Is strong $CP$ invariance due to a massless up quark?

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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, $\theta < 10^{-9}$. The unnatural smallness of $\theta$ 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 $M$ shift $\theta$,

$$\dot{\theta} = \theta + \arg \det M,$$

where $\theta$ is a fundamental parameter of the Standard Model. However, if $m_u = 0$, then $\det M = 0$ and $\arg \det M$ is unphysical, leaving one free to remove the $CP$ violating term through a simple field redefinition.

At leading order, 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 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 non-zero up quark mass and certain large NLO corrections. This is known as the Kaplan-Manohar ambiguity.

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 $2\alpha_8 - \alpha_5$ which appears in $\Delta_M$, the NLO correction to the quark mass ratios. If this combination falls within a certain range, $-3.3 < 2\alpha_8 - \alpha_5 < -1.5$, current experimental results can not 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. However, because these coefficients are physically determined by the low-energy non-perturbative behavior of QCD, the lattice offers the best opportunity for a truly first-principles calculation.

PARTIALLY QUENCHED CHIRAL PERTURBATION THEORY (pqChPT)

pqChPT 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.

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

where $U = \exp(2i\Phi/f)$, $\chi = 2\mu a^{-1} \text{diag}\{\{m_s, m_V\}\}$. $\Phi$ contains the pseudo-Goldstone “mesons” of the spontaneously broken $SU(N_f + N_V - \bar{N}_V) L \otimes SU(N_f + \bar{N}_V - \bar{N}_V) R$ 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, $m_x^{\text{dim}} = a^{-1} m_x$. 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 $f$, $\mu$, 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. 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**

$pq$ChPT 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 $\Lambda_{\chi} = 4\pi f$.

\[
M^2_{\pi} = (4\pi f)^2 z m_V \left\{ 1 + z m_V \left( 2\alpha_s - \alpha_5 + \frac{1}{N_f} \right) + \frac{z}{N_f} (2m_V - m_S) \ln z m_V \right\},
\]

\[
f_{\pi} = f \left\{ 1 + \frac{\alpha_5}{2} z m_V + \frac{zN_f}{4} (m_V + m_S) \ln \frac{z}{2} (m_V + m_S) \right\},
\]

where $z = 2\mu a^{-1}/(4\pi f)^2$. These forms differ slightly from those in [4], as the NLO dependence in the sea

![Figure 1](image1.png)

**FIG. 1:** $16^3 \times 32$, $\beta = 5.3$, $m_S = 0.01$, hypercubic blocked. Data consistent with the dashed curve (diamonds and solid curve) are before (after) hypercubic blocking to several of our ensembles, using the blocking was recently presented in [10]. A detailed analysis of this effect with dynamical quarks also allows one to work at $N_f = 3$, but involves taking the coarse lattices generates significant flavor symmetry breaking, and thus a splitting of the light meson masses. However, our use of staggered fermions on some-what 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 [4]. 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 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 [4].

![Figure 2](image2.png)

**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 dashed-dotted curve. The square mass has been absorbed into $\mu$ 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 ensembles were generated using staggered fermions via the inexact HMD R-algorithm [12], which allows one to work at $N_f = 3$, but involves taking the

**TABLE I:** Simulation details.

| $L$ | $T$ | $\beta$ | $m_S$ | start$^a$ | traj | block | $a^{-1}$ (MeV) | $M_0(m_V = m_S)$ (MeV) | $2\alpha_s - \alpha_5$ |
|-----|-----|---------|-------|-------|------|-------|----------------|-----------------|-----------------|
| 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) |
| 12  | 32  | 5.3     | 0.01  | D     | 250-1850 | 200  | 1470(130) | 1419(26)  | 438(39) | 289.1(70) | 0.196(15) | 0.226(44) |
| 8   | 32  | 5.15    | 0.015 | O     | 300-10300 | 100  | 679.8(14) | 710.9(24) | 214.58(45) | 218.00(75) | 0.328(12) | 0.343(96) |
| 8   | 32  | 5.125   | 0.02  | O     | 300-10300 | 100  | 683.5(12) | 723.3(22) | 249.27(44) | 254.18(79) | 0.343(11) | 0.381(77) |
| 8   | 32  | 5.132   | 0.025 | T     | 0-10000  | 100  | 686.1(15) | 734.6(22) | 279.54(62) | 286.79(88) | 0.388(10) | 0.415(94) |
| 8   | 32  | 5.151   | 0.035 | T     | 0-10000  | 100  | 695.0(14) | 744.3(25) | 334.45(68) | 341.00(12) | 0.475(12) | 0.470(94) |

$^a$Starting configuration state: ordered, disordered, or thermal.

$^b$Denotes a hypercubic blocked ensemble.

$^c$Spatial volume is $12^2 \times 16$. 

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$m$ denotes an ensemble’s valence quark mass at which the chiral cutoff is changed, the hypercubic blocked ensemble, at which 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 $\pm 0.14$ in $m_V/m_K$ shifted $2\alpha_8 - \alpha_5$ by $\pm 0.12$.

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 $M_2^2$ and $f_\pi$, 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 [13].

**RESULTS**

Figure 3 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 dashed-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 $12^3 \times 16 \times 32$ 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.
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 $\beta_i$ and $m_u$ for the $N_f = 3, N_t = 4$ finite temperature transition \cite{14}. 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 Figure \ref{fig:5}. This trend can be attributed to the sea quark mass dependence which was dropped from Equations \ref{eq:1.0} and \ref{eq:1.1}. A systematic study of this dependence would allow a determination of the parameter within the dropped term, $2\alpha_8 - \alpha_5$ \cite{14}.

Fully quenched and partially quenched ChPT predict different forms for $R_M$. Thus, one might hope to see the effects of quenching through an ensemble’s $R_M$ plot. Figure \ref{fig:1} shows the $16^3 \times 32$ partially quenched hypercubic blocked ensemble along side a fully quenched ensemble with similar lattice spacing. The quenched ensemble was analyzed as thought 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 Figure \ref{fig:1} 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 Figure \ref{fig:4}. 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 $2\alpha_8 - \alpha_5 = 0.287 \pm 0.018^{\text{stat}} \pm 0.18^{\text{sys}}$ 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 $(\pm 0.12)$, hypercubic blocking $(\pm 0.05)$, doubling the lattice spacing $(\pm 0.11)$, and reducing the lattice volume $(\pm 0.06)$. Assuming Dashen’s rule \cite{18}, 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 $\Delta_M$ are assumed to be on the order of $\Delta_M^2$. Using the values for the electromagnetic contributions to the light meson masses from \cite{18} 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 $m_u/m_d = 0.553 \pm 0.043$ \cite{20} and $m_u/m_d = 0.46 \pm 0.09$ \cite{21}.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5.png}
\caption{Compiled results. The UKQCD Collaboration data point is taken from \cite{19}, 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 $m_u = 0$.}
\end{figure}

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