Up Quark Mass in Lattice QCD with Three Light Dynamical Quarks and Implications for Strong *CP* Invariance

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A standing mystery in the standard model is the unnatural smallness of the strong CP violating phase. A massless up quark has long been proposed as one potential solution. A lattice calculation of the constants of the chiral Lagrangian essential for the determination of the up quark mass, $2\alpha_8 - \alpha_5$, is presented. We find $2\alpha_8 - \alpha_5 = 0.29 \pm 0.18$, which corresponds to $m_u/m_d = 0.410 \pm 0.036$. This is the first such calculation using a physical number of dynamical light quarks, $N_f = 3$.

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Introduction.—The nontrivial topological structure of the QCD gauge vacuum generates a CP breaking term in the QCD Lagrangian. However, measurements of the neutron electric dipole moment have placed a restrictive upper bound on this term's coefficient, $\bar{\theta} \leq 10^{-9}$ [1]. The unnatural smallness of $\bar{\theta}$ is known as the strong CP problem.

A massless up quark ($m_u = 0$) has long been proposed as a potential elegant solution to the problem. Chiral rotations of the quark mass matrix $\mathcal{M}$ shift $\bar{\theta}$,

$$\bar{\theta} = \theta + \mathrm{argdet}\mathcal{M}, \qquad (1)$$

where θ is a fundamental parameter of the standard model. However, if $m_u = 0$, then $\det\mathcal{M} = 0$ and $\mathrm{argdet}\mathcal{M}$ is unphysical, leaving one free to remove the CP violating term through a simple field redefinition.

At leading order (LO), chiral perturbation theory (ChPT) appears to rule out the possibility of $m_u = 0$. The quark mass ratios, including m_u/m_d, can be determined using ChPT's LO predictions for the light meson masses.

At next-to-leading order (NLO), however, new coefficients appear in the chiral expansion which contribute to the meson masses. The parameters of ChPT are no longer fully determined by experimental data. In fact, it is impossible for ChPT to distinguish between the effects of a nonzero up quark mass and certain large NLO corrections. This is known as the Kaplan-Manohar ambiguity [2].

Distinguishing between a light and a massless up quark requires knowledge of the coefficients of the NLO terms in the chiral Lagrangian, the Gasser-Leutwyler (GL) coefficients. Specifically, it is the combination of constants $2\alpha_8 - \alpha_5$ [3] which appears in Δ_M, the NLO correction to the quark mass ratios [4]. If this combination falls within a certain range, $-3.3 < 2\alpha_8 - \alpha_5 < -1.5$, current experimental results cannot rule out $m_u = 0$.

Various assumptions and phenomenological arguments have been used in the past to assemble a somewhat standard set of values for the coefficients [5]. However, because these coefficients are physically determined by the low-energy nonperturbative behavior of QCD, the lattice offers the best opportunity for a truly first-principles calculation.

Partially quenched chiral perturbation theory (pqChPT).—pqChPT [6,7] is the tool through which one can calculate the GL coefficients on the lattice. pqChPT is distinct from standard ChPT in that it is constructed from the symmetry of a graded group. This graded group follows from the presumed quark content of partially quenched QCD (pqQCD): separate valence and sea quark flavors in addition to ghost quark flavors, which in perturbation theory cancel loop corrections due to valence quarks.

The Lagrangian of pqChPT up to $O(p^4)$ follows, with only relevant NLO terms shown.

$$\begin{aligned}\mathcal{L} = {}& \frac{f^2}{4}\mathrm{sTr}[\partial_\mu U \partial^\mu U^\dagger] - \frac{f^2}{4}\mathrm{sTr}[\chi U^\dagger + U\chi] + L_4 \mathrm{sTr}[\partial_\mu U \partial^\mu U^\dagger]\mathrm{sTr}[\chi U^\dagger + U\chi] + L_5 \mathrm{sTr}[\partial_\mu U \partial^\mu U^\dagger(\chi U^\dagger + U\chi)] \\ & - L_6 \mathrm{sTr}[\chi U^\dagger + U\chi]\mathrm{sTr}[\chi U^\dagger + U\chi] - L_8 \mathrm{sTr}[\chi U^\dagger \chi U^\dagger + U\chi U\chi] + \cdots, \end{aligned} \qquad (2)$$

where $U = \exp(2i\Phi/f)$, $\chi = 2\mu a^{-1}\mathrm{diag}(\{m_S, m_V\})$, Φ contains the pseudo-Goldstone "mesons" of the spontaneously broken $\mathrm{SU}(N_f + N_V|N_V)_L \otimes \mathrm{SU}(N_f + N_V|N_V)_R$ symmetry, and U is an element of that group. m_S and m_V refer to the bare lattice quark mass parameters, which are related to their dimensionful equivalents via the lattice spacing, $m_x^{\mathrm{dim}} = a^{-1}m_x$. Three degenerate sea quarks were used, $N_f = 3$, while the number of valence quarks N_V cancels in all expressions, affecting only the counting of external states. The constants f, μ, and the L_i's are unknown, determined by the low-energy dynamics of pqQCD.

Because the valence and sea quark mass dependence of the Lagrangian of pqChPT is explicit and full QCD is within the parameter space of pqQCD ($m_V = m_S$), the values obtained for the GL coefficients in a pqQCD calculation are the exact values for the coefficients in full QCD [8,9]. Furthermore, independent variation of valence and sea quark masses allows additional lever arms in the determination the the coefficients. Because the N_f dependence of the Lagrangian is not explicit, the GL coefficients are functions of N_f. Thus, it is important to use a physical number of light sea quarks, as we have, when extracting physical results.

Predicted forms.—pqChPT predicts forms for the dependence of the pseudoscalar mass and decay constant on the valence quark mass, here assuming degenerate sea quarks and degenerate valence quarks, and cutting off loops at $\Lambda_\chi = 4\pi f$.

$$M_\pi^2 = (4\pi f)^2 z m_V \left\{ 1 + z m_V \left(2\alpha_8 - \alpha_5 + \frac{1}{N_f} \right) + \frac{z}{N_f}(2m_V - m_S) \ln z m_V \right\}, \quad (3)$$

$$f_\pi = f \left\{ 1 + \frac{\alpha_5}{2} z m_V + \frac{z N_f}{4}(m_V + m_S) \ln \frac{z}{2}(m_V + m_S) \right\}, \quad (4)$$

where $z = 2\mu a^{-1}/(4\pi f)^2$. These forms differ slightly from those in [10], as the NLO dependence in the sea quark mass has been absorbed into μ and f. This is allowed as the error due to this change is manifest when z appears in the NLO terms, pushing the discrepancy up to NNLO. Accounting for these absorbed terms would require a systematic study at several sea quark masses.

The forms above are derived assuming degenerate light mesons. However, our use of staggered fermions on somewhat coarse lattices generates significant flavor symmetry breaking, and thus a splitting of the light meson masses. A detailed analysis of this effect with dynamical quarks was recently presented in [11].

In order to study this error, we applied hypercubic blocking to several of our ensembles, using the blocking coefficients found in [12]. Because hypercubic blocked dynamical quarks were not used when generating these ensembles, we are using different Dirac operators for the valence and sea quarks. While this procedure may not have a clean continuum limit, it is still useful for estimating the systematic error due to flavor symmetry breaking.

The ensembles were generated using staggered fermions and the inexact hybrid molecular dynamics (HMD) R algorithm [13], which allows one to work at $N_f = 3$, but involves taking the $\frac{3}{4}$ root of the quark determinant. The result is a quark action which is nonlocal at finite lattice spacing, but should become local in the continuum limit. The details of the simulations and results are summarized in Table I.

To determine the value of $2\alpha_8 - \alpha_5$, the local pseudoscalar correlator was calculated using several valence quark masses. The correlators were fit to exponentials, while the meson mass and decay constants were simultaneously fit to the predicted forms. The results of the fit are the values μ, f, α_5, and $2\alpha_8 - \alpha_5$. Figure 1 displays an example of one such fit.

When fitting, a chiral cutoff point in the valence quark mass beyond which one expects pqChPT to break down must be chosen. To choose our cutoff, we added m_V values to our fit keeping $m_V/m_K \leq 1$ and keeping $\chi^2/\mathrm{dof} \approx 1$. The cutoff determined for the $16^3 \times 32$ hypercubic blocked ensemble, in terms of m_V/m_K, was used for all of the $\beta = 5.3$, $m_S = 0.01$ ensembles. m_K denotes an ensemble's valence quark mass at which the mass of the lightest pseudoscalar meson with degenerate quarks equals the physical kaon mass. We found $2\alpha_8 - \alpha_5$ to be very sensitive to our cutoff choice. For the $16^3 \times 32$ hypercubic blocked ensemble, changing the chiral cutoff by ± 0.14 in m_V/m_K shifted $2\alpha_8 - \alpha_5$ by ± 0.12.

Figures 2–4 display the quantity

$$R_M = \frac{M_\pi^2(m_S) m_V}{M_\pi^2(m_V) m_S} \quad (5)$$

TABLE I. Simulation details.

L	T	β	m_S	Start[a]	Traj	Block	a^{-1} (MeV)	hyp[b]	$M_\pi(m_V = m_S)$ (MeV)	hyp[c]	$2\alpha_8 - \alpha_5$	hyp[c]
16	32	5.3	0.01	O	250–2250	200	1271 (85)	1376.9 (74)	378 (25)	271.3 (19)	0.236 (12)	0.287 (18)
				D	250–2250	200						
12[c]	32	5.3	0.01	O	250–1850	200	1470 (130)	1419 (26)	438 (39)	289.1 (70)	0.196 (15)	0.226 (64)
8	32	5.115	0.015	O	300–10 300	100	679.8 (14)	710.9 (24)	214.58 (45)	218.00 (75)	0.326 (12)	0.3439 (76)
8	32	5.1235	0.02	O	300–10 300	100	683.5 (12)	723.3 (22)	249.27 (44)	254.18 (79)	0.343 (11)	0.3817 (87)
8	32	5.132	0.025	T	0–10 000	100	686.1 (15)	734.6 (22)	279.54 (62)	286.79 (88)	0.388 (10)	0.4150 (91)
8	32	5.151	0.035	T	0–10 000	100	695.0 (14)	744.3 (25)	334.45 (68)	341.0 (12)	0.475 (12)	0.4704 (94)
16	32	5.8	∞		144 configs			1408.4 (42)		274.2 (13)		0.231 (31)

[a]Starting configuration state: ordered, disordered, or thermal.
[b]Denotes a hypercubic blocked ensemble.
[c]Spatial volume is $12^2 \times 16$.

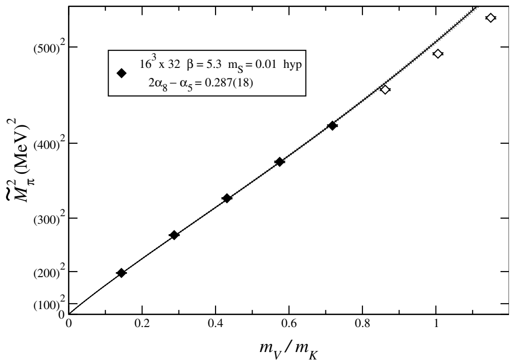

FIG. 1. $16^3 \times 32$, $\beta = 5.3$, $m_S = 0.01$, hypercubic blocked.

suggested by [14]. This quantity accentuates the NLO terms in $\tilde{M}_\pi^2$, as is evident by comparing Fig. 1 to Figs. 2–4. It should be noted, however, that the full forms of M_π^2 and f_π, (3) and (4), were used when fitting. When calculating R_M, we did not use the simplification shown in [14], but rather used a full numerator and denominator.

For each of the plots, the data points are the result of individual fits of the correlator at each valence quark mass, with jackknife error bars. The curves display the result of a simultaneous fit of all the correlators below a cutoff in m_V/m_K to the predicted forms of M_π^2 and f_π, (3) and (4), with jackknife error bounds. Solid symbols are used below the cutoff, while open symbols are used beyond it. Because of our small ensemble sizes, the full correlation matrix for many of the ensembles proved to be nearly singular. Thus, several of the fits do not fully account for data correlation.

We determined the lattice spacing of our ensembles via the static quark potential, using a tree-level corrected Coulomb term. The form of this term for hypercubic blocked ensembles was taken from [15].

Results.—Figure 2 presents R_M for the $16^3 \times 32$ ensemble both before and after hypercubic blocking. The application of hypercubic blocking altered results significantly, suggesting that the effect of flavor symmetry breaking at these lattice spacings is significant. The dash-dotted curve uses the results from the hypercubic blocked ensemble's fit, but replaces the value found for $2\alpha_8 - \alpha_5$ with one consistent with a zero up quark mass. The data clearly fall well outside this range.

To estimate the finite volume error in our result, we repeated the calculation in a smaller $12^2 \times 16 \times 32$ volume, holding all other parameters fixed. Fitting this ensemble with the same chiral cutoff as the $16^3 \times 32$ ensemble resulted in the value $2\alpha_8 - \alpha_5 = 0.226 \pm 0.064$. This matches our quoted result, suggesting that the finite volume of our $16^3 \times 32$ ensemble is not a large source of systematic error.

Figure 3 presents R_M for several ensembles with a variety of sea quark masses and matched lattice spacing. The physical volume of these lattices is similar to the physical volume of our $16^3 \times 32$ ensemble. The Columbia group has determined several values of the critical β_c and m_c for the $N_f = 3$, $N_t = 4$ finite temperature transition [16]. These ensembles were generated using those bare parameters. The trend in $2\alpha_8 - \alpha_5$ with the changing sea quark mass is inset in Fig. 3. This trend can be attributed to the sea quark mass dependence which was dropped from Eqs. (3) and (4). A systematic study of this dependence would allow a determination of the parameter within the dropped term, $2\alpha_6 - \alpha_4$ [17].

Fully quenched and partially quenched ChPT predict different forms for R_M. Thus, one might hope to see the effects of quenching though an ensemble's R_M plot. Figure 4 shows the $16^3 \times 32$ partially quenched hypercubic blocked ensemble alongside a fully quenched

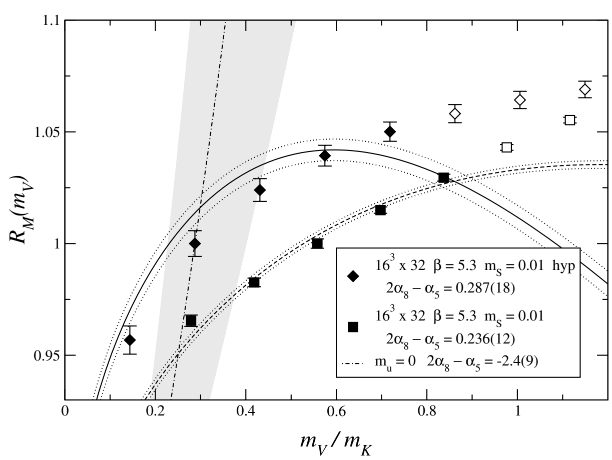

FIG. 2. $16^3 \times 32$, $\beta = 5.3$, $m_S = 0.01$. The squares and dashed curve (diamonds and solid curve) are before (after) hypercubic blocking. Data consistent with $m_u = 0$ would fall within the range centered on the dash-dotted curve.

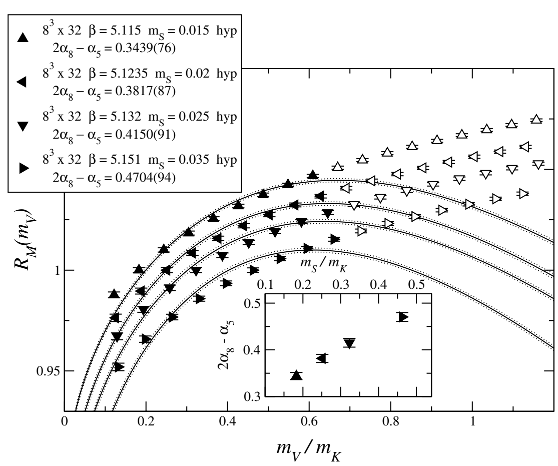

FIG. 3. $8^3 \times 32$, several values of β and m_S with matched lattice spacing, hypercubic blocked. The inset shows the effect of varying m_S on $2\alpha_8 - \alpha_5$ when $2\alpha_6 - \alpha_4$ terms are neglected.

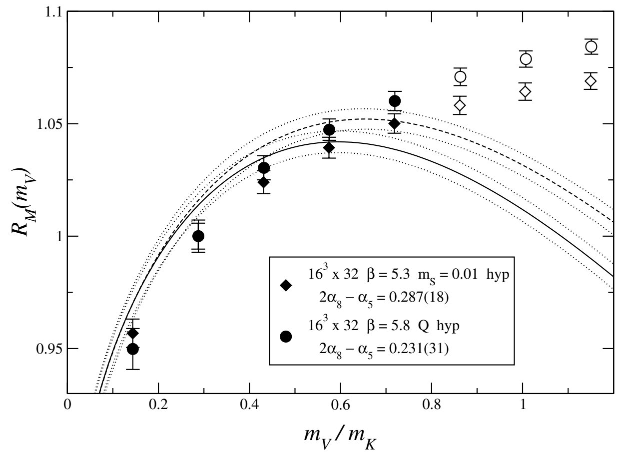

FIG. 4. $16^3 \times 32$, hypercubic blocked with similar lattice spacings. The circles and dashed curve (diamonds and solid curve) are fully (partially) quenched. The quenched data were fit as though partially quenched with $m_s = 0.01$, $N_f = 3$.

ensemble with similar lattice spacing. The quenched ensemble was analyzed as though partially quenched, using $m_S = 0.01$, $N_f = 3$. This procedure does not generate a rigorous value for $2\alpha_8 - \alpha_5$, as this would require the use of fully quenched ChPT. However, it could offer insight into the magnitude of quenching effects. As Fig. 4 shows, the effects of quenching are not pronounced. This analysis, at its current level of precision, is unable to distinguish a fully quenched ensemble from a partially quenched ensemble of equal lattice spacing.

The results for $2\alpha_8 - \alpha_5$ from each ensemble are compiled in Fig. 5. While these values vary significantly, they do so well outside the range required for a zero up quark mass, $-3.3 < 2\alpha_8 - \alpha_5 < -1.5$. Our quoted result of $2\alpha_8 - \alpha_5 = 0.287 \pm 0.018^{\text{stat}} \pm 0.18^{\text{syst}}$ comes from our hypercubic blocked $16^3 \times 32$ ensemble, where the reported systematic error is the result of adding in quadrature the determined effects of shifting the chiral cutoff (± 0.12), hypercubic blocking (± 0.05), doubling the lattice spacing (± 0.11), and reducing the lattice volume (± 0.06). Assuming Dashen's rule [19], this corresponds to $\Delta_M = -0.0897 \pm 0.0313$ and $m_u/m_d = 0.484 \pm 0.027$, where the quoted error arises primarily from the systematic error of our measurement. The error from experimental input is negligible and the size of NNLO corrections to Δ_M are assumed to be on the order of Δ_M^2. Using the values for the electromagnetic contributions to the light meson masses from [20] in place of Dashen's rule results in $\Delta_M = -0.0898 \pm 0.0313$ and $m_u/m_d = 0.410 \pm 0.036$. This can be compared to previous calculations in the literature, which have given $m_u/m_d = 0.553 \pm 0.043$ [21] and $m_u/m_d = 0.46 \pm 0.09$ [22].

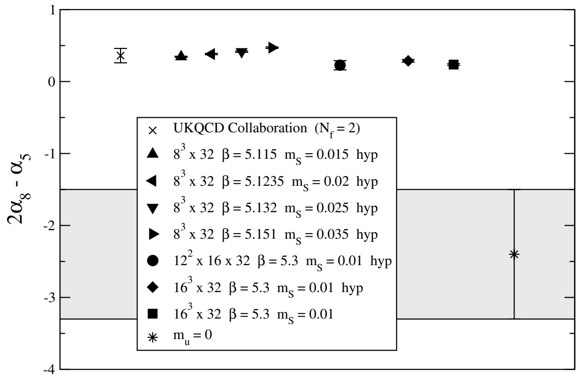

FIG. 5. Compiled results. The UKQCD Collaboration data point is taken from [18], showing their statistical error only. This point was calculated using $N_f = 2$ Wilson fermions, and thus its relative agreement suggests small N_f dependence. The rightmost point denotes the range allowed by $m_u = 0$.

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