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To cite this version:

Sz. Borsanyi, S. Dürr, Z. Fodor, J. Frison, C. Hoelbling, et al.. Isospin splittings in the light baryon octet from lattice QCD and QED. 2023. hal-01258926

HAL Id: hal-01258926

https://hal.science/hal-01258926v1

Preprint submitted on 5 Sep 2023

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Isospin Splittings in the Light-Baryon Octet from Lattice QCD and QED

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(Dated: June 19, 2018)

While electromagnetic and up-down quark mass difference effects on octet baryon masses are very small, they have important consequences. The stability of the hydrogen atom against beta decay is a prominent example. Here we include these effects by adding them to valence quarks in a lattice QCD calculation based on N_f=2+1 simulations with 5 lattice spacings down to 0.054 fm, lattice sizes up to 6 fm and average up-down quark masses all the way down to their physical value. This allows us to gain control over all systematic errors, except for the one associated with neglecting electromagnetism in the sea. We compute the octet baryon isomultiplet mass splittings, as well as the individual contributions from electromagnetism and the up-down quark mass difference. Our results for the total splittings are in good agreement with experiment.

arXiv:1306.2287v2 [hep-lat] 6 Jan 2014

The existence and stability of atoms and ordinary matter rely heavily on the fact that neutrons are slightly more massive than protons. The difference in the mass of these two particles has been measured very precisely and is only 0.14% of their average mass [1]. Although it has yet to be shown from first principles, we believe that this tiny difference results from the competition between electromagnetic (EM) effects proportional to the fine structure constant $\alpha \equiv e^2/(4\pi)$ and mass isospin breaking effects proportional to the mass difference of up and down quarks $\delta m \equiv m_u - m_d$. Here, we study this issue in the light-baryon octet. In particular, we compute mass splittings in the nucleon (N), Σ, and Ξ isospin multiplets using lattice QCD, to which we add QED in the valence quark sector. Although one would also have to account for QED contributions from sea quarks to have a complete calculation, these effects are suppressed, as discussed below. Moreover, the approach taken here allows us to use a very rich set of QCD gauge configurations that we have already generated [2–4]. Eliminating the uncertainty associated with neglecting QED sea-quark contributions would require performing completely new simulations, implementing reweighting techniques [5, 6], or using EM current insertion methods [7] and including quark-disconnected contributions. Such a computation is beyond the scope of the present work.

Because mass and EM isospin symmetry breaking corrections are small and of comparable size, it is legitimate to expand the standard model in powers of δm and α, assuming $O(\delta m) \sim O(\alpha)$ [8]. This expansion is expected to converge very rapidly, with each subsequent order contributing $\sim 1\%$ of the previous one. Given the size of other uncertainties in our calculation, we can safely work at LO in this expansion, i.e. at $O(\delta m, \alpha)$.

The physical point.– In the absence of weak interactions and for energies smaller than the charm-anticharm threshold, the standard model of quarks has five parameters that must be fixed by comparison to experiment. Here we trade these parameters for observables which are particularly sensitive to them: 1) the lattice spacing, a, for the mass of the decuplet baryon Ω^-–alternatively the isospin averaged Ξ mass–as in [9], 2) the average u-d mass, m_{ud}, for $M^2_{\pi^+}$, 3) the strange mass, m_s, for $M^2_{K^\times} \equiv (M^2_{K^+} + M^2_{K^0} - M^2_{\pi^+})/2$, 4) δm for the mass-squared difference $\Delta M^2_K \equiv M^2_{K^+} - M^2_{K^0}$, and 5) bare α for its renormalized value because it does not renormalize in our quenched QED calculation. The *physical point* is then reached by tuning these observables to their physical values given in [1], while taking the continuum $a \to 0$ and infinite-volume $L \to \infty$ limits.

Separating EM and δm contributions.– In addition to computing the total splittings, it is interesting to separate them into a contribution coming from δm and one coming from QED. We define the EM contribution by setting $\delta m = 0$ via $\Delta M^2 = M^2_{\bar{u}u} - M^2_{dd} = 0$, with all other parameters tuned to their physical values. Here, $M_{\bar{q}q}$ is the mass of a neutral meson $\bar{q}q$, $q = u, d$, whose propagator includes only quark-connected diagrams. Using the χPT results of [10], it is straightforward to show that the difference of these mesons' squared masses is $\Delta M^2 = 2B_2\delta m + O(\alpha m_{ud}, \delta m m_{ud}, \alpha\delta m, \alpha^2)$, where B_2 is the N_f=2 quark condensate parameter. Close to the physical point, $O(m_{ud})$ can be counted like $O(\delta m)$. Thus, our definition of the EM contribution differs from any other valid one by corrections of the size of NLO isospin

breaking terms, which are one order higher than the one to which we work here. To obtain the contribution from δm, we set $\alpha = 0$ and all other parameters to their physical values. In particular, the physical value of ΔM^2 is obtained from the analysis of ΔM_K^2 briefly described below and by computing the value of ΔM^2 corresponding to the physical ΔM_K^2. This analysis and its implications for Dashen's theorem [11] and $m_{u,d}$, which are very interesting in their own right, will be discussed elsewhere [12].

Simulation details and parameters.– We start from our 47, isospin symmetric, N_f=2+1, QCD ensembles, obtained from simulations with pion masses down to 120 MeV, lattice sizes up to 6 fm, five lattice spacings down to 0.054 fm, and more than 1000 trajectories each [4]. To these ensembles, we add QED gauge degrees of freedom in a way which has now become standard [13–15]. For each QCD gauge configuration, we generate an EM field $A_\mu(x)$ defined on the links, using the noncompact EM action (in Coulomb gauge) and the methods detailed in [14]. The gauge potential is then exponentiated as $U_\mu^{\rm QED}(x) = \exp\left[iqeA_\mu(x)\right]$. Unlike the QCD links, our QED links undergo no smearing before being coupled to quarks. Similarly, we have not added a clover improvement term for the U(1) field. The U(1) fields are then multiplied with the SU(3) gauge variable on each link and inserted into the Wilson-Dirac operator associated with the quark of charge q before inversion. The resulting quark propagators are combined into meson and baryon two-point functions. The extended sources and sinks used are the same as in [3, 4].

For most of our SU(3) ensembles, we have generated two valence data sets, which include QED with the physical value of α. In the first set (set 1), the bare, valence u, d, and s quark masses are individually tuned so that their PCAC values approximately reproduce the corresponding ensemble's light and strange sea-quark PCAC masses. Thus, we subtract the α/a divergences in the valence bare quark masses, which come from the EM self-energy, as described in [15]. In the second set (set 2), we choose m_d to be slightly more massive than in the first set so that ΔM^2 scatters around its physical value from ensemble to ensemble. We have one additional valence data set (set 3) in which α is varied. The latter includes a point with $\alpha \sim 2\alpha^{\rm ph}$ and $\Delta M^2 \simeq \Delta M^{2,{\rm ph}}$, a second with $\alpha \sim \alpha^{\rm ph}/4$ and a similar ΔM^2, and a third with $\alpha \sim 0$ and $\Delta M^2 \simeq 0$. The superscript ph indicates that we are referring to the physical value of a quantity. We have 74 valence points in total, which are shown in the $M_{\bar{u}u}^2$-$M_{\bar{d}d}^2$ plane in Fig. 1. This rich collection of data allows us to gain full control over the dependence of the splittings on all of the relevant parameters.

Analysis of meson and baryon correlators.– The time dependence of the π^+, K^+, K^0, and the Ω^- or Ξ two-point functions is fitted, in the asymptotic regime, to a hyperbolic cosine and an exponential, respectively. For the isospin multiplets whose splittings we wish to determine, we perform a simultaneous, correlated fit to the two-point functions of the two members of the multiplet in which we replace the individual hadron mass parameters by their average and their difference. The time ranges for correlator fits are determined after a systematic study of the goodness of fit as a function of initial and final fitting times. The choices made here are very similar to those of [3, 4].

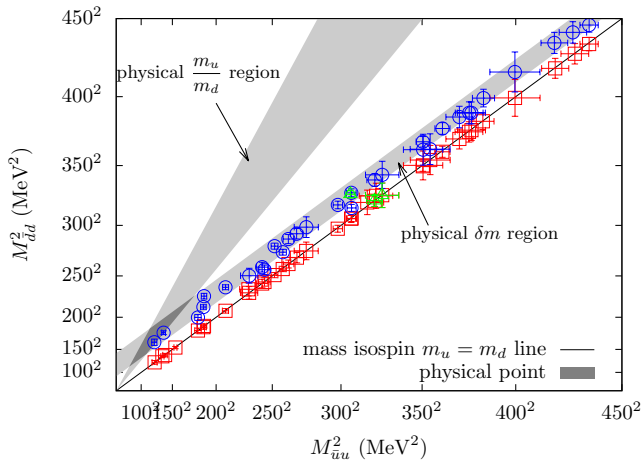

FIG. 1. *Valence data sets plotted in the $M_{\bar{d}d}^2$ vs $M_{\bar{u}u}^2$ plane. The red squares (set 1) lie along the mass isospin line $M_{\bar{u}u}^2$=$M_{\bar{d}d}^2$, and the blue circles (set 2) are scattered around an estimate of the $\Delta M^{2,{\rm ph}}$ region, obtained from the results of [1, 16]. The green triangles (set 3) are points in which α is varied away from its physical value. For clarity, points with $M_\pi > 450$ MeV are not shown.*

Interpolating to the physical point and determining the individual EM and δm contributions.– Having determined the isospin splittings and relevant hadron masses in lattice units for each of our QCD plus QED data sets, we have to convert them to physical units and extrapolate them to the continuum and infinite-volume limits. We also must interpolate the splittings to the physical mass point, as well as to the mass and EM isospin limits.

We determine the five lattice spacings simultaneously from a combined fit of the data with $\Delta M^2 \simeq 0$, for the isospin symmetric observable aM_{Ω^-} or, alternatively, aM_Ξ, using the techniques of [3, 4, 9]. The isospin mass splitting ΔM_X of a hadron X is naturally described by the LO isospin expansion

$$\Delta M_X = A_X \alpha + B_X \Delta M^2 \ , \qquad (1)$$

where ΔM^2 substitutes for δm. The coefficients A_X and B_X still depend on the isospin symmetric parameters of the theory, e.g. m_{ud} or m_s. We find that their dependences on these parameters are well described by a linear expansion in $M_{\pi^+}^2$ and in $M_{K^\chi}^2$ for the range of masses retained below.

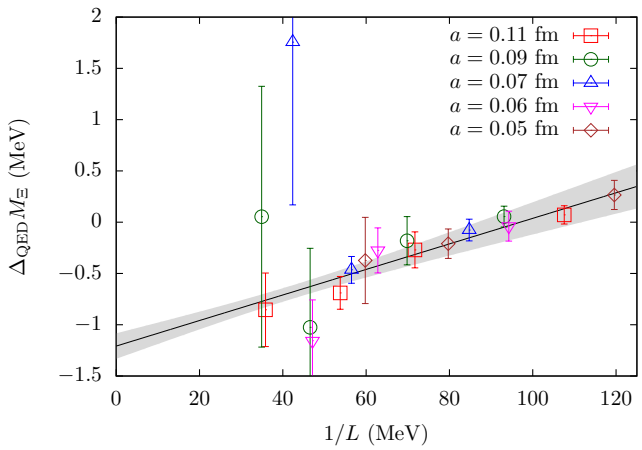

FIG. 2. *Example of FV corrections to $\Delta_{\rm QED} M_\Xi$, plotted as a function of $1/L$. The dependence of the lattice results on all other variables has been subtracted using a fit of the type described in the text. Results with a same $1/L$ and a are averaged because they show no systematic residual dependence on the other simulation parameters, in particular on quark mass. The linear fit in $1/L$, which is performed for points with $M_{\pi^+} \leq 500$ MeV, has a $\chi^2/\mathrm{DOF} = 59./67$. It is plotted as a solid curve, with its 1σ band.*

We must also account for discretization and finite-volume (FV) effects. The latter are particularly important because of the presence of the massless photon. Using techniques from [17], and performing appropriate asymptotic expansions, it is straightforward to show that the leading finite-volume term in scalar and spinor QED is proportional to $1/L$. We find these corrections to be generically large. For instance, in boxes with $L = 1.6$–2.6 fm, which is the largest range of sizes considered in all but the preliminary work of [18] on pseudoscalar masses, the correction to $\Delta_{\rm QED} M_\Xi$, the QED contribution to $\Delta M_\Xi \equiv M_{\Xi^0} - M_{\Xi^-}$, ranges from 123% to 76%. This is illustrated in Fig. 2. In our calculation, L extends up to 6 fm, where the figure indicates a 36% FV correction. While still large, our corrections are sufficiently small that they may be described with a low-order polynomial in $1/L$. This is confirmed by the data in Fig. 2, which show no sensitivity to terms beyond linear order in $1/L$. The same is true of our results for $\Delta M_N \equiv M_p - M_n$, which have a slope in $1/L$ which is compatible with that of $\Delta_{\rm QED} M_\Xi$, but with larger statistical errors. Not surprisingly, the slope in $\Delta M_\Sigma \equiv \Delta_{[\Delta I_3=2]} M_\Sigma = M_{\Sigma^+} - M_{\Sigma^-}$ is consistent with zero: the absolute values of the two particles' charges are equal.

Concerning discretization effects, the improvement of the QCD action implies $O(\alpha_s a, a^2)$ corrections to A_X and B_X. However, due to the lack of improvement in the QED sector, discretization effects on A_X are $O(a)$. In our analysis, we include $O(a)$ QED discretization effects to A_X as well as $O(\alpha_s a, a^2)$ QCD ones to B_X.

Combining all of this information yields a nine parameter description of each of the mass splittings. In the notation of Eq. (1), this corresponds to

$$A_X = a_0^X + a_1^X [M_\pi^2 - (M_\pi^{\rm ph})^2] + a_2^X [M_{K^\chi}^2 - (M_{K^\chi}^{\rm ph})^2] + a_3^X a + a_4^X \frac{1}{L} \,, \tag{2}$$

$$B_X = b_0^X + b_1^X [M_\pi^2 - (M_\pi^{\rm ph})^2] + b_2^X [M_{K^\chi}^2 - (M_{K^\chi}^{\rm ph})^2] + b_3^X f(a) \tag{3}$$

where the a_i^X and b_i^X are the parameters and $f(a) = \alpha_s a$ or a^2, alternatively. For each splitting, among the nine possible parameters, we have retained all combinations which are such that adding one more dependence to the fit causes the associated parameter to be consistent with zero within one standard deviation.

Error estimation– Our analysis methodology makes no assumptions beyond those of the fundamental theory, except for the isospin symmetry which is maintained in the sea and whose consequences we discuss below. However the analysis does depend on several choices that can be sources of systematic uncertainties.

To deal with these uncertainties, we proceed with the method put forward in [9]. More specifically, we consider the following variations in our analysis procedure. For the time ranges of the correlator fits, we consider two initial red fit times, one for which we expect negligible excited state contributions and a red second, more aggressive one. This estimates the uncertainty due to contributions from excited states. Regarding the choice of scale setting quantities, we consider two possibilities: the mass of the Ω^- and that of the isospin averaged Ξ. To estimate the uncertainty associated with the truncation of the Taylor expansion used to interpolate these two masses to physical M_{π^+}, we vary the fit ranges by excluding all data with pion mass above 400 and 450 MeV. To estimate part of this same uncertainty for the isospin splittings, we consider cuts at $M_{\pi^+} = 450$ and 500 MeV, since their $M_{\pi^+}^2$ dependence is very mild. These cuts also provide an estimate of the uncertainty associated with FV corrections, as our simulations keep $LM_\pi \sim 4$, implying cuts on $1/L$ as low as $1/L < 100$ MeV. Part of the uncertainty associated with the continuum extrapolation is determined by considering either $\alpha_s a$ or a^2 discretization errors. Finally, to estimate any additional uncertainty arising from the truncation of these expansions, we consider the result of replacing either A_X or B_X by Padé expressions. These are obtained by considering that the expansions of A_X and B_X in Eqs. (2) and (3) are the first two terms of a geometric series which we resum. This resummation is not applied to the FV corrections. Instead, we try adding a $1/L^2$ term to either the Taylor or Padé forms. In all cases, we find the coefficient of this term to be consistent with zero.

X	ΔM_X	$\Delta_{\rm QED} M_X$	$\Delta_{\rm QCD} M_X$
N	$-0.68(39)(36)$	$1.59(30)(35)$	$-2.28(25)(7)$
Σ	$-7.84(87)(72)$	$0.08(12)(34)$	$-7.67(79)(105)$
Ξ	$-7.16(76)(47)$	$-1.29(15)(8)$	$-5.87(76)(43)$

TABLE I. *Isospin breaking mass differences in MeV for members of the baryon octet. The first error is statistical and the second is systematic. As discussed in the text, we guesstimate the QED quenching uncertainties on the EM contributions to be $O(10\%)$. Propagating the uncertainty in $\Delta_{\rm QED} M_K^2$ yields an $O(4\%)$ error on the δm contributions. The quenching uncertainties on the total splittings can then be obtained by adding those of the EM and δm contributions in quadrature. These guesstimates are not included in the results.*

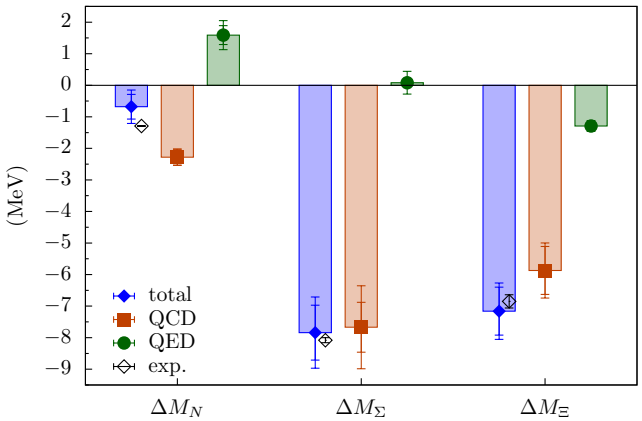

FIG. 3. *Results for the isospin mass splittings of the octet baryons (total), the individual contributions to these splittings from the mass difference $m_u - m_d$ (QCD) and from EM (QED). The bands denote the size of these results. The error bars are the statistical and total uncertainties (statistical and systematic combined in quadrature). For comparison, the experimental values for the total splittings are also displayed.*

These variations lead to $2^7 = 128$ different fits for each of the isospin splittings and parameter combinations. Correlating these with the 128 fits used to determine $\Delta M^{2,\rm ph}$ and allowing various parameter combinations but discarding fits with irrelevant parameters, we obtain between 64 and 256 results for each observable. The central value of a splitting is then the mean of these results, weighted by the p-value. The systematic error is the standard deviation. Because we account for all correlations, these fit qualities are meaningful. The whole procedure is repeated for 2000 bootstrap samples and the statistical error is the standard deviation of the weighted mean over these samples. We have also checked that the results are changed only negligibly (far less than the calculated errors) if they are weighted by 1 instead of by the p-value.

The δm corrections that we do not include in the sea are NLO in isospin breaking and can safely be neglected. The neglected $O(\alpha)$ sea-quark contributions break flavor SU(3). Moreover, large-N_c counting indicates that they are $O(1/N_c)$. Combining the two suppression factors yields an estimate $(M_\Sigma - M_N)/(N_c M_N) \simeq 0.09$. A smaller estimate is obtained by supposing that these corrections are typical quenching effects [19] that are SU(3) suppressed, or by using [20] the NLO χPT results of [10]. However, in the absence of direct quantitative evidence, it is safer to assume that the EM contributions to the splittings carry an $O(10\%)$ QED quenching uncertainty.

Final results and discussion.– Combining the methods described above, we obtain our final results for the total octet baryon isospin splittings ΔM_N, ΔM_Σ, and ΔM_Ξ defined above. These results, together with those obtained for the EM and δm contributions, are summarized in Table I. We also plot them in Fig. 3, with the experimental values for the full splittings. Our results are compatible with experiment.

Concerning the separation into δm and EM contributions, there exist very few determinations of these quantities up to now. In the review [21], hadron EM splittings were estimated using a variety of models and Cottingham's formula for the nucleon. These estimates are compatible with our results within $\sim 1.5\sigma$. The EM nucleon splitting has recently been reevaluated with Cottingham's formula in [22], yielding a result which is in better agreement with ours. ΔM_N has further been studied with sum rules in [23].

Besides the entirely quenched, pioneering work of [24], ours is the only one in which the baryon octet isosplittings are fully computed. The only other lattice calculation of the full nucleon splitting is presented in [25]. Like ours, it implements QED only for valence quarks. While their $\Delta_{\rm QCD} M_N$ agrees very well with ours, agreement is less good for the EM contribution and total splitting, which they find to be 0.38(7) MeV and $-2.1(7)$ MeV, respectively. That study was performed in rather small volumes with a limited set of simulation parameters, making an estimate of systematic errors difficult. The few other lattice calculations consider only the δm contributions to the baryon splittings, in N_f=2 [7, 26] and N_f=2+1 [27, 28] simulations. The results of [26–28] rely on imprecise phenomenological input to fix m_u/m_d or $(m_u - m_d)$. The estimate for $\Delta_{\rm QED} M_K^2$ of [16] is used directly in [26, 28] and that of [29], indirectly in [27]. The most recent N_f=2 calculation [7] actually determines $\Delta_{\rm QED} M_K^2$ in quenched QED, as we do here for N_f=2+1. $\Delta_{\rm QCD} M_N$ is computed in [7, 26, 27] while all three QCD splittings are obtained in [28]. The latter is also true in [30], where N_f=2+1 lattice results are combined with SU(3) χPT and phenomenology. Agreement with our results is typically good. In all of these calculations, the range of parameters explored is smaller than in ours, making it more difficult to control the physical limit.

L.L. thanks Heiri Leutwyler for enlightening discus-

sions. We also thank Jérôme Charles and Marc Knecht for helpful conversations. Computations were performed using the PRACE Research Infrastructure Resource JUGENE at FZ Jülich, with further HPC resources provided by GENCI-[IDRIS/CCRT] (Grant No. 52275) and FZ Jülich, as well as using clusters at Wuppertal and CPT. This work was supported in part by the OCEVU Labex (ANR-11-LABX-0060) and the A*MIDEX Project (ANR-11-IDEX-0001-02) funded by the "Investissements d'Avenir" French government program managed by the ANR, by CNRS Grants GDR No. 2921 and PICS No. 4707, by EU Grants FP7/2007-2013/ERC No. 208740 and No. MRTN-CT-2006-035482 (FLAVIAnet), and by DFG Grants No. FO 502/2 and No. SFB-TR 55.

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