-u} = 2.26 \pm 0.57 \pm 0.42 \pm 0.10 \text{ MeV} \quad , \quad (3.2)$$

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

This is to be compared with a value of $M_n - M_p|^{d-u} = 2.05 \mp 0.30$ MeV as determined via the Cottingham sum-rule.

4. Conclusions

We have performed partially-quenched calculations of the proton mass with domain-wall valence quarks on the isospin-symmetric coarse staggered MILC lattices [6]. These calculations have allowed us to isolate the contribution to the neutron-proton mass-splitting due to the light-quark mass-splitting at leading and next-to-leading order in the $SU(2)_L \otimes SU(2)_R$ chiral expansion. We find a value that is consistent with the estimate arrived at from the experimental mass-splitting and the best estimate of the electromagnetic contribution. It is clear that with more computer power, this important quantity will be calculated to high precision.

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