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Up and down quark masses and corrections to Dashen's theorem from lattice QCD and quenched QED

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In a previous letter [1] we determined the isospin mass splittings of the baryon octet from a lattice calculation based on quenched QED and N_f=2+1 QCD 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. Using the same data we determine here the corrections to Dashen's theorem and the individual up and down quark masses. For the parameter which quantifies violations to Dashens's theorem, we obtain $\varepsilon = 0.73(2)(5)(17)$, where the first error is statistical, the second is systematic, and the third is an estimate of the QED quenching error. For the light quark masses we obtain, $m_u = 2.27(6)(5)(4)$ MeV and $m_d = 4.67(6)(5)(4)$ MeV in the $\overline{\text{MS}}$ scheme at 2 GeV and the isospin breaking ratios $m_u/m_d = 0.485(11)(8)(14)$, $R = 38.2(1.1)(0.8)(1.4)$ and $Q = 23.4(0.4)(0.3)(0.4)$. Our results exclude the $m_u = 0$ solution to the strong CP problem by more than 24 standard deviations.

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The up (u) and down (d) quark masses are two fundamental parameters of the Standard Model of Particle Physics. These masses cannot be directly determined through experiment because of the confinement of quarks within hadrons. Lattice QCD provides an *ab-initio* approach to the non-perturbative calculation of QCD correlation functions. This method can be used to determine the light quark masses from the experimental values of hadron masses. In earlier work [2, 3], we determined precisely m_{ud}, the average of the up and down quark masses, using lattice QCD simulations at the physical values of the quark masses. This quantity has also been studied by many other lattice collaborations (*cf.* the FLAG review [4]) and considerable progress has been made on its determination. Thus, it is now relevant to aim for the calculation of the light-quark mass difference $\delta m = m_u - m_d$. This quantity is more difficult to obtain than m_{ud}. Its small effect on hadron masses, of order $\mathrm{O}(\delta m/\Lambda_{\mathrm{QCD}}) \simeq \mathrm{O}(1\%)$, is expected to be comparable in size to the leading $\mathrm{O}(\alpha)$ electromagnetic (EM) corrections, usually not included in lattice simulations. Thus, earlier lattice calculations of this mass difference [2, 3, 5, 6] relied on phenomenological estimates of EM corrections. The inclusion of quenched QED effects was first performed in [7] on quenched QCD configurations, in [8, 9] on $N_f = 2$ QCD configurations and in [10] on $N_f = 2 + 1$ configurations, at a single lattice spacing, with rather large pion masses and in small volumes. Preliminary results for the present calculation can be found in [11–13] and preliminary results by MILC, in [14]. Very recently, an $N_f = 2 + 1$ calculation of m_u/m_d in which QED effects are unquenched was presented in [15]. This calculation is performed on three ensembles at a single lattice spacing, in volumes up to $(3.3\text{ fm})^3$ and with sea quark masses fixed at the SU(3) symmetric point $M_\pi = M_K \simeq 412$ MeV.

Here we include QED effects to the dynamics of the valence quarks, atop $N_f = 2 + 1$ QCD configurations generated directly at the physical value of the light-quark masses, with full continuum and infinite-volume extrapolations, as well as with full non-perturbative renormalization and running. This is a sequel to the letter [1] which uses the same data set to compute light octet baryon isospin mass splittings. Note that a fully unquenched calculation of octet baryon and other hadron mass isospin splittings, with pion masses down to 195 MeV, can now be found in [16]. Here, because we are dealing with light quark masses whose extraction requires reaching deep into the chiral regime [17], we favor the simulations used in [1]. This data set also has the notable advantage that it has been used to determine the s and average u-d quark masses in [2, 3]. Thus, all of the relevant non-perturbative renormalization and running has already been performed in pure QCD [2].

The light quark mass difference δm is connected, through a low energy theorem [18], to the pseudoscalar meson EM mass splittings. In the late 1960's, Dashen showed that pions and kaons receive the same EM contributions in the SU(3) chiral limit [19]. This result is commonly known as *Dashen's theorem*. During the 1990's,

attempts to compute the chiral corrections to Dashen's theorem in effective field theories led to controversial and surprisingly large results (*cf.* the review [13] for more details). In this letter we present a computation of these corrections from our lattice QCD and quenched QED simulations.

General strategy. We consider in this work only the leading $\mathrm{O}(\alpha, \delta m)$ corrections to isospin symmetry. As was done in [1], we define ΔM^2 to be the difference of the squared masses of the "connected" $\overline{u}u$ and $\overline{d}d$ pseudoscalar mesons. It is known from partially-quenched chiral perturbation theory coupled to photons (PQχPT+QED) [20] that this quantity is related to δm by the following expansion:

$$\Delta M^2 = 2B_2\delta m + \mathrm{O}(m_{ud}\alpha, m_{ud}\delta m, \alpha^2, \alpha\delta m, \delta m^2) \quad (1)$$

where B_2 is the two-flavor chiral condensate parameter. If the quark masses have their physical values, we can safely make the assumption that $\mathrm{O}(m_{ud}) = \mathrm{O}(\delta m)$. Then at the level of precision considered here, ΔM^2 is proportional to δm. So to extract δm one needs to know the physical value of ΔM^2 and the constant B_2.

B_2 was recently computed in [17], using the same QCD simulations as the ones considered in the present paper. To determine ΔM^2, we consider the leading isospin expansion of the kaon mass splitting $\Delta M_K^2 = M_{K^+}^2 - M_{K_0}^2$:

$$\Delta M_K^2 = C_K\alpha + D_K\Delta M^2 \quad (2)$$

Results for ΔM_K^2 obtained for different values of α and δm from lattice QCD and QED simulations can be fitted to this expression to obtain the coefficients C_K and D_K and subsequently the value of ΔM^2 corresponding to physical quark masses, from the experimental value of ΔM_K^2.

Summary of the lattice methodology. The lattice setup used for this project is very similar to the one already described in [1]. The work is based on our set of lattice QCD simulations presented in [2]. It is composed of 47 $N_f = 2+1$ QCD ensembles with pion masses down to 120 MeV, 5 lattice spacings down to 0.054 fm and 16 different volumes up to $(6\,\mathrm{fm})^3$. These simulations were performed using a tree-level $\mathrm{O}(a)$-improved Wilson fermion action with 2 steps of HEX smearing. For each QCD configuration, a QED one is generated using the non-compact Maxwell action in Coulomb gauge with the four-momentum zero mode fixed to 0. The resulting $SU(3)\times U(1)$ configuration is then included in the Wilson-Dirac operator used to compute the valence quark propagators, with the appropriate electric charge. The valence light quark masses are tuned to explore the region where δm varies between 0 and its physical value. For most QCD ensembles, the unit of charge for valence quarks is set to its physical value. On one particular QCD ensemble, we perform three valence analyses: two

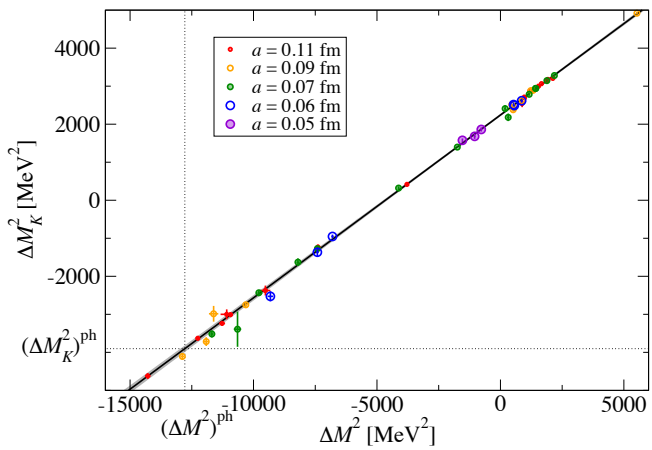

Figure 1. Example of a fit of the dependence of ΔM_K^2 on α and ΔM^2 to the expression of Eq. (2). Here, ΔM_K^2 is plotted as a function of ΔM^2. The dependence of the lattice results on all other variables has been subtracted using the fit. The fit has a correlated χ^2/dof equal to 1.59. It is plotted as a solid curve, with its 1σ band.

with close to physical δm and a value of α either about twice or one-fourth its physical value, and a third with $\alpha \simeq 0$ and $\delta m \simeq 0$. A plot of the values of $M_{\overline{d}d}^2$ versus $M_{\overline{u}u}^2$ used in our valence datasets can be found in [1, Fig. 1].

In this setup, two approximations are made: the sea u and d quark masses have the same mass and they carry no electric charge (QED is quenched). It is straightforward to show that the splitting of the sea light-quark masses only affects isospin splittings at orders in the isospin expansion which are beyond those considered. Regarding the quenching of QED, large N_c counting and SU(3) flavor symmetry suggests that the sea QED effects may represent O(10%) of the $\mathrm{O}(\alpha)$ contribution to a given isospin splitting [1]. Considering the EM part of the kaon splitting, which is of particular interest here, the next-to-leading order (NLO) PQχPT+QED calculation of [20] can be used to estimate the QED quenching effects. In [21] we argue that they may represent 5% of the $\mathrm{O}(\alpha)$ correction. Nevertheless, for giving the reader an idea of how such a quenching uncertainty may propagate to the other quantities studied in this paper, we retain the more conservative 10% quenching uncertainty on $\Delta_{\mathrm{QED}} M_K^2 = \alpha C_K$.

The EM contribution to the kaon splitting. In the expansion (2), the coefficients C_K and D_K still depends on m_{ud}, m_s, a, and the temporal and spatial extents T and L. We fix m_{ud} and m_s to their physical values by matching to the experimental values of $M_{\pi^+}^2$ and the combination $(M_{K^+}^2 + M_{K^0}^2 - M_{\pi^+}^2)/2$. Then, as explained in detail in [1], we use as a model for ΔM_K^2 a first order expansion of C_K and D_K in these mass parameters around the physical mass point. Additionally, we allow for $\mathrm{O}(a)$ dis-

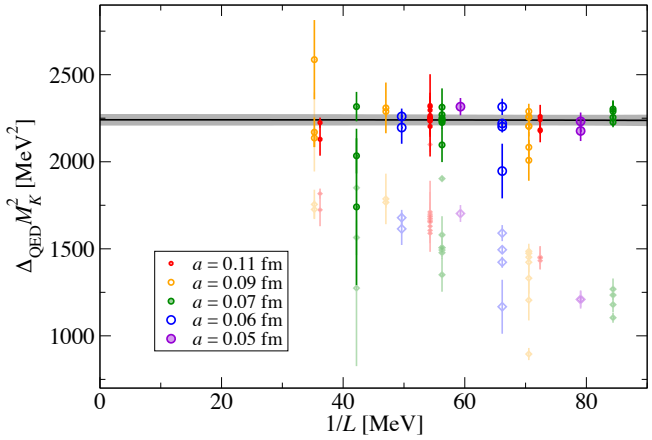

Figure 2. Same fit as in Fig. 1. Here $\Delta_{\rm QED} M_K^2$ is plotted as a function of $1/L$. The greyed symbols show the full volume dependence of the data. For the plain symbols, the universal $O(1/L)$ and $O(1/L^2)$ finite volume effects from (3) have been subtracted and the fit to the $O(1/L^3)$ correction is plotted.

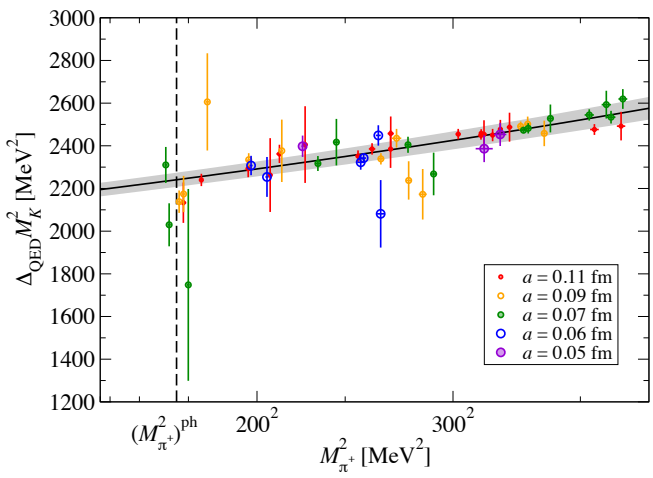

Figure 3. Same fit as in Fig. 1. Here $\Delta_{\rm QED} M_K^2$ is plotted as a function of $M_{\pi^+}^2$.

cretization effects and power-like $O(1/L)$ finite-volume effects [16, 22] in the QED contribution proportional to C_K, as required in our setup. The finite volume effects are taken into account by adding the following term to the aforementioned expansion of C_K:

$$C_K^{\rm FV} = -\frac{\kappa M_K}{L}\left[1 + \frac{2}{M_K L}\left(1 - \frac{\pi}{2\kappa}\frac{T}{L}\right)\right] + \frac{\rho}{L^3} \qquad (3)$$

where $\kappa = 2.837\ldots$ is a known number, $M_K = \frac{1}{2}(M_{K^+} + M_{K^0})$ is the isospin averaged kaon mass and ρ is a fit parameter. In the parametrization (3), the $O(1/L)$ and $O(1/L^2)$ coefficients have been fixed to their known universal value [16] and the $O(1/L^3)$ term is fitted to take into account additional structure-dependent effects. For the QCD contribution proportional to D_K, we assume $O(\alpha_s a, a^2)$ discretization effects and negligible finite-volume effects, which is justified in our large volumes given our present precision. To estimate systematic uncertainties, we consider a variety of analysis procedures. These variations are identical to those performed in [1]. They include (please see [1] for justifications and additional details): fitting the needed correlators on a conservative or a more aggressive time range; setting the scale with the mass of the Ω^- or the isospin-averaged Ξ; eliminating points with M_{π^+} either greater than 400 MeV or than 450 MeV for the Ω^- and the Ξ mass, and greater than 350 MeV or than 400 MeV for ΔM_K^2; including either $\alpha_s a$ or a^2 contributions in D_K; replacing individually the Taylor mass expansions in C_K and D_K by the inverse of these expansions (for a total of 4 choices). This leads to 128 different determinations of C_K and D_K. An example of such a fit is illustrated in Figs. 1 – 3. Finally, using the histogram method developed in [23], we combine all of these results to obtain:

$$\Delta_{\rm QED} M_K^2 = 2186(26)(68)(219)\ {\rm MeV}^2 \qquad (4)$$

where C_K is taken at the physical mass point, in the continuum and infinite volume limits. Here the first error is statistical, the second is systematic, and the third is an estimation of the quenching uncertainty as discussed above. Our result can be compared to an estimate obtained from the input of FLAG [4], $\Delta_{\rm QED} M_K^2 = 2090(380)$ MeV^2. The results are entirely compatible and ours has a total precision which is more than 5 times higher omitting the generous estimate for the quenching error and more than 1.6 times including it. For completeness, we also give the value of the slope of ΔM_K^2 in ΔM^2 at the physical point, obtained from our analysis: $D_K = 0.484(5)(4)$. This result is compatible with the value $D_K = 0.45(9)$, obtained by appropriately combining results from FLAG [4]. Its total error is 15 times more precise.

Corrections to Dashen's theorem. As defined in [4], one can quantify corrections to Dashen's theorem with the parameter:

$$\varepsilon = \frac{\Delta_{\rm QED} M_K^2 - \Delta_{\rm QED} M_\pi^2}{\Delta M_\pi^2} \qquad (5)$$

The pion isospin mass splitting, needed to evaluate ε, is challenging to obtain through a lattice computation. Because the neutral pion is diagonal in flavor, correlation functions for this state will contain quark disconnected diagrams. These diagrams are known to be expensive and hard to evaluate on the lattice. Thus, we choose not to compute the pion splitting here. Fortunately, using G-parity, one can easily show that the leading $O(\delta m)$ corrections to ΔM_π^2 vanishes. Therefore, at the level of precision considered in this paper, we have $\Delta_{\rm QED} M_\pi^2 = \Delta M_\pi^2$, which is very well known experimentally [24].

Using our result (4) for $\Delta_{\rm QED} M_K^2$ and the experimen-

tal value of ΔM_π^2, we obtain:

$$\varepsilon = 0.73(2)(5)(17) \tag{6}$$

Here the relative quenching error, obtained by propagating a 10% uncertainty in $\Delta_{\rm QED} M_K^2$, is 23%. Now, if we include an estimate of the δm^2 corrections in the relation of $\Delta_{\rm QED} M_\pi^2$ to ΔM_π^2, as given in [4] with the parameter $\varepsilon_m = \Delta_{\rm QCD} M_\pi^2 / \Delta M_\pi^2 = 0.04(2)$, we find $\varepsilon = 0.77(2)(5)(17)(2)$, with the fourth uncertainty coming from the one in ε_m. Our result of (6) can be compared to the FLAG estimate $\varepsilon = 0.7(3)$ [4]. Again, it is entirely compatible with this estimate, and has a total precision which is more than 5 times higher without the quenching uncertainty estimate and about 1.8 times higher with it.

Up and down quark masses. Using our analysis of the kaon splitting, the experimental value of this splitting, our lattice result $B_2 = 2.61(6)(1)\,\text{GeV}$ [17] in the $\overline{\rm MS}$ scheme at 2 GeV and formula (2), we obtain:

$$\delta m = m_u - m_d = -2.41(6)(4)(9)\ \text{MeV} \tag{7}$$

in the same scheme and at the same scale. If one assumes a 10% QED quenching error on $\Delta_{\rm QED} M_K^2$, this error propagates to 3.7% on δm. It is interesting to note that the quenching of QED has a rather small impact on the determination of δm. This comes essentially from the fact that the QCD part of the kaon splitting is roughly 3 times larger than the QED part. Our result is entirely compatible with the value $\delta m = -2.53(16)$ MeV, derived from FLAG input [4]. Its precision is a factor of 2.1 to 1.3 higher, depending on whether the quenching error is taken into account.

If we combine (7) with our previous result $m_{ud} = 3.469(47)(48)\,\text{MeV}$ [3], we get:

$$m_u = m_{ud} + \frac{\delta m}{2} = 2.27(6)(5)(4)\ \text{MeV} \tag{8}$$

$$m_d = m_{ud} - \frac{\delta m}{2} = 4.67(6)(5)(4)\ \text{MeV} \tag{9}$$

still in the $\overline{\rm MS}$ scheme at 2 GeV. With the same assumptions as before, the QED quenching error on the individual quark masses is estimated to be 1.8 and 0.9%, respectively. Our results are nicely compatible with the FLAG values $m_u = 2.16(9)(7)$ MeV and $m_d = 4.68(14)(7)$ MeV.

From the results of (8) and (9), we obtain the ratio of light quark masses:

$$\frac{m_u}{m_d} = 0.485(11)(8)(14) \tag{10}$$

Strictly speaking, because u and d have different electric charges, this ratio is scale dependent in QCD plus QED. However it is easy to see that this dependency is beyond the leading isospin order considered in this work. Error propagations give a 2.9% QED quenching uncertainty on this ratio. Our result is compatible with the FLAG average $m_u/m_d = 0.46(2)(2)$. Moreover, our total precision is between 1.5 and 2.2 times higher, depending on whether our estimate of quenching uncertainties is included.

We can further use our previous result $m_s/m_{ud} = 27.53(20)(8)$ [3] to build the flavor breaking ratios R and Q:

$$R = \frac{m_s - m_{ud}}{m_d - m_u} = 38.2(1.1)(0.8)(1.4) \tag{11}$$

$$Q = \sqrt{\frac{m_s^2 - m_{ud}^2}{m_d^2 - m_u^2}} = 23.4(0.4)(0.3)(0.4) \tag{12}$$

QED quenching effects of order 4% and 2%, respectively, cannot be excluded on these quantities. It is also interesting to compare our results for R to those obtained from χPT applied to $\eta \to 3\pi$ decays [18, 25–28]. The convergence of χPT for this process is very poor and it is usually supplemented by a dispersive analysis. Without such an analysis, the results vary from 19.1 at LO to 31.8 at NLO and 42.2 (or 38.7 setting the $O(p^6)$ low-energy constants to 0) at NNLO [25]. The most recent NNLO χPT dispersive analysis [27] gives $R = 37.7(2.2)$, in good agreement with our result.

To summarize, our results are compatible with the estimates of [4], which already include input from the quenched QED studies mentioned above [29]. In most cases, they significantly improve on their precision. In all isospin symmetry breaking quantities the quenching uncertainty is the dominant one. Therefore, it is now important to determine these quantities using a fully unquenched calculation with significantly higher statistics, such as the one carried out in [16] for the splitting of stable hadrons.

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[29] In fact, preliminary versions of the results presented here [11, 13, 21] impacted the analysis of [4].