Can $\theta_{\rm QCD} = \pi$?

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Recent work suggests that wormholes in spacetime may drive θ_{QCD} to π , and it has been argued that this is not in conflict with any observations. We have therefore determined current-mass ratios of the light quarks in second-order chiral perturbation theory, with attention to the relative sign of the upquark mass. We discuss an ambiguity which makes it impossible to determine the quark mass ratios from chiral-Lagrangian considerations alone. Using results from lattice QCD we resolve the ambiguity to obtain $m_u/m_d = 0.61 \pm 0.26$, $m_s/m_d = 21 \pm 2$, implying that $\theta_{QCD} = 0$.

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Since the invention of axions twelve years ago, several hundred papers have been written about them. Less effort seems to have gone into trying to determine whether the up quark is massless, which would render axions superfluous, or has a wrong-sign mass, which would rule them out. In the latter case, the physical θ parameter of QCD would take the *CP*-conserving value π rather than zero. It has long been thought that current-quark-mass ratios, hence θ_{QCD} , can be determined from comparing predictions of the chiral Lagrangian for pseudo Goldstone bosons with measurable quantities like their masses.¹ Such calculations,² including Weinberg's determination³ $m_u/m_d = 0.56$, $m_s/m_d = 20.1$, indicate a positive up-quark mass, or $\theta_{QCD} = 0$.

However, Kaplan and Manohar have pointed out that such predictions could plausibly be upset by second-order corrections in chiral perturbation theory.⁴ They found that if one allows mesons to get up to 30% of their theoretical (mass)² from second-order corrections, the ratio m_u/m_d could vary between 0 and 0.8. It would thus seem possible that m_{μ} could be zero or negative. But can a more definite prediction be made? Although this question is interesting in its own right, our immediate motivation for trying to answer it stems from recent attempts to solve the strong CP problem using wormholes in spacetime, 5-7 which were originally proposed as a solution to the cosmological-constant problem.⁸ Nielsen and Ninomiya argue rather generally that wormholes should cause the wave function of the Universe to be strongly peaked at $\theta_{QCD} = 0$ or π , while Choi and Holman, and Preskill, Trivedi, and Wise, argue that the preferred value is π . Reference 7 further claims that instanton effects could make this value of θ_{OCD} phenomenologically acceptable.

The reason Kaplan and Manohar did not get a definite prediction for the sign of m_{μ} is that their expressions for the five meson masses depended on six undetermined parameters of the Lagrangian. To do better one needs to compute an additional measurable quantity to the same accuracy, preferably one that is sensitive to the updown-quark mass difference. We have chosen to use the partial width for the isospin-violating decay $\eta \rightarrow 3\pi^0$ because it is free from annoving electromagnetic corrections at one loop. Although $\Gamma(\eta \rightarrow 3\pi)$ was previously computed in second-order chiral perturbation theory by Gasser and Leutwyler,⁹ they did not try to extract any constraints on quark mass ratios from it. We find that $m_u/m_d = 0.31 \pm 0.06$, $m_s/m_d = 23.3 \pm 0.1$ for the current-quark-mass ratios, which would appear to rule out $\theta_{\rm QCD} = \pi.$

After completing the above calculation we were made aware of an ambiguity that appears to cast serious doubt on the validity of *any* attempt to get information about current quark masses from chiral Lagrangians alone.¹⁰ The point is that effective Lagrangians can only give information about an *effective* quark mass matrix which is some function of the true mass matrix M that transforms the same way under SU(3)_L×SU(3)_R as M does. This function could be determined only with a detailed understanding of nonperturbative QCD dynamics, as would be afforded by a lattice computation. After describing our calculation we will discuss this issue more fully and show how existing lattice results can be used to resolve the ambiguity, with the effect of shifting the above mass ratios to $m_u/m_d = 0.61 \pm 0.26$, $m_s/m_d = 21 \pm 2$.

One starts with the second-order Lagrangian⁴ $\mathcal{L} = \mathcal{L}_2 + \mathcal{L}_4$,

$$\mathcal{L}_{2} = (f^{2}/4) \operatorname{tr}(\partial_{\mu}\Sigma \partial_{\mu}\Sigma^{\dagger}) + (f^{2}/2) \operatorname{tr}(\mu M\Sigma + \mathrm{H.c.}); \qquad (1)$$

$$\mathcal{L}_{4} = (f^{2}/2\Lambda^{2}) \{c_{1} | \operatorname{tr}(\mu M\Sigma) |^{2} + c_{2} [\operatorname{tr}(\mu M\Sigma)]^{2} + \mathrm{H.c.} + c_{3} \operatorname{tr}[(\mu M\Sigma)]^{2} + \mathrm{H.c.} + c_{4} (\alpha/4\pi) \Lambda^{4} \operatorname{tr}(Q\Sigma Q\Sigma^{\dagger}) + c_{5} \operatorname{tr}(\mu M\Sigma) \operatorname{tr}(\partial_{\mu}\Sigma \partial_{\mu}\Sigma^{\dagger}) + \mathrm{H.c.} + c_{6} \operatorname{tr}(\mu M \partial_{\mu}\Sigma \partial_{\mu}\Sigma^{\dagger}\Sigma) + \mathrm{H.c.} + c_{7} \operatorname{tr}(\partial^{2}\Sigma \partial^{2}\Sigma^{\dagger}) \} + O((\partial\pi)^{4}), \qquad (2)$$

where $\Sigma = \exp(2i\pi_a T_a/f)$ and $f \cong f_{\pi} = 93$ MeV; π_a are the components of the pseudoscalar-meson octet; M and Q are, respectively, the quark mass and charge matrices, $M = \operatorname{diag}(m_u, m_d, m_s)$, $Q = \operatorname{diag}(\frac{2}{3}, -\frac{1}{3}, -\frac{1}{3})$; μ is an indeterminate mass scale of order 1 GeV. As noted in Ref. 4, all the effects of the c_6 and c_7 terms can be absorbed into other

coefficients by an appropriate $SU(3)_L \times SU(3)_R$ transformation, so they can be ignored. Let $\Lambda = 4\pi f_{\pi}$ be the cutoff scale for the theory and $\epsilon = \mu m_s / \Lambda^2$. Using the above Lagrangian, including one-loop effects from \mathcal{L}_2 , we obtain the following expressions for the meson masses to second order in ϵ :

$$m_{\pi^{0}}^{2} = \Lambda^{2} \epsilon(x+y) [E - \frac{2}{9} \ln(4\epsilon/3)], \quad m_{\pi^{+}}^{2} = m_{\pi^{0}}^{2} + \Lambda^{2}(\alpha/4\pi)D,$$

$$m_{K^{0}}^{2} = \Lambda^{2} \epsilon[(1+y)E + \epsilon B(1+2y) + \epsilon(x+y)/9 + (4\epsilon/9)(1-x/2+2y)\ln(4\epsilon/3)],$$

$$m_{K^{+}}^{2} = (m_{K^{0}}^{2} \text{ with } x \leftrightarrow y) + \Lambda^{2}(\alpha/4\pi)D,$$

$$m_{\eta}^{2} = \Lambda^{2} \epsilon((4+x+y)E/3 + 8\epsilon B/3 + 2\epsilon(1-x-y)C/3) + \epsilon\{(\frac{10}{27} + \frac{20}{9} \ln[4(x+y)/3] + \frac{64}{9} \ln \frac{4}{3}\} + (\epsilon/27)[4+26(x+y)]\ln\epsilon),$$
(3)

where $x = m_u/m_s$, $y = m_d/m_s$, $A = c_1/2 + c_2 - 2c_5$, $B = 2c_3$, $C = 4c_2 - 2c_1$, $D = c_4$, and $E = 1 + 2\epsilon A \operatorname{tr} M/\mu m_s$. We used dimensional regularization with the renormalization scale Λ for the loop graphs, and subtracted the combination $\Gamma(2 - d/2)(4\pi)^{d/2} + 1$ wherever it appeared. As in Ref. 4 we have ignored contributions of order x^2, xy, y^2 compared to x, y since the latter are small, $-\frac{1}{20}$. The tree diagrams in (3) agree with Ref. 4,¹¹ and the loop contributions agree with Refs. 12 and 13 (both of which assume x = y). The only possibly subtle point in the calculation is that although $\eta - \pi^0$ mixing can be ignored almost completely, there is one diagram in which it is important, Fig. 1. This makes a contribution of order $\epsilon(x - y) \ln \epsilon$ to $m_{K^+}^2$ and $m_{K^0}^2$.

Although Eqs. (3) may appear to depend on seven parameters, A can be removed by defining a new expansion parameter $\epsilon = \tilde{\epsilon}(1 - 2\tilde{\epsilon}A \operatorname{tr} M/\mu m_s)$. D and B can then

be eliminated from the equations for the pion and kaon masses to obtain parametric expressions for x and y as functions of $\tilde{\epsilon}$. This curve, shown dotted in Fig. 2, differs somewhat from the one displayed by Kaplan and Manohar. (We come very close to their curve if we leave out the contribution in Fig. 1.)

The next step is to calculate the $\eta \rightarrow 3\pi^0$ amplitude to the same order in ϵ , x, and y. This could be very tedious, but happily one may reduce a month's work into a day using the background-field method, by making the replacement $\Sigma \rightarrow \xi \Sigma_q \xi$ (Ref. 13) in the Lagrangian (1) +(2). Here Σ_q is the quantum field and $\xi^2 = \Sigma_b$ is the background field. One could imagine other ways of making the split between quantum and background fields, but this one seems to be the most convenient. (For instance, using $\Sigma \rightarrow \Sigma_q \Sigma_b$ is not parity invariant and introduces cubic couplings, making more diagrams to compute.) We find the amplitude to be

$$i\mathcal{M} = (1/\sqrt{3})(4\pi)^{2} \epsilon(x-y) \left(1 + (3\epsilon/4) \sum_{s \to t \to u} \hat{s}^{2} f_{2}(s,\pi) - (\hat{s}^{2} - 2\hat{s} + \frac{4}{3}) f_{2}(s,K) + (3\epsilon/16) \sum_{s \to t \to u} \hat{s}(\hat{s} - \frac{4}{3}) [f_{2}(s,K^{+}) - f_{2}(s,K^{0})]/(x-y) + \epsilon [f_{1}(K) - f_{1}(\eta)/6] + \epsilon (2A - C) \right) + O(\epsilon^{3}) + O(x^{2}, xy, y^{2}),$$
(4)
where $\hat{s} = s/\mu m_{s} = (q_{1} + q_{2})^{2}/\mu m_{s}, q_{i}$ are the pion momenta, $t = (q_{1} + q_{3})^{2}, u = (q_{2} + q_{3})^{2},$ and

$$f_{1}(P) = (m_{P}^{2}/\mu m_{s}) \ln(m_{P}^{2}/\Lambda^{2}),$$

$$f_{2}(s,P) = 1 - \ln(m_{P}^{2}/\Lambda^{2}) + \begin{cases} -a_{P} \arctan[sa_{P}/(2\mu m_{s} - s)], P = K^{+}, K^{0} \\ a_{P} \ln[(1 - a_{P})/(1 + a_{P})], P = \pi, \end{cases}$$

$$a_{P} = (|1 - 4m_{P}^{2}/s|)^{1/2}.$$
(5)

The values of m_F^2 appearing in the loop contributions f_1 and f_2 can be taken to be the leading-order terms in Eqs. (3). Actually f_2 also has an imaginary part, but when the matrix element is squared this would appear at order



FIG. 1. A nonnegligible contribution to the kaon masses involving $\eta - \pi^0$ mixing.

 ϵ^4 , which we are ignoring.

Amazingly, Eq. (4) depends only on the same combinations of Lagrangian parameters that contribute to the masses. This was not guaranteed by chiral symmetry or any other principle. For example, the operator $c_8 \operatorname{tr}(\partial_{\mu} \Sigma \partial_{\mu} \Sigma^{\dagger} \partial_{\nu} \Sigma \partial_{\nu} \Sigma^{\dagger})$ [which Ref. 13 showed to be the only independent operator of order $(\partial \pi)^4$ once the \mathcal{L}_2 equations of motions are imposed] contributes to $\eta \rightarrow \pi^+ \pi^- \pi^0$, but not to $\eta \rightarrow 3\pi^0$. Similarly, there is no reason that c_5 should combine with c_1 and c_2 to make $A = c_1/2 + c_2 - 2c_5$, but it does. A subtle way in which it appears is through rewriting the Lagrangian parameter f



FIG. 2. Dotted curve: effective quark mass ratios, constrained by a second-order chiral-perturbation-theory fit to the meson masses and the Kaplan-Manohar bound. Solid curves: the true quark mass ratios, obtained from the dotted curve using Eq. (11) with $\alpha \epsilon = -0.10$, -0.37, and -0.64, from left to right. The brackets indicate the extreme values consistent with the $\eta \rightarrow 3\pi^0$ partial width; the heavy dot is the preferred value; the range of $\alpha \epsilon$ values reflects lattice-QCD uncertainties. Cross: Weinberg's lowest-order determination.

in terms of the physically measurable decay constant f_{π} in the leading contribution to $\mathcal{M}(\eta \rightarrow 3\pi)$: $f_{\pi} = f(1 + 2\epsilon c_5 \operatorname{tr} \hat{M} - \frac{1}{2} \epsilon \ln \epsilon)$.

We can check the S-matrix elements (3) and (4) for consistency by demanding that they be renormalizationgroup invariant. Any change of the arbitrary renormalization scale entering through the logarithms must be absorbable into a redefinition of the couplings in \mathcal{L}_4 , ¹³ which is a nontrivial constraint. We find that (3) and (4) are indeed invariant under the combined transformations $\ln \epsilon \rightarrow \ln \alpha \epsilon$; $A \rightarrow A + \frac{1}{9} \ln \alpha$; $B \rightarrow B + \frac{2}{3} \ln \alpha$; $C \rightarrow C$ $+ 2 \ln \alpha$.

The partial width for $\eta \rightarrow 3\pi^0$ can now be computed numerically using Eq. (3) for m_η^2 to determine C in (4). Stepping through the values of $\tilde{\epsilon}$ that parametrize the curve in Fig. 2, we obtain Table I for the couplings consistent with the uncertainty in $\Gamma(\eta \rightarrow 3\pi^0)$ as given by the Particle Data Group.¹⁴ In particular,

$$\tilde{m}_u/\tilde{m}_d = 0.31 \pm 0.06; \quad \tilde{m}_s/\tilde{m}_d = 23.3 \pm 0.1$$
. (6)

(The meaning of the tildes will be explained presently.) No attempt is given here to estimate the theoretical uncertainty, but one can form an opinion by comparing Eq. (6) with Weinberg's first-order results, 0.56 and 20.1.

On the face of it, (6) would appear to rule out θ_{QCD} - π . But now we must discuss an unpleasant surprise. The chiral Lagrangian's form is dictated by the formal $SU(3)_L \times SU(3)_R$ symmetry¹⁵

$$\Sigma \to L\Sigma R^{\dagger}, \quad M \to RML^{\dagger}. \tag{7}$$

M does not really transform, but this rule tells one how it

TABLE I. Values of the Lagrangian parameters corresponding to experimental limits on the $\eta \rightarrow 3\pi^0$ partial width.

ĩ	\tilde{m}_u/\tilde{m}_d	\tilde{m}_s/\tilde{m}_d	В	С	Width (keV)
0.20	0.37	23.2	-0.3	-4.9	0.283
0.21	0.31	23.3	-0.3	-4.4	0.347
0.22	0.26	23.3	-0.4	-4.0	0.406

is allowed to break the symmetry. Choi has pointed out to us that the combination 16

$$\tilde{M} = M + (\alpha \mu / \Lambda^2) (\det M) (M^{-1})^{\dagger}$$
(8)

transforms just like M under (7). Therefore one can never know, solely on the basis of chiral-Lagrangian calculations, whether mass ratios thereby computed are those of the true current quark masses M, or just some effective quark masses \tilde{M} . This is true to any order in the chiral expansion, essentially because only S-matrix elements, and not the mass ratios, are determined as power series in ϵ . Nevertheless we can still say a few things. First of all, the same ambiguity that applies to our calculation also afflicts Preskill, Trivedi, and Wise's (and perhaps Choi and Holman's) prediction $\theta_{OCD} = \pi$, for it shows that what they predict is not the sign of the true up-quark mass, but rather the effective up-quark mass \tilde{m}_u in \tilde{M} , since they also used chiral perturbation theory. Our result indicates it is unlikely that \tilde{m}_u is negative.

However, we can do even better than this. We have argued that the coefficient α in (8) can never be determined from chiral Lagrangians alone, but there already exist lattice calculations which, taken together with our result (6) can be used to solve for the true quark mass ratios. Hamber¹⁷ finds that

$$m_u/m_s + m_d/m_s \equiv x + y = 1/(13 \pm 2.5)$$
 (9)

in a simulation using dynamical fermions. Maiani and Martinelli¹⁸ obtained a similar number in the quenched approximation, $1/(12 \pm 3)$, which agrees with Hamber's earlier quenched calculations.¹⁹ If we write the true quark mass ratios as x and y, and the effective ones as \tilde{x} and \tilde{y} , then (8) can be inverted to give

$$x = \tilde{x} - \alpha \epsilon \tilde{y}, \quad y = \tilde{y} - \alpha \epsilon \tilde{x} , \tag{10}$$

ignoring terms quadratic in \tilde{x} and \tilde{y} as usual. Of course we expect there to be higher-order contributions to (8) such as $(\beta\mu^3/\Lambda^6)(\det M)M$ that would add terms of order $\beta\epsilon^3 x^2 y$ to (10). It seems reasonable to assume (and we shall show it for α) that the dimensionless coefficients α,β are ~ 1 so that these higher-order contributions should be negligible. Equations (9) and (10) can be solved for x, y, and $\alpha\epsilon$ with the result

$$m_u/m_d = 0.61 \pm 0.26, \quad m_s/m_d = 21 \pm 2,$$

 $\alpha \epsilon = -0.37 \pm 0.27.$ (11)

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Therefore the ambiguity in the true identity of the current masses, when resolved via lattice QCD, only tends to bound m_u farther away from zero, resulting in a stronger determination that $\theta_{\rm QCD} = 0$.

It should be emphasized that these conclusions do not exclude wormholes as a solution to the strong *CP* problem (although other difficulties may well do so²⁰). Wormholes unequivocally drive θ_{QCD} to 0 or π , but the argument that π is favored depends upon unproved assumptions about the infrared properties of QCD. Whatever the mechanism of *CP* conservation in the strong interactions, it appears that there is little room for the possibility that $\theta_{QCD} = \pi$.

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Note added.—I have been informed of the following: (1) Gasser and Leutwyler extensively reviewed the results of various methods (different from ours) for determining quark masses in Ref. 21. (2) Leutwyler says that the ambiguity Eq. (9) can be removed using sum rules derived from spectral representations of current-current correlations. Although this is unpublished, the SU(2) version of these sum rules is given in Ref. 22. (3) Some experts question the accuracy of the lattice results quoted here. If a different value for $(m_u + m_d)/m_s$ should emerge as the consensus of the lattice-gauge community, it is trivial to revise Eqs. (9)-(11). Better yet, perhaps lattice workers will soon determine m_u and m_d independently, providing additional evidence about θ_{QCD} .

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