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Testing $m_u = 0$ on the lattice

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Abstract: A massless up quark is an intriguing possible solution to the strong CP problem. We discuss how lattice computations can be used in conjunction with chiral perturbation theory to address the consistency of $m_u = 0$ with the observed hadron spectrum and interactions. It is not necessary to simulate very light quarks — three flavor partially quenched computations with comparable sea and valence quark masses on the order of the strange quark mass could suffice.

Keywords: Quark Masses and SM Parameters, CP violation, Lattice QCD, Chiral Lagrangians.

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Contents

1. Introduction

QCD allows violation of the symmetry CP through the parameter $\bar{\theta} \equiv \theta_{QCD} - \arg \det\mathcal{M}$, where $\mathcal{M}$ is the quark mass matrix. All experimental evidence implies that $\bar{\theta} < 10^{-9}$, and thus CP is nearly preserved by the strong interactions. The absence of a symmetry to ensure $\bar{\theta} = 0$ is one of the most perplexing features of the Standard Model. Three different solutions are commonly considered for this "strong CP puzzle": dynamical relaxation of $\bar{\theta}$ by means of an axion field [1]; spontaneous CP violation at high energy with a Nelson-Barr mechanism [2, 3] to ensure reality of the quark mass determinant; and a vanishing up quark mass $m_u = 0$. In the particularly simple case of vanishing m_u the determinant of the quark mass matrix is zero, and $\bar{\theta}$ is no longer a physical parameter. Models in which the up-type quark mass matrix has rank two at short distance as an accidental consequence of symmetry are easily constructed [4, 5, 6, 7, 8].

The viability of a massless up quark can in principle be determined by comparing the predictions of QCD with the observed spectrum and interactions of hadrons. However, *effective* hadronic theories whose sole input from QCD is the approximate SU(3) $\times$ SU(3) chiral flavor symmetry cannot settle this question. Under $\mathrm{SU}(3)_L \times \mathrm{SU}(3)_R$, the quark mass matrix $\mathcal{M}$ transforms as the $(3, \bar{3})$ representation, and therefore so does the matrix ${\mathcal{M}^{\dagger}}^{-1}|\mathcal{M}|$. Thus, symmetry considerations alone can never rule out the possibility that explicit symmetry breaking occurs in hadronic physics through combinations of the form $\mathcal{M}_{eff} = \mathcal{M} + {\mathcal{M}^{\dagger}}^{-1}|\mathcal{M}|/\Lambda$, with

Λ a scale determined by strong interactions, an ambiguity pointed out by Kaplan and Manohar [9]. In the case $m_u = 0$, this gives an effective quark mass matrix

$$\mathcal{M}_{eff} = \begin{pmatrix} m_d^* m_s^*/\Lambda & & \\ & m_d & \\ & & m_s \end{pmatrix} \tag{1.1}$$

which allows the quantity $m_d^* m_s^*/\Lambda$ to fulfill the role conventionally played by m_u. Note, however, that in this case $\det \mathcal{M}_{eff}$ is real, and there is no strong CP problem. The nonlinear term in $\mathcal{M}_{eff}$ could arise from instantons, for example, where the d and s quark zero-mode propagators are connected by m_d and m_s insertions respectively [9, 10, 11]. Appropriate values for the Λ in this scenario would correctly fit all hadron data. The conventional extraction of quark mass ratios from chiral perturbation theory [12] would nevertheless incorrectly yield a nonzero value for m_u/m_d.

To resolve the ambiguity chiral symmetry may be supplemented with additional assumptions. In ref. [13], Leutwyler gives a list of three plausible assumptions, each of which independently rules out $m_u = 0$. The assumptions are: SU(3) symmetry is always approximately valid, and all physical quantities can be reliably expanded in powers of m_s; dispersion relations are saturated by the lowest lying states; and the large-N_c explanation for Zweig's rule (suppression of virtual quark loops by $1/N_c$) is valid.

We consider the above arguments against $m_u = 0$ to be quite reasonable. Each of these assumptions can be experimentally tested in various ways, and none has yet been disproven. Yet it is possible that an effective up quark mass, although sub-leading in $1/N_c$, is numerically large enough to account for the hadron spectrum without implying a general breakdown of chiral symmetry. Due to the importance of the strong CP problem, we consider it essential to pin down the value of m_u without assumptions.

Lattice simulation of QCD can, in principle, decide whether or not a massive up quark is required, particularly in light of recent advances in realizing chiral symmetry on the lattice [14, 15, 16]. With the aid of chiral perturbation theory, it is not necessary to simulate QCD with a massless or extremely light quark. We begin by reviewing chiral perturbation theory in the continuum, and then we consider in turn full, partially quenched, and quenched QCD on the lattice. We find that lattice simulations in either full QCD or partially quenched QCD with all quark masses comparable to the strange quark mass could largely settle the issue.

2. m_u in the continuum

The light quark masses (m_u, m_d, m_s) are small compared with the characteristic mass scale of the strong interactions, and QCD possesses an approximate $\mathrm{SU}(3) \otimes \mathrm{SU}(3)$ chiral symmetry broken spontaneously to the vector SU(3) subgroup, resulting in a light pseudo-Goldstone boson octet with predictable low energy interactions [12, 17, 18, 19, 20, 21]. For sufficiently light quarks, the pseudo-Goldstone masses squared are nearly linear in the quark masses, and the quark mass ratios may be extracted from the pseudoscalar spectrum with values $m_u/m_d = 0.56$, $m_s/m_d = 20.1$ [17].[1] However, the strange quark mass is large enough that the lowest order predictions from chiral symmetry receive significant corrections, of size m_s/Λ_χ, where Λ_χ is the chiral symmetry breaking scale of order a GeV. The simplest way of extracting predictions from chiral symmetry to any given order in m_s and in pion momenta is to use a phenomenological chiral lagrangean [18]. Using the parametrization of Gasser and Leutwyler [12, 19, 20, 21] the lagrangean relevant for the extraction of quark masses to second order in m_s is

$$\mathcal{L} = \mathcal{L}_2 + \mathcal{L}_4 + \cdots \tag{2.1}$$

$$\mathcal{L}_2 = \frac{f^2}{4}\,\mathrm{Tr}\left(\partial_\mu U^\dagger \partial^\mu U\right) + \frac{f^2}{2}\,\mathrm{Tr}\left(\chi^\dagger U + \chi U^\dagger\right) \tag{2.2}$$

$$\begin{aligned}\mathcal{L}_4 = {} & \cdots + L_4\,\mathrm{Tr}\left(\partial_\mu U^\dagger \partial^\mu U\right)\mathrm{Tr}\left(U^\dagger\chi + \chi^\dagger U\right) + \\ & + L_5\,\mathrm{Tr}\left[\partial_\mu U^\dagger \partial^\mu U\left(U^\dagger\chi + \chi^\dagger U\right)\right] + \\ & + L_6\left[\mathrm{Tr}\left(U^\dagger\chi + \chi^\dagger U\right)\right]^2 + L_7\left[\mathrm{Tr}\left(U^\dagger\chi - \chi^\dagger U\right)\right]^2 + \\ & + L_8\,\mathrm{Tr}\left(\chi^\dagger U \chi^\dagger U + \chi U^\dagger \chi U^\dagger\right) + \cdots + L_{12}\,\mathrm{Tr}\,\chi\chi^\dagger\,,\end{aligned} \tag{2.3}$$

where

$$\begin{aligned}\mathcal{M} &\equiv \mathrm{diag}(m_u, m_d, m_s)\,, \\ U &\equiv \exp\left(\frac{i2T_a\pi_a}{f}\right), \\ \chi &\equiv 2\mathcal{M}B\,,\end{aligned} \tag{2.4}$$

T_a are SU(3) generators, π_a are pseudoscalar fields, and B, L_i, f are phenomenological parameters characterizing QCD dynamics. (It is not possible to separately determine $\mathcal{M}$ and B from experiment.) Most of these parameters are renormalization scale dependent — we follow the usual practice in the chiral perturbation theory literature of quoting all parameters at the ρ mass. They are then easily run to a different scale by using the renormalization group. For convenience electromagnetism has been left out of this effective theory, although electromagnetic effects contribute to the pseudoscalar meson masses. We therefore define "QCD" masses which have electromagnetic effects subtracted — to leading order these are just the physical meson masses with the exception of the electrically charged mesons [23]

$$\begin{aligned}M^2_{\pi^\pm QCD} &\approx M^2_{\pi^0\,\mathrm{phys}}\,, \\ M^2_{K^\pm QCD} &\approx M^2_{K^\pm\,\mathrm{phys}} - M^2_{\pi^\pm\,\mathrm{phys}} + M^2_{\pi^0\,\mathrm{phys}}\,.\end{aligned} \tag{2.5}$$

[1] Similar earlier quark mass estimates were given in ref. [22].

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These lowest order formula for the QCD masses can be improved beyond leading order [24]–[29]. All meson masses used in subsequent formulæ are these QCD masses. From this effective theory, it is possible to determine a constraint on quark mass ratios, up to corrections of order m_s^2, [20, 21, 30]

$$\frac{{m_s}^2 - \hat{m}^2}{{m_d}^2 - {m_u}^2} \equiv Q^2 \approx Q_D^2 \equiv \frac{M_K^2}{M_\pi^2} \frac{(M_K^2 - M_\pi^2)}{(M_{K^0}^2 - M_{K^\pm}^2)} \approx (24.2)^2 \,, \tag{2.6}$$

where

$$\hat{m} \equiv \frac{1}{2}\,(m_u + m_d)\,. \tag{2.7}$$

If the values of the L's are known, the quark mass ratios may be found:

$$\begin{aligned} \frac{m_s}{\hat{m}} &= \frac{2M_K^2}{M_\pi^2(1+\Delta_M)} - 1 \\ \frac{m_u}{\hat{m}} &= 1 - \frac{M_K^2}{M_\pi^2} \frac{M_K^2 - (1+\Delta_M)M_\pi^2}{Q^2(1+\Delta_M^2)^2} \end{aligned} \tag{2.8}$$

where

$$\Delta_M \equiv \mu_\pi + \mu_\eta + \frac{8}{f^2}(M_K^2 - M_\pi^2)(2L_8 - L_5) \tag{2.9}$$

and

$$\mu_P \equiv \frac{M_P^2}{32\pi^2 f^2} \log\left(\frac{M_P^2}{\mu^2}\right). \tag{2.10}$$

To decide whether m_u can be zero, the value of $2L_8 - L_5$ is required. L_5 can be determined from the ratio f_K/f_π, with a value $10^3 L_5 \approx 1.4 \pm 0.5$. The linear combination $L_5 - 12L_7 - 6L_8$ can be extracted from the pseudoscalar masses, giving $10^3(2L_7 + L_8) = \pm 0.2$. (The quoted errors represent the estimated theoretical uncertainty due to higher order corrections in m_s.) In principle (but not in practice) L_4 and $L_6 - L_7$ can be determined from meson-meson interactions. However data cannot be used *even in principle* to completely specify the L's. The Gasser-Leutwyler lagrangean is invariant under the replacement [21]

$$\begin{gathered} \chi \to \chi + \beta(\det\chi)\chi^{-1} \\ L_6 \to L_6 - \delta \qquad L_7 \to L_7 - \delta \qquad L_8 \to L_8 + 2\delta \end{gathered} \tag{2.11}$$

with

$$\delta \equiv \frac{\beta f^2}{32}\,. \tag{2.12}$$

This invariance is a necessary consequence of the Kaplan-Manohar ambiguity, and leads to a corresponding ambiguity in the L's.

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A combination of phenomenological and large N_c constraints *can* be used to determine all the L's with an estimated 30% precision [30, 31, 32]. The results agree (by design) with the picture that all terms in $\mathcal{L}_4$ are consistent with the values obtained by integrating out light resonances, and are inconsistent with $m_u = 0$ [30]. In particular, a conventional estimate of this kind gives [33, 34, 35, 36] $10^3 L_8 \approx 0.9 \pm 0.3$, $10^3 L_7 \approx (-0.4 \pm 0.2)$, while the hypothesis $m_u = 0$ would require $10^3 L_8 = -0.4 \pm 0.3$, and $10^3 L_7 = 0.2 \pm 0.2$. Thus any method which can directly determine the L's, even with errors as large as 100%, can distinguish between these two possibilities.

3. m_u on the lattice

Simulating QCD on a lattice is, in principle, the most reliable way of determining quantities which are not predicted from symmetry alone. For instance, although it is only possible to constrain ratios of light quark masses phenomenologically, recent lattice computations of the hadron spectrum have suggested an absolute range for the strange quark mass [37]–[46] and the parameter B. It is difficult to simulate quarks with realistic masses: light quarks require large lattices to avoid finite volume artifacts. However with the aid of chiral symmetry lattice computations done at moderate quark masses can be extrapolated to lighter quark masses. Unfortunately this extrapolation is complicated and plagued with unphysical artifacts in the usual quenched approximation, where quark dynamics are not included.

3.1 Unquenched lattice QCD

With computing power sufficient to simulate unquenched QCD with quark masses light enough to apply chiral symmetry, there are several possible methods[2] to extract the chiral lagrangean coefficients and determine m_u. One way is to use the chiral symmetry prediction for the pion mass squared [21]:

$$M_\pi^2 = 2\hat{m}B\left(1 + \mu_\pi - \frac{1}{3}\mu_\eta + 2\hat{m}K_3 + \frac{m_u + m_d + m_s}{3}K_4\right), \tag{3.1}$$

where

$$\begin{aligned} K_3 &\equiv \frac{8B}{f^2}(2L_8 - L_5)\,, \\ K_4 &\equiv \frac{48B}{f^2}(2L_6 - L_4)\,. \end{aligned} \tag{3.2}$$

By measuring the pion mass as a function of $\hat{m}$ and m_s the combination $2L_8 - L_5$, needed in determining the quark mass ratios, as well as the combination $2L_6 - L_4$, which provides an interesting test of conventional assumptions and the large N_c expansion, may be extracted. Independently varying $\hat{m}$ and m_s requires a lot of

[2] For earlier work on lattice computations of chiral coefficients see refs. [47, 48].

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different simulations, however. It may be simpler to work with equal quark masses $m_u = m_d = m_s = \hat{m} = \bar{m}$ and vary $\bar{m}$. A fit to the quadratic dependence of the pion mass squared then yields the linear combination $2L_8 - L_5 + 6L_6 - 3L_4$ from

$$\frac{\partial^2 M_\pi^2}{\partial \bar{m}^2} = \frac{B^2}{12\pi^2 f^2}\left[3 + 2\log\left(\frac{2\bar{m}B}{\mu^2}\right) + 768\pi^2(2L_8 - L_5 + 6L_6 - 3L_4)\right]. \quad (3.3)$$

With equal quark masses, the combination $2L_6 - L_4$ may be separately extracted by a measurement of the matrix element of $\bar{s}s$ in the pion, using

$$\langle\pi|\bar{s}s|\pi\rangle = -\frac{\bar{m}B}{36\pi^2 f^2}\left[1 + \log\left(\frac{2\bar{m}B}{\mu^2}\right) + 1152\pi^2(L_4 - 2L_6)\right]. \quad (3.4)$$

L_6 may be independently extracted from the vacuum expectation value $\langle\int \bar{s}s \int \bar{d}d\rangle$, and L_4 may also be measured from the dependence of f_π on $\bar{m}$. Thus in principle by simulating QCD on the lattice with several different quark masses it is possible to verify the conventional estimates of those L's for which there is no direct experimental data. Even a measurement of $2L_8 - L_5$ with 100% errors provides an interesting test of the large N_c expansion and, depending on the result, could rule out the possibility that $m_u = 0$. Note that measurement of L_4 and L_6 would also be quite interesting theoretically, although not directly needed to extract quark mass ratios. Available data provides no constraints on $L_{4,6}$.

Ruling out $m_u = 0$ along the above lines may not be easy. Here we define the more restrictive "effective up mass hypothesis", which may be somewhat simpler to test than whether $m_u = 0$, since this hypothesis makes a prediction for L_6. The effective up mass hypothesis is motivated by the agreement between different experimental determinations of light quark mass ratios [12, 30, 49, 50, 51]. The hypothesis is that $m_u = 0$, but that the conventional low energy theory works accurately with the replacement $m_u \to m_d^* m_s^*/\Lambda$. In the chiral lagrangean, such an effective up mass is a nonstandard contribution to the coefficients L_6, L_7, and L_8, in the combination $\Delta L_6 = \Delta L_7 = -2\Delta L_8 = 0.7 \times 10^{-3}$. With this hypothesis, all the L's are determined, and L_4 agrees with the conventional estimate $10^3 L_4 = -0.3 \pm 0.5$, while $10^3 L_6$ is 0.5 ± 0.3, in contrast to the conventional estimate $10^3 L_6 = -0.2 \pm 0.3$.

3.2 Partially quenched lattice QCD

QCD simulations in the "partially quenched" approximation, which includes the effects of N flavors of dynamical quarks with mass $m_{\rm sea}$ different from the valence quark mass, may also be of interest. Such simulations could be decisive for the determination of the Gasser-Leutwyler L coefficients.[3] For such an analysis to be reliable it is necessary that the sea quark mass is sufficiently small for the dominant artifacts

[3] After the completion of this work we were informed of the work of Sharpe and Shoresh [52] who reach similar conclusions.

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of partial quenching to be computable using partially quenched chiral perturbation theory [53]. This requires that the mass M_{SS} of a pion made of sea quarks be light compared with the scale Λ_χ. It is also desirable to take the valence quark mass to be comparable to the sea quark mass, to reduce quenching artifacts from the non-decoupling of the η' [54]. In the limit $m_{\rm sea} \sim \bar{m} \ll \Lambda_\chi$, Sharpe has calculated the following dependence of the pion masses on the valence and sea quark masses [53]:

$$M^2_{\pi^\pm} = 2\bar{m}B\Big\{1 + \frac{B}{N8\pi^2 f^2}\Big[(2\bar{m} - m_{\rm sea})\log(\frac{2\bar{m}B}{\mu^2}) + \bar{m} - m_{\rm sea}\Big] + \\ + \frac{16\bar{m}B}{f^2}(2L_8 - L_5) + \frac{N16m_{\rm sea}B}{f^2}(2L_6 - L_4)\Big\} \tag{3.5}$$

$$M^2_{SV} = (m_{\rm sea} + \bar{m})B\Big[1 + \frac{\bar{m}B}{N8\pi^2 f^2}\log\left(\frac{2\bar{m}B}{\mu^2}\right) + \frac{8(m_{\rm sea} + \bar{m})B}{f^2}(2L_8 - L_5) + \\ + \frac{N16m_{\rm sea}B}{f^2}(2L_6 - L_4)\Big] \tag{3.6}$$

$$M^2_{SS} = 2m_{\rm sea}B\Big[1 + \frac{m_{\rm sea}B}{N8\pi^2 f^2}\log\left(\frac{2m_{\rm sea}B}{\mu^2}\right) + \\ + \frac{16m_{\rm sea}B}{f^2}(2L_8 - L_5) + \frac{N16m_{\rm sea}B}{f^2}(2L_6 - L_4)\Big]. \tag{3.7}$$

Here all valence quarks have mass $\bar{m}$, $\pi^\pm$ is a pion made of different valence quarks, M_{SS} is the mass of a pion made of sea quarks and M_{SV} is the mass of a pion made of one sea and one valence quark. For $N = 3$ the parameters B and L_i are the same as those in the QCD chiral lagrangean [53, 55]. Thus for $N = 3$, the desired combination $2L_8 - L_5$ may be extracted by fitting the pion masses as a function of $\bar{m}$ with $m_{\rm sea}$ held fixed. Note that an $N = 2$ simulation, while interesting, is not sufficient to determine the L coefficients, as these may have significant dependence on the number of flavors. For instance the contributions from gauge field configurations with fermion zero modes, such as instantons, should be quite sensitive to the number of sea flavors.

Golterman and Leung [54] have extended the partially quenched chiral perturbation theory calculations to the case where the η' is light compared to the scale Λ_χ, as expected in the large N_c limit. In this limit, unless the valence and sea quark pion masses are comparable and both much lighter than the η', the pion masses depend on two new parameters associated with the η' mass and decay constant. Even with a light η' it is theoretically possible, with enough different measurements, to extract $2L_8 - L_5$ from lattice data.

3.3 Quenched lattice QCD

The quenched approximation is not a systematic approximation to QCD. Nevertheless it is generally used to facilitate lattice computations with currently available computing power, and quenched QCD does have a spectrum similar to the real

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thing [56, 57]. This suggests that the dominant effects of quark loops can be compensated for in the quenched approximation by adjusting the QCD parameters (quark masses and the scale Λ_{QCD}). However a reliable extraction of the true value of the chiral lagrangean coefficients and of m_u from the quenched spectrum is problematic; the possibility that the quenched approximation with a nonzero up quark mass mimics the true QCD spectrum with $m_u = 0$ cannot be ruled out. For instance the quenched approximation is missing the down and strange quark loop effects which, in conjunction with instantons, might mimic an effective up quark mass proportional to $m_d^* m_s^*$.

A possible way to explore the quark loop contribution to the effective up quark mass in the quenched approximation is to explicitly include sources for the sea quarks. For instance, one could measure a three-point function

$$\langle \pi | \int \bar{s} s | \pi \rangle \,. \tag{3.8}$$

In particular, the instanton effects which might give an effective up quark mass do contribute to this matrix element in the quenched approximation. In full QCD this matrix element is equivalent to $\partial M_\pi^2 / \partial m_s$, which would vanish ignoring quark loops; however the equivalence does not hold in the quenched approximation. Logarithmically enhanced quenched artifacts from an η' loop[4] give a contribution to this matrix element which are suppressed by $1/N_c^2$ but which introduce a new parameter which cannot be computed using quenched chiral perturbation theory [58, 59]. To avoid this artifact it may be better to measure

$$\langle \pi | \int (2\bar{s}s - \bar{d}d - \bar{u}u) | \pi \rangle \,. \tag{3.9}$$

4. Summary

Chiral perturbation theory makes possible the use of lattice simulations of full and partially quenched QCD with moderate quark masses to learn about the properties of QCD with light quarks. In this paper we showed how to use full or partially quenched simulations with equal, moderately sized quark masses to extract the second order coefficients in the pion chiral lagrangean. Such calculations are of interest to check the predictions of large N_c QCD, to verify chiral perturbation theory, and to test the hypothesis of resonance saturation of dispersion relations. Such computations, even with large errors, can provide a method for settling the important issue of whether the $m_u = 0$ solution to the strong CP problem is consistent with the spectrum of light pseudoscalar mesons.

[4] We thank Steve Sharpe for explaining this to us.

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