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Studies of the QCD and QED effects on Isospin breaking

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The isopin breaking effect due to different masses and electric charges between up/down quarks are stuided non-perturbatively using lattice QCD+QED. Up, down, and strange quark masses are determined using $K^{\pm}, K^0$, and $\pi^{\pm}$ meson masses as inputs. The charge splitting of *Kaon* mass, $m_{K^{\pm}} - m_{K^0}$, is broken up into the part coming from up, down quark mass difference and that from electromagnetic effects. We also report about the neucleon/proton mass splittings as well as other recent studies of isospin breakings on lattice.

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1. Introduction

In QCD, the isospin symmetry, the $SU(2)$ rotation between up and down quarks, is broken due to the electric charge difference between up and down quarks, $q_{\rm up} = 2/3 \neq q_{\rm down} = -1/3$, besides their mass difference, $m_{\rm up} - m_{\rm down}$. The isospin symmetry is realized in a good approximation, and it has led to various quantitative understandings in particle physics. Studying the breaking of the symmetry also brings us information of important quantities. For instance, the up and down quark mass difference could be extracted from the very accurately measured isospin breaking in Hadron masses,

$$m_{K^\pm} - m_{K^0} = -3.937(28)\ \text{MeV},\ \ m_{\pi^\pm} - m_{\pi^0} = 4.5936(5)\ \text{MeV}, \tag{1.1}$$

$$m_N - m_P = 1.2933317(5)\ \text{MeV}, \tag{1.2}$$

by studying the isospin breaking as we will see later. The determination of up quark mass is particularly interesting since one could check the simplest solution to the strong CP problem $m_u = 0$. The positive mass difference between neutron and proton makes proton a stable particle thus the chemistry is as it is.

The first principle non-perturbative computations of QCD using the lattice regularization including light quark degrees of freedom, $N_F = 2+1$, have successfully become a practical tool for the particle and nuclear phenomenologies as presented in this conference [1, 2, 3, 4, 5]. The mode of typical lattice computations so far is assuming isospin symmetry. Especially, the breaking, which is originates from the electromagnetic (EM) effects, are often neglected, or they are partially incorporated using phenomenological assumptions such as Dashen's theorem, which causes one of the dominant systematic errors. The lattice QCD+QED simulation, which include not only gluon field but also photon field are necessary for more accurate hadron spectrum studies and quark mass determinations.

The main focus in this contribution will be our studies of the lattice QCD+QED [6, 7, 8] and its applications including, (1) meson mass fitting to the chiral perturbation theories [9] with virtual photon (ChPT+γ), (2) determinations of up, down and strange quark masses, and (3) exercises to disentangle the two origins of isospin breaking (quark masses and charges difference) in the mass splittings of *Kaon* and nucleons. Lattice quarks used are the domain-wall fermions [11, 12, 13], which preserves chiral symmetry in a good approximation. The chiral symmetry is essential in these studies to identify the quark massless points unaffected from the fluctuations of photon and gluon.

2. Lattice QCD+QED simulation

To make the photon field couple to quarks on lattice we follow the pioneering works [14, 15] in which non-perturbative simulations of the lattice QCD+QED was carried out. The photon field, $A_{{\rm em},\mu}(x)$, in its non-compact implementation, is generated in the Feynman gauge with eliminating the diverging zero modes. Although the emission of quark and anti-quark pairs from gluon are fully incorporated, that from photon is ignored to reduce the computational costs for now. This omission will be taken into account in our estimation for the systematical error.

For each $i-$th quark flavor, the photon field is combined with the gluon field $U_\mu(x)$, which fully incorporates the vacuum polarization effects of up, down, and strange quarks:

$$U_\mu(x) \longrightarrow (U_\mu^{\rm EM})^{q_i} U_\mu(x), \quad U_\mu^{\rm EM} = e^{-ieA_{{\rm em},\mu}(x)}\ \ . \tag{2.1}$$

Here q_i is the quark's charge in the unit of the elementary electric charge, e, and $\alpha = e^2/(4\pi) = 1/137$.

The gluon ensembles are generated by RBC and UKQCD collaborations [16, 17, 18] using the domain-wall fermions (DWF) as lattice quarks, which are another key ingredients in this study. The settings and parameters of the simulation are follows: the lattice spacing determined from Omega baryon masses is $a = 0.115(2)$ fm, the quark masses in the lattice unit are $am_q = 0.005, 0.01, 0.02, 0.03$, which are roughly corresponds to $20-120$ MeV. The dynamical strange quark mass ($am_s = 0.03$) turns out to be roughly 15 % heavier than the physical one. We will extrapolate (and interpolate) results at the physical quark masses from those in the simulation.

Since the photon field is not confined, it propagates for a longer distance and we should anticipate the effect of the finite volume of lattice in QCD+QED simulation than that in QCD. This is the reason we examine two lattice volumes, $V = (16a = 1.84\mathrm{fm})^3$ and $(24a = 2.75\mathrm{fm})^3$. By comparing results from the two different volumes, we will estimate the finite volume effects.

To extract the mass of I hadron ($I = \pi, K, P, N, \cdots$) from the simulation, hadron correlation functions in Euclidean time, $C_I(t)$, are calculated on the QCD+QED ensemble, then they are fit to the exponential function form with the mass M_I as a fit parameter at large t: $\lim_{t\gg a} C_I(t) = A_I e^{-M_I t}$. We found that averaging over $C_I(t)$ of positive and negative QED charges is very useful to reduce the statistical noise [10] since its $\mathscr{O}(e)$ contribution to the noise is explicitly cancelled in the average leaving the physical signal which is $\mathscr{O}(e^2)$.

Thus, on each ensemble with dynamical light (degenerate up and down) quark masses, m_l, we measure $M_{\mathrm{PS}}(m_1, q_1, m_3, q_3; m_l)$, the mass of pseudoscalar meson, which is made of quark pairs $\psi_1(x)$ and $\psi_3(x)$, each of whose charge and mass is (m_i, q_i) with $i = 1, 3$. In Fig.1, difference between squared masses of pseudoscalar meson of QCD+QED and that of QCD alone,

$$\delta m^2(m_1, q_1, m_3, q_3; m_l) = M_{\mathrm{PS}}^2(m_1, q_1, m_3, q_3; m_l) - M_{\mathrm{PS}}^2(m_1, 0, m_3, 0; m_l) \ , \tag{2.2}$$

is plotted for the lightest sea quark mass, $m_l = 0.01/a \sim 40$ MeV. The horizontal axis is sum of valence quark masses, $m_1 + m_3$. Different colors correspond to different charge combination of quark-antiquark pairs: $q_{13} = q_1 - q_3$ is the difference of charge of quarks (total meson charge), and $\delta q = q_1 + q_3$ is the sum of the charges. To make the plot less busy, we plot only for degenerate quark mass cases, $m_1 = m_3$. We also calculated for the non-degenerate quark mass cases, and will use them in the analysis.

In total, we have measured 234 different mass and charge combinations, $(m_1, q_1, m_3, q_3; m_l)$, of quark antiquark pairs on $(2.75\mathrm{fm})^3$ lattices. Some of combination are unphysical. For example, we have fractional charges $\pm q_{13} = 1/3, 2/3, 4/3$ in Fig.1. Although there are no experimental results for meson, they are no less useful than results from physical charge combinations, $q_{13} = 0, \pm 1$, to constrain the unknown parameters in the ChPT fits .

Since the quarks in our simulation are still heavier than physical up and down quark masses due to our limited computational resources, we need to extrapolate the results of simulation into the lighter quark masses to predict for the physical points. There is no need for such extrapolations in the direction of electric charges as they are already set to be physical in the simulation.

The extrapolation is done by fitting the simulation results to the meson mass formula of ChPT. Very similar to the case of quark mass, the electric charges break the flavor-chiral symmetry $SU(3)_V \times SU(3)_A$ and. By treating the quark's 3×3 charge matrix and mass matrix as the

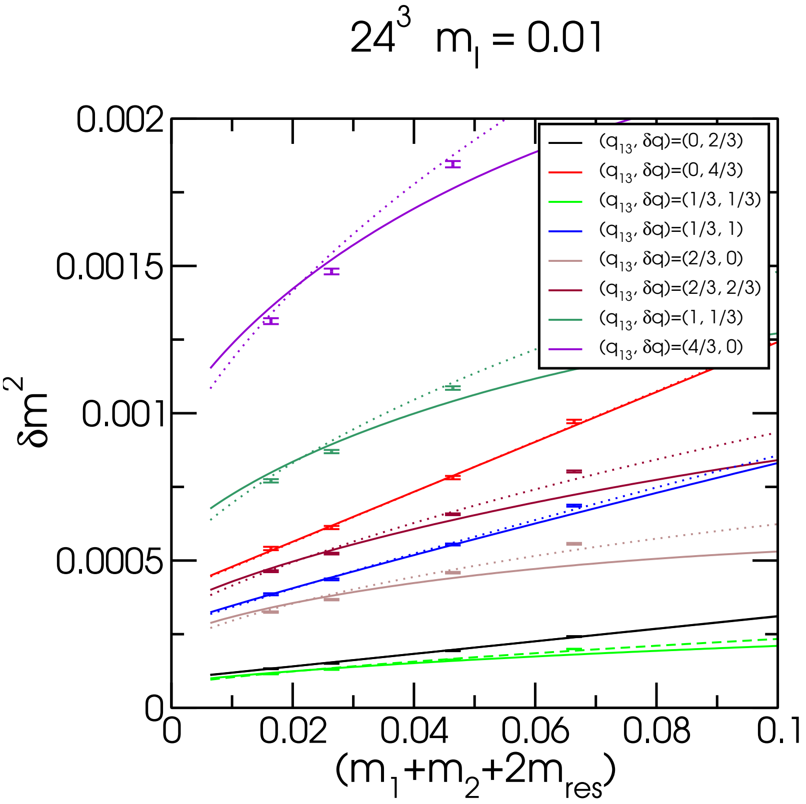

Figure 1: The squared mass difference of pseudoscalar meson mass, δm^2, defined in (2.2) in lattice unit for the lightest sea quark mass, $m_l = 0.01/a \simeq 40$ MeV and Volume is $V = (24a)^3 \simeq (2.75\text{fm})^3$. The horizontal axis is the sum of the valence quark masses in lattice unit. Different colors correspond to different charge combination of quark antiquark pairs. $q_{13} = q_1 - q_3$ is the total meson charge, and $\delta q = q_1 + q_3$ is difference of charges between quark and anti-quark. The result of the SU(3) partially quenched ChPT+γ fit are shown for $m_{\text{cut}}/a = 0.01/a \simeq 40$ MeV (solid curves) and $m_{\text{cut}}/a = 0.02/a \simeq 70$ MeV (dotted curves).

spurion field, the chiral symmetric low energy effective theory including the virtual photon is constructed order by order in the double powers of e^2 and m_q. We treat $\mathcal{O}(e^2)$ as the same order as $\mathcal{O}(m_q)$.

The ChPT mass formula we will mainly use is the flavor $SU(3)$ ChPT with virtual photon included [19, 20], treating the up, down, and strange quarks (or pions, kaons and η) as light degrees of freedom. The mass formula allows us to fit not only for the unitary case, where the sea quarks are exactly same as valence quarks in terms of mass and the electric charge (partially quenched ChPT+γ). In future, we will also use the ChPT with finite volume correction to the next leading order [21] as well as the flavor $SU(2)$+Heavy Kaon+γ, which is expected to be a better converging power series of quark mass [18].

The squared mass of the pseudoscalar meson made of quark pairs (m_i, q_i) with $i = 1,3$ in

ChPT+γ are expanded as follows (m_l, m_s is the sea up/down and strange quark masses):

$$M^2_{\rm PS}(m_1,q_1,m_3,q_3) = M^2_{\rm PS}(m_1,0,m_3,0)+\delta m^2(m_1,q_1,m_3,q_3)+\mathscr{O}(e^4,p^6,e^2p^4) \tag{2.3}$$

$$M^2_{\rm PS}(m_1,0,m_3,0) = \chi_{13}+(48L_6-24L_4)\overline{\chi_1}\chi_{13}+(16L_8-8L_5)\chi^2_{13}+\cdots \tag{2.4}$$

$$\begin{aligned}\delta m^2(m_1,q_1,m_3,q_3) &= \frac{2Ce^2}{F_0^2}q^2_{13}\\ &-Y_1 4e^2\overline{Q_2}\chi_{13}+Y_2 4e^2(q_1^2\chi_1+q_3^2\chi_3)+Y_3 4e^2 q^2_{13}\chi_{13}-Y_4 4e^2 q_1 q_3\chi_{13}+Y_5 12e^2 q^2_{13}\overline{\chi_1}+\cdots\end{aligned} \tag{2.5}$$

Here the tree level squared pion mass, $\chi_{13}\equiv B_0(m_1+m_3)$, and average of the three sea quark masses $\overline{\chi_1}$. When QED is switched-off by $e^2=0$, there are three LECs in $M^2_{\rm PS}(m_1,0,m_3,0;m_l,m_h)$: B_0 at the LO and two NLO LECs, $2L_6-L_4$ and $2L_5-L_8$.

At $\mathscr{O}(e^2)$ level, we only have a new EM LEC C, which gives the mass to charged PS meson at the quark massless limit. C term corresponds to the Dashesn's theorem: the charge splitting δm^2 is independent of quark mass omitting $\mathscr{O}(e^2 m_q)$ terms. There are five $\mathscr{O}(e^2 m_q)$ terms, Y_i with $i=1,2,\cdots,5$, among which, only Y_1 depends on the average of squared sea quark charges, $\overline{Q_2}$. In our quenched QED simulation, electric charges of the sea quarks are zero so we couldn't fit Y_1. We will estimate the systematic error due to the omission of Y_1 term. These $\mathscr{O}(e^2 m_q)$ terms are the corrections to the Dashen's theorem.

In this formula and hereafter, the sea quark masses, m_l, m_h, are suppressed from the arguments, we have also omitted the known logarithmic terms as well as analytic terms written in terms of C and QCD's NLO LECs, but they are properly taken into account into our analysis.

3. Results

The ChPT mass formula (2.3) is used to fit the calculated PS masses. We fit the squared PS masses without QED to $M^2_{\rm PS}(m_1,0,m_3,0)$ in (2.4), and the squared mass difference to $\delta m^2(m_1,q_1,m_3,q_3)$ in (2.5). The fit parameters B_0, f (and also the lattice spacing a from Ω mass) are common in the first and the second fits. We use their values determined from the first fit as inputs to the second fit. The statistical errors of B_0 and f from the first fit are taken into account by varying them from their central values by one sigma statistical error.

Simulation data used in the fit procedure are restricted to lighter quark masses, $m_1, m_3, m_l \le m_{\rm cut}$, so that the higher order terms in the ChPT Lagrangian stay small enough. 48 partially quenched points survive for $am_{\rm cut}=0.01$, corresponding roughly 40 MeV quark mass, while 120 data are fitted for $am_{\rm cut}=0.02$ ($m_{\rm cut}\simeq$70 MeV).

The fit curves are shown for partial quenched case, $m_l \neq m_1, m_3$, in Fig. 1. The solid (dotted) curve is the fit results with $m_{\rm cut}a=0.02$ (0.04). The fit curves reproduce the data point well for quark masses lighter than $m_{\rm cut}$ and deviate for the heavier points. In Fig. 1, there are also visible deviations in larger meson charge cases, $q_{13}\ge 1$. These deviations are likely due to the omission of the higher order terms in ChPT+γ. The effects of NNLO and higher terms, which are omitted in the fit, will be estimated by comparing the results of the two different values of $m_{\rm cut}$ and by estimating $\mathscr{O}(e^4)$ effects.

PoS(KAON09)034

Fit, V	$m_{\rm cut}$	$m_{\rm up}$	$m_{\rm down}$	$m_{\rm strange}$	$m_{\rm up}/m_{\rm down}$	$2m_{\rm strange}/(m_{\rm up}+m_{\rm down})$
SU(3), (2.7 fm)^3	40 MeV	2.76(26)	4.80(46)	95(9)	0.575(14)	25.1(5)
SU(3), (2.7 fm)^3	70 MeV	2.55(23)	4.78(46)	95(9)	0.532(15)	25.9(5)
SU(3), (1.8 fm)^3	70 MeV	2.93(19)	4.85(29)	95(5)	0.605(11)	24.4(4)
SU(3)$\delta m_{\rm res}$,(2.7 fm)^3	40 MeV	2.52(24)	4.74(45)	95(9)	0.532(15)	26.1(5)

Table 1: Preliminary determinations of quark masses in MeV in $\overline{\rm MS}$(NDR) at $\mu = 2$ GeV using SU(3) ChPT+γ fit. Errors are only statistical. Values for lattice spacing and QCD LECs without QED are taken from Ref. [18]: a^{-1}=1.729(28) GeV, $\sqrt{2}aF_0$ =0.0541(40), aB_0/Z_m = 2.35(16) and Z_m = 1.656(48)(150) from Ref. [23]. The last row is the fit results with the additive shift in quark mass due to the $\mathscr{O}(e^2)$ residual breaking.

From the values of the low energy constants determined from the fit, we could obtained the physical quark masses by solving the ChPT meson mass formula (2.3),

$$M_{\rm PS}(m_{\rm up},2/3,m_{\rm down},-1/3) = 139.57018(35){\rm MeV}\ , \tag{3.1}$$
$$M_{\rm PS}(m_{\rm up},2/3,m_{\rm strange},-1/3) = 493.677(13){\rm MeV}\ , \tag{3.2}$$
$$M_{\rm PS}(m_{\rm up},-1/3,m_{\rm strange},-1/3) = 497.614(24){\rm MeV}\ , \tag{3.3}$$

for the three quark masses $m_{\rm up}, m_{\rm down}, m_{\rm strange}$. The experimental inputs are masses of $\pi^\pm, K^\pm, K^0$ [22]. The disconnected quark loops, needed for π^0, is not calculated in our simulation, so we refrain from using π^0 mass in this work. In (3.1)-(3.3), we have omitted one of $\mathscr{O}(e^2 m_q)$ term, $Y_1\overline{Q}_2\chi_{13}$, since sea quark charge is zero, $\overline{Q}_2 = 0$, in our simulation, and the low energy constant Y_1 can't be extracted from our simulation. We will estimate the systematical error by varying Y_1.

Table 3 summaries preliminary determinations for the quark masses in $\overline{\rm MS}$(NDR) at $\mu = 2$ GeV for three combinations of quark mass cuts, $m_{\rm cut} = 40, 70$ MeV, and volumes, $V \simeq (2.75\ {\rm fm})^3, (1.84\ {\rm fm})^3$. The mild dependence of the quark masses on the volume and $m_{\rm cut}$ is a measure for systematical errors due to the finite volume effects and the omission of the higher order terms in ChPT+γ. We use the lattice spacing and QCD LECs determined in Ref. [18], which are slightly different than the ones reported in the talk at the conference due to an enhancement of statistics. There are a discrepancies between the results of this work and those in Ref. [18], *e.g.* we quoted $m_{\rm strange}$=107.3(4.4) MeV in Ref. [18], while $m_{\rm strange}$ = 95(9) MeV is obtained in this work. The discrepancies are not only from the inclusion of QED in this work, but also from the difference in the fit formula: We have used SU(2) ChPT in Ref. [18] while SU(3) ChPT+γ is used in this work. Analysis based on SU(2) ChPT+γ is in progress.

As an application of the determined quark masses for *Kaon physics*, the isospin splitting of the Kaon masses, $m_{K^\pm} - m_{K^0} = -3.937(28)$ MeV from experiments [22], is broken up into two parts: $\Delta^{(m_q)}M_K$, the part coming from the up, down quark mass difference, and $\Delta^{(e^2)}M_K$, the part coming from the difference between their electric charges, modulo tiny $\mathscr{O}(e^2(m_{\rm up} - m_{\rm down}))$ ambiguity. From the fit results for $V = (2.7{\rm fm})^3, m_{\rm cut} = 40$ MeV, we find

$$\Delta^{(m_q)}M_K \equiv M_{\rm PS}(m_{\rm up},0,m_{\rm strange},0) - M_{\rm PS}(m_{\rm down},0,m_{\rm strange},0) = -5.13(11)\ \ {\rm MeV} \tag{3.4}$$
$$\Delta^{(e^2)}M_K \equiv M_{\rm PS}(\overline{m_{ud}},\frac{2}{3},m_{\rm strange},\frac{-1}{3}) - M_{\rm PS}(\overline{m_{ud}},\frac{-1}{3},m_{\rm strange},\frac{-1}{3}) = 1.20(10)\ \ {\rm MeV} \tag{3.5}$$

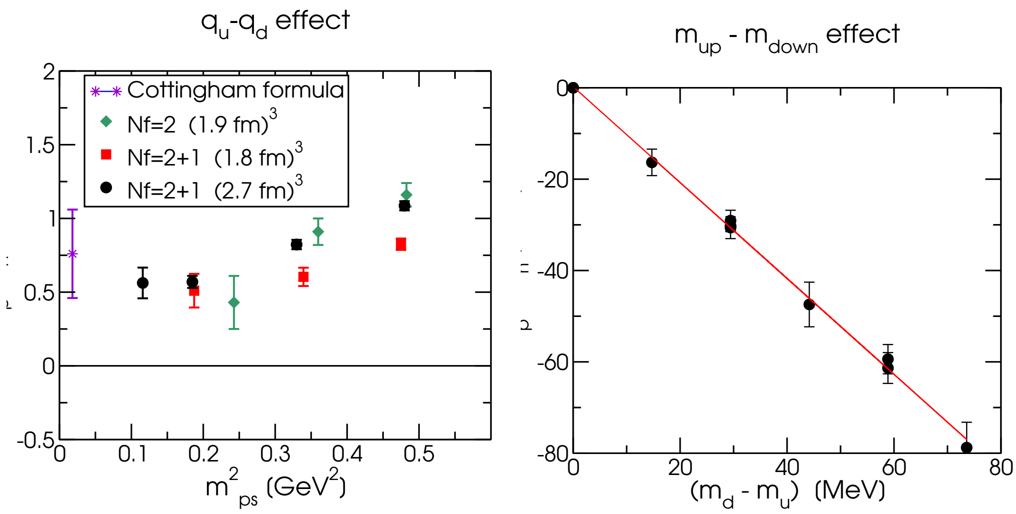

Figure 2: Proton/Neutron mass splitting, $m_p - m_n$, for $m_{\rm up} = m_{\rm down}$ (left) and for $e^2 = 0$ (right). Error bars are only statistical.

where $\overline{m_{ud}} = (m_{\rm up} + m_{\rm down})/2$ and errors are only statistical. In terms of the difference of squared Kaon masses, roughly +130% of the difference comes from $m_{\rm down} - m_{\rm up}$ while the QED effects are responsible for its -30%.

The mass splitting between neutron and proton [10], $m_n - m_p = 1.2933317(5)$ MeV, is also decomposed into the part originated from $m_{\rm up} - m_{\rm down}$ and that from $q_{\rm up} - q_{down}$ in Fig.2. In the left panel, $m_n - m_p$ as a function of $M^2_{\rm PS}$ for $m_{\rm up} = m_{\rm down}$ are plotted. $m_n - m_p$ in this plot entirely comes from the EM effects. The left most star is the estimation for the same quantity using ChPT [24], $m_p - m_n|_{\rm QED} = 0.76(30)$ MeV. $m_{\rm up} - m_{\rm down}$ dependence of the mass splitting is shown in the left panel for the case without QED. Assuming a linear function, $m_p - m_n \propto (m_{\rm up} - m_{\rm down})$, we get $m_p - m_n|_{\text{quark mass}} = -2.3(3)$ MeV, at the physical point $m_{\rm down} - m_{\rm up} = 2.0(2)$ MeV with only statistical error are shown. This value is comparable to the ChPT prediction, -2.05(30) MeV, from [24] or, -2.3(6) MeV from other lattice computation [25].

4. Summary and Discussion

Studies of isospin breaking effects using lattice QCD+QED are presented. By fitting the hadron masses computed in the simulation to ChPT+γ, the three light quark masses and their ratios are determined. Although the whole systematic errors are still under the final assessments, we have seen that the major two errors, the finite volume errors and the chiral extrapolation errors, are likely under control: the central values in Table.3 from the two volumes and the two ranges of quark masses in the fits scatter roughly within $\simeq$ 10% for both quark masses and their ratios. Other sources of errors including omission of $\mathcal{O}(e^2)$ correction in the mass renormalization constant, Z_m, lattice discretization error, effect of up/down sea quark mass difference, sea strange quark mass uncertainties, the sea quark charge, and the residual chiral symmetry breaking are expected to give another 10 % or so.

The determined quark masses are used to break up the Kaon mass splittings, $M_{K^\pm} - M_{K^0}$, into the each part from the two sources of isospin breaking: the quark mass difference $m_{\rm up} - m_{\rm down}$ and the electric charge difference $q_{\rm up} - q_{\rm down}$. Similar decomposition for the mass difference between proton and neutron is examined.

There are other isospin breaking studies recently done on lattice. MILC collaboration (Basak *et al.*) performed the electromagnetic splittings of charged and neutral mesons using asqtad staggered quarks and determined the violation of Dashen's theorem [26]. In Ref. [27], ETMC collaboration (McNeile *et.al.*) carried out $\rho - \omega$ mass splitting using the twisted Wilson fermions. They also discussed about $\rho - \omega$ mixing due to $m_{\rm up} - m_{\rm down}$. JLQCD collaboration (Shintani *et al.*)[28, 29] calculated the vacuum polarization functions on the lattice using the overlap quarks. The squared mass splitting between charged and neutral pions at the chiral limit is calculated using a sum rule. There are further applications of QCD+QED simulations such as the baryon mass splittings [10] or the $\mathcal{O}(\alpha^3)$ hadronic contribution to the muon's anomalous magnetic moment (light-by-light) [30].

Isospin breaking physics are interesting and inevitable for precise understandings of hadron physics, which could be addressed by QCD+QED simulations from the first principle.

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PoS(KAON09)034