

Light quark masses beyond leading order

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We describe the measurement of the light quark mass ratios when one calculates to second order in the quark masses. At this order there is an ambiguity in the meaning of the quark mass, which afflicts the past attempts to provide a model-independent measurement of the ratios. We argue that this is similar to the regularization-scheme dependence of coupling constants. We study the anomalous Ward identities and the effects of strong CP violation in an attempt to resolve the ambiguity. The ambiguity persists even with singlet fields, such as the η' , but can be resolved by observing the θ dependence of the theory. Since matrix elements of $F\bar{F}$ are related to $\partial\mathcal{L}_{\text{QCD}}/\partial\theta$, they are useful probes of quark masses. We give a procedure by which quark mass ratios can be measured in a model-independent way through the matrix elements $\langle 0|F\bar{F}|\pi^0\rangle$, $\langle 0|F\bar{F}|\eta\rangle$, and $\langle 0|F\bar{F}|3\pi\rangle$, which in turn are observable in $V\rightarrow V\pi^0$ ($\eta, 3\pi$), with V being ψ or Υ , when analyzed using a heavy-quark multipole expansion. Present data are not sufficient to complete this program, but we use available results to provide the value $[(m_d - m_u)/(m_d + m_u)](m_s + \hat{m})/(m_s - \hat{m}) = 0.59 \pm 0.07 \pm 0.08$ (i.e., $m_u/m_d = 0.30 \pm 0.05 \pm 0.05$), where the first error is experimental and the second is our estimate of the remaining theoretical model dependence.

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I. INTRODUCTION

In most field theories, the masses of the particles are the most obvious and accessible properties. However, in QCD the masses of the light quarks (u, d, s) have a very different character. They are not directly measurable in inertial experiments, but enter the theory only indirectly as parameters in the fundamental Lagrangian. In this respect they are much more similar to coupling constants than they are to inertial masses. Both coupling constants and the light quark masses must be measured by their influence on observables. To do this properly, one has to be able to calculate the observables in terms of the renormalized coupling constants and masses, defined in a specified regularization and renormalization scheme. Generally this is accomplished order by order in a perturbative scheme. In the case of the light quark masses, our inability to calculate hadronic properties at low energy makes it difficult to use this method to extract the renormalized masses.

There is, however, a rigorous, semiphenomenological method, chiral perturbation theory [1–3], to extract information about the *ratios* of quark masses, order by order, in an expansion in the masses themselves. It relies on the fact that there would be an exact chiral symmetry in the limit that the masses vanish. Deviations from the exact-symmetry predictions are then functions of the masses which, to the extent that the masses are small, can

be expanded in a series in the mass. To first order,¹ the results are extremely simple [4]:

$$\frac{m_u + m_d}{2m_s} \equiv \frac{\hat{m}}{m_s} = \frac{m_\pi^2}{2m_K^2 - m_\pi^2} = \frac{1}{25}, \quad (1a)$$

$$\frac{m_d - m_u}{m_s + \hat{m}} = \frac{m_{K^0}^2 - m_{K^+}^2 + m_\pi^2 - m_{\pi^0}^2}{m_K^2} = \frac{1}{46},$$

or

$$\frac{m_u}{m_s} = \frac{1}{35}, \quad \frac{m_d}{m_s} = \frac{1}{19}, \quad (1b)$$

$$\frac{m_u}{m_d} = \frac{1}{1.8}, \quad \frac{m_d - m_u}{m_d + m_u} = 0.28.$$

To this order, the interpretation is equally simple. Since the leading-order QCD renormalization is mass independent, these ratios are equally well the ratios of renormalized masses or of bare parameters in the Lagrangian. These measurements of mass ratios will be modified if the

¹We would like to emphasize that here and throughout the rest of the paper, when we describe the order of the expansion, it refers to an expansion in the mass. A perturbative expansion in the QCD coupling constant is never implied.

theoretical analysis is carried out to next order, when the subtleties appear. It is the purpose of this paper to discuss the analysis of quark mass ratios at next order.

There are several motivations for this work. In the first place, the quark masses are some of the basic parameters of the standard model, and it is important to document our level of understanding of them. There is in the community an almost universal acceptance of the lowest-order mass ratios of Eq. (1). This is not warranted, as we will demonstrate that sizable corrections to these ratios are allowed. A second motivation is a known ambiguity which first surfaces at second order [5]. While we will leave the precise statement of the ambiguity to the next section, it states that we can obtain the same phenomenological consequences either from a mass matrix m , or from a changed mass matrix

$$m^{(\lambda)} \equiv m + \bar{\lambda} \det(m) m^{-1}, \quad (2)$$

where $\bar{\lambda}$ is an arbitrary constant. Specifically (at second order)

$$\begin{aligned} m_u^{(\lambda)} &= m_u + \bar{\lambda} m_d m_s, \\ m_d^{(\lambda)} &= m_d + \bar{\lambda} m_u m_s, \\ m_s^{(\lambda)} &= m_s + \bar{\lambda} m_u m_d. \end{aligned} \quad (3)$$

As far as phenomenology is concerned, any one in this family of mass matrices can be chosen as the primary mass matrix. There have been conflicting claims about the effect of this ambiguity [5–7], including an interesting recent investigation by Leutwyler to resolve the ambiguity [7], and we will spend a good deal of the paper in an attempt to clarify this issue.

A further motivation comes from the strong CP problem [8]. The only solution which does not require physics outside the standard model is the option with $m_u = 0$, in which case the effect of the θ term vanishes. Put another way, the physical CP -violating parameter is $\theta \det m$, which would vanish if $\det m = 0$. Although it has been argued in the past that this option is not viable phenomenologically, this conclusion has been questioned because of the ambiguity mentioned above [5]. We note, however, that, even if it were to be allowed phenomenologically, the “ $m_u = 0$ option” does not resolve the naturalness problem within the standard model as it is no more natural to set $m_u = 0$ than to set $\theta = 0$.

There is, in addition, a stimulating calculation by Kim, Choi, and Sze [9]. These authors consider a massless up quark in an instanton gas and show that, through the instanton quantum effects of Fig. 1 (the 't Hooft determinant), the up quark would pick up a nonzero mass

$$m_u^{\text{eff}} = C m_d m_s e^{-i\theta}, \quad (4)$$

where the constant C depends on the details of the calculations including the cutoff on the integration over instanton sizes. More important than the precise numerical coefficient C is the explicit demonstrations that this form of mass shift takes place in QCD. This calculation raises questions about how one defines the quark mass, and which quark mass plays a role in the chiral $U(1)_A$ rota-

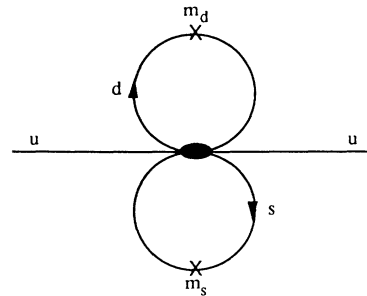


FIG. 1. The diagram used to generate an effective up quark mass in Ref. [9]. The symbol \times indicates a mass insertion.

tion needed to remove θ . This phenomenon will fit naturally into the description of mass effects which are considered in chiral perturbation theory.

One of our goals is to provide a procedure by which quark mass ratios can be unambiguously measured. At this stage, we should distinguish between a “measurement” and a “model.” For our purposes, a “measurement” means a determination (from experiment) which follows rigorously from QCD to the order that one is working. In contrast, a “model” implies that one uses results from nonrigorous calculations which attempt to mimic low-energy QCD. Past attempts to extract quark masses at second order have all had some aspects which are in the model category. This is not to say that they are bad estimates; they may, in fact, be successful at mimicking QCD. However, because models involve adjustable assumptions, they do not form a controlled approximation scheme to QCD, and we cannot be truly confident of the results.

We will find that the θ dependence of the theory can be used to probe the quark masses. While it is unfortunately not possible to measure the θ dependence from the observation of strong CP -violating effects, the matrix elements of $F\tilde{F}$ are related to $\partial\mathcal{L}_{\text{QCD}}/\partial\theta$. Fortunately, the multipole expansion [10,11] for heavy quarks shows that the decays $V \rightarrow V + M$, where $V = \Upsilon$ or ψ and $M = \pi^0, \eta, 3\pi$, are dominated by the $F\tilde{F}$ matrix elements, to leading order in the heavy-quark expansion. This then yields an operational procedure for the measurement of quark masses. Sufficient data do not yet exist to carry out that measurement, so we provide a weaker estimate based on available data. The result is slightly, but not dramatically, different from previous estimates.

II. QUARK MASSES AND CHIRAL PERTURBATION THEORY

The fundamental fact of low-energy QCD is that the approximate chiral symmetry (which would be exact if $m_q \rightarrow 0$) is dynamically broken with the pions, kaons, and η being the approximate Goldstone bosons. The interaction of these bosons is best described by an effective Lagrangian, which expands low-energy matrix elements in powers of the energy and quark masses. While there are many ways to present and parametrize this effective Lagrangian, we will follow the notation of Gasser and

Leutwyler [2].

Consider QCD coupled to external sources $l_\mu, r_\mu, s, p, \theta$,

$$\begin{aligned} \mathcal{L}_{\text{QCD}} = & -\frac{1}{4}F_{\mu\nu}^A F_{\mu\nu}^A + \bar{\psi} i \not{D} \psi - \bar{\psi}_L (s + ip) \psi_R \\ & - \bar{\psi}_R (s - ip) \psi_L + \frac{\theta \alpha_s}{8\pi} F_{\mu\nu}^A \tilde{F}^{A\mu\nu}, \\ iD_\mu = & i\partial_\mu + g \frac{t^A}{2} A_\mu^A + l_\mu \frac{(1+\gamma_5)}{2} + r_\mu \frac{(1-\gamma_5)}{2}, \quad (5) \\ \tilde{F}_{\mu\nu}^A = & \frac{1}{2} \epsilon_{\mu\nu\alpha\beta} F^{A\alpha\beta}. \end{aligned}$$

The sources l, r, p, s are matrices in the flavor space, and QCD without sources is reproduced with $s=m, p=l_\mu=r_\mu=0, \theta=\bar{\theta}$. This Lagrangian has an exact local chiral symmetry

$$\psi_L \rightarrow L(x)\psi_L, \quad \psi_R \rightarrow R(x)\psi_R \quad (6)$$

with L in $SU(3)_L$ and R in $SU(3)_R$, if we also transform the source fields

$$\begin{aligned} l_\mu & \rightarrow L(l_\mu - iL^\dagger \partial_\mu L)L^\dagger, \\ r_\mu & \rightarrow R(r_\mu - iR^\dagger \partial_\mu R)R^\dagger, \\ (s + ip) & \rightarrow L(s + ip)R^\dagger. \end{aligned} \quad (7)$$

The response of QCD to these sources is described by the functional

$$\begin{aligned} e^{iZ(l, r, s, p, \theta)} & = \int d\psi d\bar{\psi} dA_\mu \\ & \times \exp \left[i \int d^4x \mathcal{L}_{\text{QCD}}(\psi, A, l_\mu, r_\mu, s, p, \theta) \right]. \end{aligned} \quad (8)$$

This functional can also be described in terms of the physical particles of QCD, the hadrons. While this description is too complicated to be useful, in general, it simplifies at very low energy. This is because all of the heavy particles can be “integrated out” of the theory, as they cannot be excited at very low energy. Their effects appear in the renormalized parameters of the low-energy Lagrangian. Only the Goldstone bosons appear dynamically and must be explicitly included in the effective Lagrangian. One then writes the functional in terms of the sources and the low-energy particles

$$e^{iZ(l_\mu, r_\mu, s, p, \theta)} = \int dU \exp \left[i \int d^4x \mathcal{L}_{\text{eff}}(U, l_\mu, r_\mu, s, p, \theta) \right], \quad (9)$$

where U is an $SU(3)$ matrix field describing the Goldstone bosons. For the rest of this section we will set $\theta=0$, and will treat $\theta \neq 0$ in Sec. IV.

The effective Lagrangian has an infinite number of terms. However, it can be expanded in powers of the energy, E :

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_2 + \mathcal{L}_4 + \mathcal{L}_6 + \dots, \quad (10)$$

where \mathcal{L}_n produces matrix elements at order E^n . At low enough energy, only the first few \mathcal{L}_n are required. \mathcal{L}_2 yields the leading-order results, and corresponds to the

soft-pion predictions explored in the 1960's. In the past decade, the phenomenology at the next to leading order, \mathcal{L}_4 , has been studied.

The effective Lagrangian must share the chiral symmetry of Eq. (5). To lowest order this is accomplished by

$$\begin{aligned} \mathcal{L}_2 = & \frac{F^2}{4} \text{Tr}(D_\mu U D^\mu U^\dagger) + \frac{F^2}{4} \text{Tr}(\chi^\dagger U + U^\dagger \chi), \\ iD_\mu U \equiv & i\partial_\mu U + l_\mu U - U r_\mu, \quad (11) \\ \chi \equiv & 2B_0(s + ip). \end{aligned}$$

Here the matrix U has been chosen to transform as

$$U \rightarrow LUR^\dagger \quad (12)$$

under the chiral transformation. To describe the pseudoscalar mesons, ϕ^A , one expands

$$U = \exp \left[i \frac{\lambda^A \phi^A}{F_0} \right] = 1 + i \frac{\lambda^A \phi^A}{F_0} + \dots, \quad A = 1, 2, \dots, 8. \quad (13)$$

At leading order, the unknown parameters in this Lagrangian correspond to $F = F_0 = F_\pi = 92.4 \text{ MeV}$, and

$$F_\pi^2 B_0 = \frac{-\partial \mathcal{L}_{\text{eff}}}{\partial s^0} = -\langle 0 | \bar{\psi} \psi | 0 \rangle, \quad (14)$$

where $s = s^0 \mathbf{1} + s^A \lambda^A$. The meson masses are

$$\begin{aligned} m_\pi^2 & = (m_u + m_d) B_0, \\ m_{K^+}^2 & = (m_s + m_u) B_0, \\ m_{K^0}^2 & = (m_s + m_d) B_0, \\ m_{\eta_8}^2 & = \left(\frac{4}{3} m_s + \frac{2}{3} \hat{m} \right) B_0 = \frac{1}{3} (4m_K^2 - m_\pi^2). \end{aligned} \quad (15)$$

Note that in the QCD Lagrangian the quark mass enters only multiplied by $\bar{\psi} \psi$, i.e., $m \bar{\psi} \psi$. The mass itself is not a renormalization-group invariant, nor is $\bar{\psi} \psi$. In order to define a mass, one must specify how one renormalizes and defines $\bar{\psi} \psi$. In the effective Lagrangian, the mass always appears multiplied by B_0 , and, hence, one cannot separately identify the m_i but only the product $m_i B_0$. However, in ratios, B_0 cancels. We will also use the shorthand notation

$$\begin{aligned} M & = m B_0, \\ M_u & = m_u B_0, \\ \text{etc.} & , \end{aligned} \quad (16)$$

in this paper. Note that, since B_0 carries mass dimension of one, the parameters M are of dimension (meson mass)².

At order E^4 , the effective Lagrangian involves more terms whose coefficients must be determined phenomenologically. The possible combinations depending on the masses [2] are

$$\begin{aligned}
\mathcal{L}_4 = & \cdots + L_4 \text{Tr}(D_\mu U D^\mu U^\dagger) \text{Tr}(\chi^\dagger U + U^\dagger \chi) + L_5 \text{Tr}[D_\mu U D^\mu U^\dagger (\chi U^\dagger + U \chi^\dagger)] \\
& + L_6 [\text{Tr}(\chi U^\dagger + U \chi^\dagger)]^2 + L_7 [\text{Tr}(\chi U^\dagger - U \chi^\dagger)]^2 + L_8 \text{Tr}(\chi U^\dagger \chi U^\dagger + U \chi^\dagger U \chi^\dagger) \\
= & \cdots + 2L_4 \text{Tr}(D_\mu U D^\mu U^\dagger) \text{Tr}[M(U + U^\dagger)] + 2L_5 \text{Tr}[D_\mu U D^\mu U^\dagger (MU^\dagger + UM)] \\
& + 4L_6 \{\text{Tr}[M(U + U^\dagger)]\}^2 + 4L_7 \{\text{Tr}[M(U - U^\dagger)]\}^2 + 4L_8 \text{Tr}(MU^\dagger MU^\dagger + MUMU), \tag{17}
\end{aligned}$$

where L_i are dimensionless constants of order 10^{-3} . Other terms, not involving masses in the general $O(E^4)$ Lagrangian, are given in Ref. [2]. These terms parametrize all of the allowed ways by which the masses can influence physics at second order. Our general ignorance of the dynamics of low-energy QCD has been reduced to a few constants, L_i .

Phenomenologically, the terms proportional to L_4, L_5 influence the meson decay constants. In particular,

$$\frac{F_K}{F_\pi} = 1 + 4 \frac{L_5}{F^2} (m_K^2 - m_\pi^2), \quad F_\eta = F_K \left(\frac{F_K}{F_\pi} \right)^{1/3}, \quad \frac{F_{K^0}^2}{F_{K^+}^2} = 1 + \left(\frac{F_K^2}{F_\pi^2} - 1 \right) \left[\frac{m_d - m_u}{m_s - \hat{m}} \right]. \tag{18}$$

Formulas including one-loop quantum corrections are given in Ref. [2]. From F_K/F_π , one extracts $L_5^2(\mu = m_\eta) = (2.2 \pm 0.5) \times 10^{-3}$ and obtains $F_\eta/F_\pi = 1.3$, $F_{K^0}/F_{K^+} = 1.004$.

In addition, the formulas for the meson masses exhibit the expected character of an expansion in the quark masses. To write them, we have found it convenient to use effective masses M_i^* defined by

$$\begin{aligned}
M_u^* = & M_u \left[1 + 32 \frac{L_6}{F_\pi^2} (M_u + M_d + M_s) + 32 \frac{L_8}{F_\pi^2} M_u - 3\mu_\pi - 2\mu_{K^+} - \frac{1}{3}\mu_\eta + \frac{1}{2} \left(\frac{M_d - M_u}{M_s - \hat{M}} \right) (\mu_\mu - \mu_\pi) \right] \\
& + 32 \frac{L_7}{F_\pi^2} (M_u - M_d)(M_u - M_s), \\
M_d^* = & M_d \left[1 + 32 \frac{L_6}{F_\pi^2} (M_u + M_d + M_s) + 32 \frac{L_8}{F_\pi^2} M_d - 3\mu_\pi - 2\mu_{K^0} - \frac{1}{3}\mu_\eta - \frac{1}{2} \left(\frac{M_d - M_u}{M_s - \hat{M}} \right) (\mu_\eta - \mu_\pi) \right] \\
& + 32 \frac{L_7}{F_\pi^2} (M_d - M_u)(M_d - M_s), \\
M_s^* = & M_s \left[1 + 32 \frac{L_6}{F_\pi^2} (M_u + M_d + M_s) + 32 \frac{L_8}{F_\pi^2} M_s - 2\mu_{K^0} - 2\mu_{K^+} - \frac{4}{3}\mu_\eta \right] + 32 \frac{L_7}{F_\pi^2} (M_s - M_u)(M_s - M_d). \tag{19}
\end{aligned}$$

Here we have included one-loop chiral correction; all coefficients L_i are renormalized at a scale μ , and

$$\mu_i = \frac{m_i^2}{32\pi^2 F_\pi^2} \ln \frac{m_i^2}{\mu^2}. \tag{20}$$

These definitions are independent of the scale μ , and will be shown below to be reparametrization invariant. We now have

$$\begin{aligned}
F_\pi^2 m_\pi^2 &= F^2 [M_u^* + M_d^*], \\
F_K^2 + m_{K^+}^2 &= F^2 \{ [M_s^* + M_u^*] + \delta_{\text{GMO}}(m_K^2 - m_\pi^2) \}, \\
F_{K^0}^2 m_{K^0}^2 &= F^2 \{ [M_s^* + M_d^*] + \delta_{\text{GMO}}(m_K^2 - m_\pi^2) \}, \\
F_\eta^2 m_\eta^2 &= F^2 \left[\frac{4}{3} M_s^* + \frac{2}{3} \hat{M}^* \right], \tag{21}
\end{aligned}$$

where

$$\begin{aligned}
\delta_{\text{GMO}} &= \frac{4F_K^2 m_K^2 - 3F_\eta^2 m_\eta^2 - F_\pi^2 m_\pi^2}{4(F_K^2 m_K^2 - F_\pi^2 m_\pi^2)} \\
&= \frac{16}{F_\pi^2} (2L_7 + L_8) (m_\pi^2 - m_K^2) - \frac{3}{2}\mu_\pi + \mu_{K^+} + \frac{1}{2}\mu_\eta \\
&= -0.06. \tag{22}
\end{aligned}$$

In these expressions, we have dropped some extremely small terms in $(M_u - M_d)^2$. Writing the results in terms of $F_i^2 m_i^2$, instead of simply m_i^2 , is useful because it removes all dependence on the low-energy constants L_4, L_5 . Note that δ_{GMO} determines the combination $(2L_7 + L_8) = 0.2 \times 10^{-3}$ at $\mu = m_\eta$.

At this stage, the ambiguity mentioned in the Introduction can be seen [5]. The effective Lagrangian has been constructed using only chiral SU(3) symmetry as a constraint. However, χ and $\chi^{(\lambda)}$, defined by

$$\chi^{(\lambda)} = \chi + \lambda [\det \chi^\dagger] \chi (\chi^\dagger \chi)^{-1}, \tag{23}$$

where λ is an arbitrary constant, have the same symmetry transformation property

$$\begin{aligned}\chi &\rightarrow L\chi R^\dagger, \\ \chi^{(\lambda)} &\rightarrow L\chi^{(\lambda)}R^\dagger.\end{aligned}\quad (24)$$

In terms of the quark mass matrix m or $M = B_0 m$, Eq. (23) has the form

$$\begin{aligned}M^{(\lambda)} &= M + 2\lambda(\det M)M^{-1}, \\ m^{(\lambda)} &= m + \bar{\lambda}(\det m)m^{-1}\end{aligned}\quad (25)$$

with $\bar{\lambda} = 2B_0\lambda$. This means that, in constructing the effective Lagrangian, we could have used $\chi^{(\lambda)}$ everywhere that we used χ . Either choice is equally valid. The only difference is that the low-energy constants L_i have different values in the two cases. This can be seen through an identity for 3×3 matrices. Recall that the characteristic equation for a 3×3 matrix A is

$$\begin{aligned}\det(A - \lambda I) = 0 &= -\lambda^3 + \lambda^2 \text{Tr} A \\ &+ \frac{\lambda}{2} [\text{Tr}(A^2) - (\text{Tr} A)^2] + \det A.\end{aligned}\quad (26)$$

The Cayley-Hamilton theorem says that the matrix A also satisfies this relation, i.e.,

$$-A^3 + A^2 \text{Tr} A + \frac{A}{2} [\text{Tr}(A^2) - (\text{Tr} A)^2] + \det A = 0.\quad (27)$$

When applied to the matrix χ^\dagger , one has

$$\begin{aligned}[\det \chi^\dagger] \chi \frac{1}{\chi^\dagger \chi} &= [\det U \chi^\dagger] \chi \frac{1}{\chi^\dagger \chi} \\ &= U \chi^\dagger U \chi^\dagger U - \text{Tr}(U \chi^\dagger) U \chi^\dagger \\ &\quad - \frac{U}{2} \{ \text{Tr}(U \chi^\dagger U \chi^\dagger) - [\text{Tr}(U \chi^\dagger)]^2 \},\end{aligned}\quad (28)$$

where $\det U = 1$ has been used.² Thus, we have

$$\begin{aligned}\text{Tr}(\chi^{(\lambda)} U^\dagger) &= \text{Tr}(\chi U^\dagger) - \frac{\lambda}{2} \{ \text{Tr}(\chi^\dagger U \chi^\dagger U) - [\text{Tr}(U \chi^\dagger)]^2 \}, \\ \text{Tr}(\chi^{(\lambda)} U^\dagger) &= \text{Tr}(\chi^\dagger U) - \frac{\lambda}{2} \{ \text{Tr}(\chi U^\dagger \chi U^\dagger) - [\text{Tr}(\chi U^\dagger)]^2 \}.\end{aligned}\quad (29)$$

In the effective Lagrangian, the mass term becomes

$$\begin{aligned}\text{Tr}[M^{(\lambda)}(U + U^\dagger)] &= \text{Tr}[M(U + U^\dagger)] \\ &\quad - \lambda \text{Tr}(MUMU + MU^\dagger MU^\dagger) \\ &\quad + \frac{\lambda}{2} \{ \text{Tr}[M(U - U^\dagger)] \}^2 \\ &\quad + \frac{\lambda}{2} \text{Tr}[M(U + U^\dagger)]^2.\end{aligned}\quad (30)$$

The terms proportional to λ are of the same structure as some terms in \mathcal{L}_4 . Thus, the precise statement of the

Kaplan-Manohar ambiguity is that any phenomenology described by the mass matrix M and the low-energy coefficients $\{L_6, L_7, L_8\}$ can be equally well described by $M^{(\lambda)}$ and the coefficients $\{L_6 - \bar{\lambda}, L_7 - \bar{\lambda}, L_8 + 2\bar{\lambda}\}$ with $\bar{\lambda} \equiv F_\pi^2 \lambda / 16$. Since λ is an arbitrary parameter, this, in fact, corresponds to a continuous family of equivalent Lagrangians.

The meson masses displayed above exhibit the feature of being invariant under the reparametrization transformation, as can be readily verified with a slight algebraic effort. In fact, we have chosen the effective masses M_u^* , M_d^* , and M_s^* to each be invariant both under the reparametrization transformation and also under a change in scale μ in the chiral logs. The combination δ_{GMO} also exhibits these properties. These invariant masses M_i^* , which are different from the original masses, are the combinations which enter into observables.

In order to proceed, we really should have an evaluation of the electromagnetic splittings of K^+ and K^0 valid to second order in the masses. Unfortunately, this analysis does not yet exist. In order to illustrate the effect of the reparametrization ambiguity, we follow Ref. [2] and proceed by continuing to use Dashen's theorem to estimate the electromagnetic contribution. This yields

$$\frac{\hat{M}^*}{M_s^*} = \frac{F_\pi^2 m_\pi^2}{2F_K^2 m_K^2 - F_\pi^2 m_\pi^2 + \frac{1}{2} \rho_{\text{GMO}} F_K^2 (m_K^2 - m_\pi^2)} = \frac{1}{37},\quad (31)$$

$$\frac{M_d^* - M_u^*}{M_d^* + M_u^*} = \left[\frac{F_{K^0}^2 m_{K^0}^2 - F_{K^+}^2 m_{K^+}^2}{F_\pi^2 m_\pi^2} \right]_{\text{QCD}} = 0.57.$$

The invariant masses are fixed, but because of the reparametrization transformation, there is a continuous family of input quark masses which can generate a given M_i^* . This means that several different parameter sets may represent the data. For example, the values of Refs. [2,7]

$$\begin{aligned}\frac{m_u}{m_s} &= \frac{1}{34}, \quad \frac{m_d}{m_s} = \frac{1}{19}, \\ L_7 &= -0.4 \times 10^{-3}, \quad L_8 = 1.1 \times 10^{-3},\end{aligned}\quad (32)$$

yields a mass matrix which differs very little from the lowest-order ratios of Eq. (1). However, by using the reparametrization transformation with $\lambda = -1.15$, we may obtain a set with $m_u = 0$

$$\begin{aligned}\frac{m_u}{m_s} &= 0, \quad \frac{m_d}{m_s} = \frac{1}{26}, \\ L_7 &= 0.2 \times 10^{-3}, \quad L_8 = -0.1 \times 10^{-3}.\end{aligned}\quad (33)$$

Alternatively, we could increase the size of \hat{m}/m_s by 30% using $\lambda = +0.6$, resulting in

$$\begin{aligned}\frac{m_u}{m_s} &= \frac{1}{22}, \quad \frac{m_d}{m_s} = \frac{1}{16}, \\ L_7 &= -0.8 \times 10^{-3}, \quad L_8 = 1.9 \times 10^{-3},\end{aligned}\quad (34)$$

which might be useful in the phenomenology of the σ

²Note that this form makes it clear that the factors of $\chi^\dagger \chi$ in the denominator are harmless and do not introduce any singularities as $\chi \rightarrow 0$.

term [3]. Note that the m_d/m_s is rather stable, but it is easy to shift m_u/m_s by significant amounts.

The parameter sets defined in Eqs. (32)–(34) are equivalent. There is nothing intrinsic to the sets that would suggest that one is superior to the other. Others might be tempted to question the second set with $m_u=0$, arguing that a 100% shift in m_u from lowest order to second order represents a breakdown of chiral perturbation theory. However, this is misleading and we would like to explain it in some detail. It is natural that the smallest parameter in the theory receive the largest percentage shift, and the shift in m_u is not any larger than could be expected. We would claim that the expected shift from a second-order analysis of m_u should be of the size

$$\Delta m_u = a m_d \frac{m_K^2}{\Lambda^2}, \quad (35)$$

where Λ is some measure of the chiral scale and a is a number of order unity. This occurs because it is a chiral $SU(3)$ analysis that separates m_u, m_d from \hat{m} , and, hence, the extracted values receive corrections of order m_K^2/Λ^2 . Since, in many applications, the expansion scale is $\Lambda \sim m_\rho$ or $\Lambda \sim 1$ GeV, and $m_d \approx 2m_u$ at lowest order, we naturally expect $\Delta m_u \approx (\frac{1}{4} \rightarrow \frac{1}{2}) m_d \approx O(m_u)$. In fact, we could make the case for the expected size of the shift in m_u more explicitly by setting $L_6=L_7=L_8=0$ in the formulas for the masses and only retaining the *known* lowest $SU(3)$ breaking in $F_K=1.22F_\pi$. In this case we have

$$\begin{aligned} \frac{m_u}{m_s + \hat{m}} &= \frac{1}{2} \left[\frac{F_\pi^2 m_\pi^2}{F_K^2 m_K^2} - \frac{(F_{K^0}^2 m_{K^0}^2 - F_K^2 + m_K^2)_{\text{QCD}}}{F_K^2 m_K^2} \right] \\ &\approx \left[\frac{m_u}{m_s + \hat{m}} \right]_{\text{lowest order}} \\ &\quad - \left[\frac{F_K^2}{F_\pi^2} - 1 \right] \left[\frac{m_d}{m_s + m_d} \right]_{\text{lowest order}}, \quad (36) \end{aligned}$$

where the lowest-order result is obtained by setting all the F_i equal to each other. Equation (31) corresponds to a shift in the measurement of the up-quark mass

$$\begin{aligned} \Delta m_u &= - \left[\frac{F_K^2}{F_\pi^2} - 1 \right] (m_d)_{\text{lowest order}} \\ &\approx -0.88 (m_u)_{\text{lowest order}}. \quad (37) \end{aligned}$$

A change in m_u of this size is as natural as in $F_K/F_\pi=1.22$, and, indeed, to obtain a small shift one must adjust L_7, L_8 to cancel off this known effect. The $m_u=0$ set, in fact, has the smallest values of L_7, L_8 .

One *can* define a criterion that describes the naturalness of a given second-order analysis. The natural size of the L_1 is few $\times 10^{-3}$. For example, the largest of the known values are $L_9=7.4 \times 10^{-3}$, $L_{10}=-6.0 \times 10^{-3}$, $L_3=-3.06 \times 10^{-3}$, $L_5=2.2 \times 10^{-3}$. If a mass matrix $m^{(\lambda)}$ was to require L_6, L_7, L_8 larger than these, then it could be considered as a unnatural choice. However, none of our examples contradict this criterion.

We would also like to argue that the reparametrization invariance is a feature of *all* known physical observables when one uses only chiral $SU(3)$ symmetry. One might hope that, by leaving the purely Goldstone-boson sector and using baryons or other mesons, the quark masses could be determined without reference to this problem. However, as long as we only employ chiral $SU(3)$ invariance, there is an equivalent reparametrization invariance in the other sectors also. As an example, consider η_8 - η_0 mixing. The coupling of η_0 and η_8 is driven by the quark mass difference and can be described by an effective Lagrangian

$$\begin{aligned} \mathcal{L}_{\eta\eta'} &= i\eta_0 [\alpha \text{Tr}[M(U-U^\dagger)] \\ &\quad + \beta_1 \text{Tr}[M(U-U^\dagger)] \text{Tr}[M(U+U^\dagger)] \\ &\quad + \beta_2 \text{Tr}(MUMU - MU^\dagger MU^\dagger) \cdots]. \quad (38) \end{aligned}$$

Here η_0 does not occur in the chiral matrix, but appears as an unrelated matter field. We included terms at both order E^2 and E^4 , and α, β_1, β_2 are constants. There is also a reparametrization invariance of $\mathcal{L}_{\eta\eta'}$ associated with the redefinition of the masses. Using previous identities we find

$$\begin{aligned} \text{Tr}[M^{(\lambda)}(U-U^\dagger)] &= \text{Tr}[M(U-U^\dagger)] \\ &\quad + \lambda \text{Tr}(MUMU - MU^\dagger MU^\dagger) \\ &\quad + \lambda \text{Tr}[M(U-U^\dagger)] \\ &\quad \times \text{Tr}[M(U+U^\dagger)]. \quad (39) \end{aligned}$$

Thus, any physics described by the mass matrix M and the low-energy constants $\{\alpha, \beta_1, \beta_2\}$ can be equally well described by $M^{(\lambda)}$ plus the set $\{\alpha, \beta_1 + \lambda\alpha, \beta_2 - \lambda\alpha\}$. The $\eta\eta'$ mixing element demonstrates this invariance and the experimental $\eta\eta'$ mixing angle is compatible with any of the quark mass matrices $m^{(\lambda)}$.

Similar discussions can be given for baryon matrix elements or for transitions involving other mesons (such as ρ - ω mixing). In each case, there can be derived exact identities involving effective Lagrangian such that the difference between using M or $M^{(\lambda)}$ (for any λ) will only amount to a change in the coefficients of higher-order effective Lagrangians. Unfortunately, most other systems have been treated at lowest order only, so that information from them is not phenomenologically useful at next order. The lowest-order analyses are summarized in Appendix A. That lowest-order estimates are consistent does not imply that higher-order corrections are absent, but only that the corrections, if present, are similar in different systems. In practice, however, the lowest-order analyses are sufficiently varied to allow for sizable second-order corrections.

Leutwyler [7] has attempted to resolve the quark mass ambiguity by consideration of $\eta\eta'$ mixing. He uses a sum rule of pseudoscalar bilinears together with assumptions of single-particle saturation to argue that L_7 is dominated by $\eta\eta'$ mixing. Then the phenomenological value for the η - η' mixing angle, analyzed with $\beta_1=\beta_2=0$ in Eq. (38), suggests the numerical value for L_7 given in Eq. (32). With the further input of the lowest-order elec-

tromagnetic $K^+ - K^0$ mass splitting, this reproduces the quark mass ratios quoted in Eq. (32). The assumptions of single-particle saturation and lowest-order electromagnetic splitting are aspects that fall into the model-dependent category. Although not unreasonable, they are not guaranteed to be correct. For example, all of our experience of single-particle saturation comes from phenomenology which is invariant under the reparametrization transformation. However, since L_7 changes under this transformation, a new set of issues arises when one applies single-particle saturation, such as which of the mass bases $M^{(\lambda)}$ best corresponds to our experience of $\eta - \eta'$ mixing (with $\beta_1 = \beta_2 = 0$) and whether there are new contributions to the sum rule.

III. REPARAMETRIZATION INVARIANCE AS A REGULARIZATION AMBIGUITY

Is the reparametrization ambiguity only an algebraic nuisance, a curiosity of effective Lagrangians which keeps us from getting a handle on quark masses? One cannot doubt the algebraic fact that this ambiguity exists, but we would like to argue that it may represent a similar ambiguity in the definition of renormalized mass in QCD. At lowest order one does not need to carefully specify the renormalization procedure for quark masses, as any dependence on it cancels in the ratio of masses. However, at second order one must proceed more carefully, and different methods of regularization and renormalization can lead to different masses.

Let us motivate the result by symmetry arguments. Consider first the limit when $m_u = m_d = 0$, but $m_s \neq 0$. Such a theory has an exact chiral SU(2) invariance, and although quantum effects may shift m_s , they cannot change the result $m_u = m_d = 0$. The masslessness of u and d has been protected by the chiral SU(2) symmetry. (Similarly, in a world with $m_u = m_s = 0$, both u and s would remain massless.) Now consider the case $m_u = 0$ but $m_d \neq 0$, $m_s \neq 0$. The chiral SU(2) symmetry has been broken by having $m_d \neq 0$. The vacuum fields of QCD do not exhibit a $U(1)_A$ invariance, and hence, an up quark moving in the QCD vacuum is not protected from acquiring a mass. However, the structure of the mass is restricted by the symmetries. It must vanish in the limit $m_d \rightarrow 0$ or in the limit $m_s \rightarrow 0$ because of the chiral SU(2) invariance of those limits. Hence, a nonzero m_u must have the form

$$\Delta m_u = \bar{\lambda} m_d m_s \quad (40)$$

for some $\bar{\lambda}$. If we now generalize to all of m_u, m_d, m_s being nonzero, we see from the permutation symmetry that, to this order in the masses, each quark must get a mass shift

$$\begin{aligned} \Delta m_d &= \bar{\lambda} m_u m_s, \\ \Delta m_s &= \bar{\lambda} m_u m_d. \end{aligned} \quad (41)$$

This, of course, is of the same form as the reparametriza-

tion transformation.

We can see now that the Kim, Choi, and Sze calculation mentioned in the Introduction [9] is a specific example of the use of quantum effects to shift the quark masses. While we need not seriously take the specific value of the constant $\bar{\lambda}$ found in an instanton gas (with a particular size cutoff), we see that the effect is more general than the specific calculation. It appears to reflect a form of mass renormalization allowed by the symmetries of QCD.

This raises the issue of the dependence of the mass on the renormalization scheme used. Even if we were able to solve QCD, we would need a procedure for defining a renormalized mass parameter and then expressing observables in terms of that parameter. Such a procedure is not unique, and differing definitions of mass may emerge. If one chooses to renormalize quark masses at a high energy (say M_W for example), the instanton effect of Kim, Choi, and Sze would not be important, and one would obtain the multiplicative mass renormalization of perturbation theory. However, if one chose instead to renormalize at a lower-energy scale, the mass-mixing effects of Eq. (25) could be included in the renormalized mass. Other schemes are also possible. Hence, the masses of any two schemes would be related by a finite renormalization, e.g.,

$$[m_u^{\text{ren}}]_{\text{scheme 2}} = [Z m_u^{\text{ren}} + \bar{\lambda} m_d^{\text{ren}} m_s^{\text{ren}}]_{\text{scheme 1}}, \quad \text{etc.} \quad (42)$$

In order for physical observables to remain invariant, one also needs a corresponding change in the low-energy constants calculated in the two schemes

$$[L_6]_{\text{scheme 2}} = [Z_6 L_6 - \lambda]_{\text{scheme 1}}. \quad (43)$$

Note that, while a high-energy scale may seem conceptually simplest for the discussion of mass, since one would then use QCD perturbation theory, it is not well suited for the calculation of the low-energy constants L_i . The complete calculation requires both the renormalized masses and the low-energy constants, and, hence, must include low-energy effects. Note, however, that all schemes must agree on the invariant masses M_i^* given in Eq. (19).

A full calculation is specified by renormalized masses $\{m_u, m_d, m_s\}$ and low-energy constants $\{L_6, L_7, L_8\}$ (plus other low-energy constants for other systems). Due to the scheme dependence, different sets of masses and low-energy constants are possible in different regularization and renormalization schemes. However, the underlying chiral symmetry requires that these differences be of the form of Eq. (19) in order to keep observables invariant. This result is similar to that which occurs with the QCD coupling constant, where the magnitude of the scale parameter Λ depends on the details of the regularization scheme, yet physical results are invariant to a given order in perturbation theory.

One might argue that the external-field formalism removes the need for this ambiguity. One defines the external field $\chi(x)$ and varies it to probe the response of the

system, determining L_6, L_7, L_8 and hence the masses. However, the use of an external field does not remove the need for a renormalization and regularization. The field χ is not a purely classical parameter. Since it couples to a bilinear that needs to be renormalized ($\bar{\psi}\psi$), the process of defining renormalized scalar densities can lead to changes in the definition of χ as in Eq. (23). An explicit example is again given by the calculational procedure of Kim, Choi, and Sze. If one considers the diagram of Fig. 1, one sees that the operators $\{\bar{u}u, \bar{d}d, \bar{s}s\}$ need not be multiplicatively renormalized, with the picture describing the mixing of $\bar{u}u$ and $\bar{d}d$. One needs to specify the renormalization procedure for $\bar{u}u$ in order to decide which component of the matrix field χ couples to $\bar{u}u$.

The issues raised above make it clear that the problem of defining a mass cannot be solved through present models such as quark models or even present versions of QCD sum rules. Masslike parameters enter these models, but the theories lack sufficient control over the dynamics of QCD to be able to precisely define a full regularization scheme based on the QCD Lagrangian mass parameters.

IV. EFFECTIVE LAGRANGIANS CONTAINING θ AND $U(1)_A$ TRANSFORMATIONS

The discussion thus far ignores the possibility of using axial $U(1)$ symmetry in the determination of quark masses. Recall that $U(1)_A$ is an approximate symmetry of the classical Lagrangian which has an anomaly [12] and which is not a symmetry of the vacuum state of QCD [13]. There are, however, anomalous Ward identities which involve the quark masses [14]. In particular, there is no strong CP violation if, in some definition, m_u vanishes [8,15]. In this section, we explore the content of the anomalous Ward identities and will argue that the strong CP -violating sector of the theory allows one, in principle, to identify a special mass matrix out of the set $m^{(\lambda)}$ which deserves to be called “the” mass matrix of QCD.

The $U(1)_A$ Noether current is not conserved even for vanishing quark mass, i.e.,

$$i\partial^\mu J_{5\mu}^{(0)} = \frac{3\alpha_s}{8\pi} F\tilde{F} + 2m_u \bar{u}\gamma_5 u + 2m_d \bar{d}\gamma_5 d + 2m_s \bar{s}\gamma_5 s. \quad (44)$$

However, because $F\tilde{F}$ is a total divergence,

$$F\tilde{F} = \partial_\mu K^\mu, \quad (45)$$

$$K_\mu = 2\epsilon^{\mu\nu\lambda\sigma} A_\lambda^a \left[F_{\lambda\sigma}^a - \frac{g}{6} F^{abc} A_\lambda^b A_\sigma^c \right],$$

there is a gauge-variant current

$$\tilde{J}_{5\mu} = J_{5\mu}^{(0)} - K_\mu, \quad (46)$$

which would be conserved if quark masses vanished. It is this current which would generate $U(1)_A$ symmetry transformations in the chiral limit. Because K^μ is related to the topological charge, a chiral rotation with the charge \tilde{Q}_5 will shift the θ vacuum of QCD with

$$e^{i\alpha\tilde{Q}_5}|\theta\rangle = |\theta - 6\alpha\rangle. \quad (47)$$

One can always then shift to the $\theta=0$ vacuum by such a rotation, but if the quark masses are nonzero, the rotation will generate a CP -violating phase in the quark mass matrix.

In order to probe the behavior of the chiral Lagrangian under $U(1)_A$ transformations, we include a θ source term in the QCD Lagrangian

$$\mathcal{L} = \mathcal{L}_{\text{QCD}}^{(0)} + \frac{\theta\alpha_s}{8\pi} F_{\mu\nu}^A \tilde{F}^{A\mu\nu}. \quad (48)$$

In the basis where the quark mass matrix is diagonal, QCD without sources is characterized by vacuum angle $\theta(x) = \bar{\theta}$. The method for adding θ to the chiral Lagrangian at order E^2 , both with and without an extra singlet field ϕ_0 in the chiral matrix U , has been given by Gasser and Leutwyler [2]. Including only the eight Goldstone fields, they obtain

$$\mathcal{L}_2 = \frac{F^2}{4} \text{Tr}(D_\mu U D^\mu U^\dagger) + \frac{F^2}{4} \text{Tr}(\tilde{\chi} U^\dagger + U \tilde{\chi}^\dagger) + \frac{\tilde{H}_0}{12} D_\mu \theta D^\mu \theta. \quad (49)$$

Here the new ingredients are contained in the definitions

$$\tilde{\chi} \equiv \chi e^{i\bar{\theta}/3}, \quad (50)$$

$$D_\mu \theta = \partial_\mu \theta + 2 \text{Tr} a_\mu,$$

and \tilde{H}_0 is a constant. Aside from the contact term $D_\mu \theta D^\mu \theta$, which has no meson matrix elements, the θ dependence is entirely contained in the source term $\tilde{\chi}$, which is invariant under global $U(1)_A$ transformations

$$\chi \rightarrow e^{i\alpha} \chi e^{i\alpha}, \quad \theta \rightarrow \theta - 6\alpha. \quad (51)$$

If the external sources are set equal to zero, we recover the mass term of QCD

$$\tilde{\chi} \rightarrow 2B_0 m e^{i\bar{\theta}/3}. \quad (52)$$

Variation of this Lagrangian with respect to θ reproduces the anomalous Ward identities involving the Goldstone fields. The Lagrangian of Gasser and Leutwyler containing an $SU(3)$ singlet field is given in Appendix B, where it is also generalized to order E^4 . Below we concentrate on the generalization of Eq. (49) since the inclusion of the singlet field is not needed for our purposes.

The order- E^4 Lagrangian containing θ will involve two distinct classes of operators

$$\mathcal{L}_4 = \mathcal{L}_4^{(\tilde{\chi})} + \mathcal{L}_4^{(D\theta)}. \quad (53)$$

In $\mathcal{L}_4^{(\tilde{\chi})}$ are the operators of the usual chiral Lagrangian, governed by the low-energy constants L_1, \dots, L_{10} , written with $\tilde{\chi}$ in place of χ . New operators involving derivatives of θ are contained in $\mathcal{L}_4^{(D\theta)}$. We find that these are

$$\begin{aligned} \mathcal{L}_4^{(D\theta)} = & iL_{14}D_\mu D^\mu \theta \text{Tr}(\tilde{\chi}^\dagger U - U^\dagger \tilde{\chi}) + iL_{15}D_\mu \theta \text{Tr}[(D^\mu \tilde{\chi}^\dagger)U - (D^\mu \tilde{\chi})U^\dagger] + L_{16}D_\mu \theta D^\mu \theta \text{Tr}(D_\nu U D^\nu U^\dagger) \\ & + L_{17}D_\mu \theta D_\nu \theta \text{Tr}(D^\mu U D^\nu U^\dagger) + L_{18}D_\mu \theta D^\mu \theta \text{Tr}(\tilde{\chi}U^\dagger + U\tilde{\chi}^\dagger) + H_6(D_\mu \theta D^\mu \theta)^2. \end{aligned} \quad (54)$$

The numbering scheme starts at L_{14} to accommodate recent work on the chiral energy-momentum tensor [17] which introduced operators characterized by low-energy constants L_{11}, L_{12}, L_{13} . Factors involving derivatives of θ are automatically invariant under global $U(1)_A$ transformations. Note that when $\theta = \bar{\theta} = \text{const}$, these new terms disappear. When $\chi = 2B_0 m$, only the first operator listed is linear in θ , and this one will be relevant in our analysis.

The original reparametrization transformation is not an invariance of $\mathcal{L}_4^{(\tilde{\chi})}$. This is because the reparametrization transformation does not respect the anomalous $U(1)_A$ behavior of the theory. Therefore, the θ dependence may be used to probe the quark masses in a way that overcomes the reparametrization ambiguity. We will utilize this in the next section. Another way to see this is to note that there exists a modified, reparametrization transformation

$$\chi \rightarrow \chi + \lambda [\det \chi^\dagger] \chi \frac{1}{\chi^\dagger \chi} e^{-i\theta} \quad (55)$$

with $L_{6,7,8}$ transforming as before.

Despite the fact that there is a modified reparametrization transformation, there is a way to single out a special quark mass matrix. The transformation of Eq. (55) involves the complex phase $e^{i\theta}$. For nonzero θ , if one starts with a real mass matrix M , the resulting $M^{(\lambda)}$ will be complex. Thus, while there exists a set of parameters with $\lambda \neq 0$ to reproduce experimental results, one does so only at the expense of a complex mass matrix. One can pick out “the” mass matrix of QCD as the only member of the family $M^{(\lambda)}$ which is purely real.

The θ dependence then provides a means to determine the correct mass matrix, at least in principle, since the terms proportional to θ are not invariant any more. The effective Lagrangian can be expanded in terms of θ , i.e., $\mathcal{L} = \mathcal{L}_0 + \theta(\partial\mathcal{L}/\partial\theta) + \dots$. Here the first term, without any factors of θ , has the original reparametrization invariance, but the θ -dependent terms are not invariant. If one is studying strong CP violation, one measures accurately a large number of CP -violating and CP -conserving processes and finds that they can be fit with a real mass matrix only for a given set of parameters. Of course, this program is impractical. In the next section, we will provide a more realistic alternative treating θ as an external source field.

The instanton-gas calculation of Kim, Choi, and Sze, in fact, already suggests that when $\theta \neq 0$, the reparametrization transformation is that of Eq. (55). The $e^{-i\theta}$ factor arose because the mass-generation mechanism involved an instanton connecting topological sectors in the θ vacuum. The agreement of that result with the effective-Lagrangian analysis is striking, but, of course, not surprising.

The possibility of defining a unique mass matrix governing $U(1)_A$ transformations does not invalidate the various mass matrices discussed in Sec. II. More than one definition of mass is possible. The θ dependence probes what might be called “ $U(1)_A$ current masses,” the vanishing of which allows the removal of effects of θ . However, the family $m^{(\lambda)}$ could all be called good “ $SU(3)$ current masses,” as they all equally well govern the chiral $SU(3)$ currents. They clearly are current masses in the usual sense, but may be generated by $U(1)_A$ violating fields in the QCD vacuum, leading to a difference from the $U(1)_A$ current masses.

V. USING THE ANOMALY TO MEASURE QUARK MASSES

The parameter θ in the effective Lagrangian can be used in two different ways. If the true ground state of QCD is specified by some $\theta = \bar{\theta} \neq 0$, there will be strong CP violation. CP odd matrix elements can be found by setting $\theta = \bar{\theta}$ in the Lagrangian, finding the ground-state solution, and calculating the amplitudes containing odd powers of $\bar{\theta}$. On the other hand, even if $\bar{\theta} = 0$, one can use θ as an external source which lets one calculate matrix elements of $F\tilde{F}$, using

$$\frac{\partial \mathcal{L}_{\text{QCD}}}{\partial \theta} = \frac{\alpha_s}{8\pi} F_{\mu\nu}^A \tilde{F}^{A\mu\nu}. \quad (56)$$

Thus, in this usage, matrix elements of $F\tilde{F}$ are found from the θ dependence of the effective Lagrangian. We can probe the $U(1)_A$ behavior through matrix elements of $F\tilde{F}$. In this section we will calculate the low-energy theorems for $F\tilde{F}$ to order E^4 , and show how they can be used to measure the quark mass in $\psi' \rightarrow J/\psi + \pi^0(\eta^0, 3\pi)$.

Before describing the technical details, we would like to comment on why this procedure can overcome the reparametrization ambiguity. The basic point is that, while the mass term $\bar{\psi}m\psi$ can be renormalized by the instanton effects, the operator $F\tilde{F}$ is not itself modified. It remains the operator which probes the θ dependence of the theory. There can be various definitions of the quark mass parameters which enter phenomenology, but the θ dependence probes the fundamental definition of mass. The matrix element of $F\tilde{F}$ measures the $U(1)_A$ dependence, for which the reparametrization transformation is not valid.

Let us first calculate the π^0 and η^0 matrix elements of $F\tilde{F}$ at low energy. We define the shorthand notation

$$F\tilde{F} \equiv \frac{\alpha_s}{8\pi} F_{\mu\nu}^A \tilde{F}^{A\mu\nu}. \quad (57)$$

From Eqs. (11), (17), and (60), the effective-Lagrangian realization of this operator is

$$\begin{aligned}
F\tilde{F} = i & \left[\frac{F^2}{4} \text{Tr}(\chi U^\dagger - U\chi^\dagger) + L_4 \text{Tr}(D_\mu U D^\mu U^\dagger) \text{Tr}(\chi U^\dagger - U\chi^\dagger) + L_5 \text{Tr}[D_\mu U D^\mu U^\dagger (\chi U^\dagger - U\chi^\dagger)] \right. \\
& + 2(L_6 + L_7) \text{Tr}(\chi U^\dagger + U\chi^\dagger) \text{Tr}(\chi U^\dagger - U\chi^\dagger) + 2L_8 \text{Tr}(\chi U^\dagger \chi U^\dagger - U\chi^\dagger U\chi^\dagger) \\
& \left. - L_{14} \square \text{Tr}(\chi U^\dagger - U\chi^\dagger) - L_{15} \partial^\mu \text{Tr}(D_\mu \chi^\dagger U - U^\dagger D_\mu \chi) \right]. \tag{58}
\end{aligned}$$

When $\chi = 2B_0 m$, the last term will not contribute and may be dropped.

In calculating quantum corrections at one loop, there is a slight subtlety. In the loop diagrams, one should use the particles of definite mass in order to have a diagonal propagator [2]. In chiral perturbation theory only, \mathcal{L}_2 is used in one-loop diagrams. The appropriate basis including η - π^0 mixing is

$$\begin{aligned}
\pi_{(2)}^0 &= \phi^3 + \varepsilon \phi^8, \\
\eta_{(2)} &= \phi^8 - \varepsilon \phi^3, \\
\varepsilon &= \frac{\sqrt{3}}{4} \left[\frac{M_u - M_d}{\hat{M} - M_s} \right].
\end{aligned} \tag{59}$$

The subscript (2) indicates that these are only field definitions appropriate to \mathcal{L}_2 , and that further mixing will take place at $\mathcal{O}(E^4)$. From this starting point, the quantum corrections are straightforward. We drop effects of order $(M_u - M_d)^2$. After wave-function and mass renormalization, the one-loop effective Lagrangian for the π^0 and η mesons is

$$\mathcal{L} = \frac{1}{2} (\partial_\mu \pi_{(2)}^0)^2 + \frac{1}{2} (\partial_\mu \eta_{(2)})^2 + Z_{\pi\eta} \partial_\mu \pi_{(2)} \partial^\mu \eta_{(2)} - \frac{1}{2} m_\pi^2 \pi_{(2)}^2 - \frac{1}{2} m_\eta^2 \eta_{(2)}^2 - m_{\pi\eta}^2 \pi_{(2)}^0 \eta_{(2)} + (A_\pi^{(0)} \pi_{(2)}^0 + A_\eta^{(0)} \eta) \theta + \dots \tag{60}$$

with

$$\begin{aligned}
Z_{\pi\eta} &= \sqrt{3} (M_u - M_d) \left[\frac{\mu_K^- - \mu_\pi}{M_s - \hat{M}} - \frac{\mu_{K^0} - \mu_{K^+}}{M_d - M_u} \right], \\
m_{\pi\eta}^2 &= \frac{M_u - M_d}{\sqrt{3}} \left[\frac{32}{F^2} (L_8 + 3L_7) (\hat{M} - M_s) - (3\mu_\pi - 2\mu_K - \mu_\eta) - 2\hat{M} \left[\frac{\mu_{K^+} - \mu_{K^0}}{M_u - M_d} - \frac{\mu_\pi - \mu_K}{\hat{M} - M_s} \right] \right], \\
A_\pi^{(0)} &= \frac{3}{2} \frac{F^2}{F_\pi} (M_u - M_d) \left[1 + \frac{32}{F^2} (L_6 + L_7) (2\hat{M} + M_s) + \frac{32}{3} \frac{L_8}{F^2} (5\hat{M} + M_s) - 2(\mu_\pi + \frac{4}{3}\mu_K + \frac{1}{3}\mu_\eta) \right. \\
&\quad \left. - \frac{4}{3} \hat{M} \left[\frac{\mu_{K^+} - \mu_{K^0}}{M_u - M_d} + \frac{1}{4} \frac{(5\mu_\pi - 2\mu_K - 3\mu_\eta)}{\hat{M} - M_s} \right] \right], \\
A_\eta^{(0)} &= \frac{2F^2}{\sqrt{3}F_\eta} (\hat{M} - M_s) \left[1 + \frac{32}{F^2} (L_6 + L_7) (2\hat{M} + M_s) + \frac{32L_8}{F^2} (\hat{M} + M_s) - 4\mu_K - \frac{4}{3}\mu_\eta - \hat{M} \frac{(3\mu_\pi - 2\mu_K - \mu_\eta)}{\hat{M} - M_s} \right].
\end{aligned} \tag{61}$$

This is diagonalized by a further field redefinition

$$\begin{aligned}
\pi^0 &= \pi_{(2)}^0 + s_\pi \eta_{(2)}, \\
\eta &= \eta_{(2)} - s_\eta \pi_{(2)}^0, \\
s_\pi &= \frac{m_{\pi\eta}^2 - Z_{\eta\pi} m_\eta^2}{m_\pi^2 - m_\eta^2}, \\
s_\eta &= \frac{m_{\pi\eta}^2 - Z_{\eta\pi} m_\pi^2}{m_\pi^2 - m_\eta^2}.
\end{aligned} \tag{62}$$

For these fields, the anomaly matrix elements are

$$\begin{aligned} \langle 0|F\tilde{F}|\pi^0\rangle = \frac{3}{2} \frac{F^2}{F_\pi} (M_u - M_d) & \left[1 + \frac{32}{F_\pi^2} (L_6 + M_7)(2\hat{M} + M_s) + \frac{64L_8}{F_\pi^2} \hat{M} + \frac{4L_{14}}{F^2} m_\pi^2 \right. \\ & \left. + \frac{32L_7}{F_\pi^2} (\hat{M} - M_s) - (3\mu_\pi + 2\mu_K + \frac{1}{3}\mu_\eta) - \hat{M} \frac{(3\mu_\pi - 2\mu_K - \mu_\eta)}{\hat{M} - M_s} \right], \end{aligned} \quad (63)$$

$$\begin{aligned} \langle 0|F\tilde{F}|\eta\rangle = \frac{2F^2}{\sqrt{3}F_\eta} (\hat{M} - M_s) & \left[1 + \frac{32}{F_\pi^2} (L_6 + L_7)(2\hat{M} + M_s) + \frac{32L_8}{F_\pi^2} (\hat{M} + M_s) + \frac{4L_{14}}{F^2} m_\eta^2 \right. \\ & \left. - 4\mu_K - \frac{4}{2}\mu_\eta - \hat{M} \frac{(3\mu_\pi - 2\mu_K - \mu_\eta)}{\hat{M} - M_s} \right]. \end{aligned}$$

Most of the higher-order corrections are the same in both the matrix elements, such that the ratio is

$$\begin{aligned} r_{F\tilde{F}} &= \frac{\langle 0|F\tilde{F}|\pi^0\rangle}{\langle 0|F\tilde{F}|\eta\rangle} \\ &= \frac{3\sqrt{3}}{4} \left[\frac{m_d - m_u}{m_s - \hat{m}} \right] \frac{F_\eta}{F_\pi} \left[1 - \frac{32}{F^2} (M_s - \hat{M})(L_7 + L_8) \right. \\ & \quad \left. + \frac{4L_{14}}{F^2} (m_\pi^2 - m_\eta^2) - (3\mu_\pi - 2\mu_K - \mu_\eta) \right]. \end{aligned} \quad (64)$$

As expected, these results are not reparametrization invariant because the matrix element is related to the θ dependence. The first term in this matrix element ratio was originally calculated in Ref. [18]. We have therefore extended the results to $O(E^4)$.

There is a set of amplitudes which will yield $(m_d - m_u)/(m_d + m_u)$ in an almost parameter-free manner. This emerges from a combination of Eqs. (21), (22), and (64). Remarkably, all of the chiral logarithms disappear, as does all but one of the low-energy constants, and we find

$$\begin{aligned} \frac{m_d - m_u}{m_d + m_u} \frac{m_s + \hat{m}}{m_s - \hat{m}} &= \frac{4(F_K^2 m_K^2 - F_\pi^2 m_\pi^2)}{3\sqrt{3}F_\pi^2 m_\pi^2} \frac{F_\pi}{F_\eta} \frac{\langle 0|F\tilde{F}|\pi^0\rangle}{\langle 0|F\tilde{F}|\eta\rangle} \\ & \times [1 - \delta_{\text{GMO}}] \left[1 + \frac{4L_{14}}{F_\pi^2} (m_\eta^2 - m_\pi^2) \right] \end{aligned} \quad (65)$$

valid to $O(E^4)$ in the chiral expansion.

The presence of the new low-energy constant L_{14} prevents this from being completely determined. However, this parameter can, in principle, be extracted from the 3π matrix element of $F\tilde{F}$. We find that

$$\begin{aligned} \frac{\langle \pi^+ \pi^- \pi^0 | F\tilde{F} | 0 \rangle}{\langle \pi^0 | F\tilde{F} | 0 \rangle} &= -\frac{2}{9F_\pi^2} \left[1 + \frac{24(2L_4 + L_5)}{F_\pi^2} p_+ \cdot p_- \right. \\ & \quad + \frac{32L_7}{F_\pi^2} (m_K^2 - m_\pi^2) \\ & \quad + \frac{96(L_6 + L_7 + L_8)}{F_\pi^2} m_\pi^2 \\ & \quad \left. + \frac{4L_{14}}{F^2} (s - m_\pi^2) \right], \end{aligned} \quad (66)$$

where $s = (p_+ + p_- + p_0)^2$. The s dependence of this matrix element is governed by L_{14} . Equivalently, the result

$$\begin{aligned} \frac{1}{\langle \pi^+ \pi^- \pi^0 | F\tilde{F} | 0 \rangle} \frac{d}{ds} \langle \pi^+ \pi^- \pi^0 | F\tilde{F} | 0 \rangle \Big|_{p_+ \cdot p_- = \text{const}} \\ = \frac{4L_{14}}{F^2} \end{aligned} \quad (67)$$

can be used to extract L_{14} . Note that chiral logs have not been included in Eqs. (66) and (67).

How can one measure these matrix elements experimentally? The answer is found in a surprising set of reactions, i.e., $V' \rightarrow VM$, where $V = \Upsilon$ and M is π^0 , η^0 , or 3π . The heavy-quarkonium system forms a compact, color-neutral system. For soft hadronic emission, where the heavy quarks do not annihilate, the transitions can be analyzed in terms of a multipole expansion [10,11]. The interaction is due to gluonic couplings to the heavy quark, and the transitions to light hadrons are then governed by matrix elements of gluonic fields. The multipole method amounts to a systematic expansion in inverse powers of the heavy-quark mass. For pseudoscalars, the expansion starts with two gluon fields, as in Fig. 2. Voloshin and Zakharov [11] have shown that the leading pseudoscalar operator is $\mathbf{E}^A \cdot \mathbf{B}^A \propto F\tilde{F}$. Thus, they obtain

$$\frac{\Gamma(V' \rightarrow V\pi^0)}{\Gamma(V' \rightarrow V\eta)} = \left[\frac{\langle 0|F\tilde{F}|\pi^0\rangle}{\langle 0|F\tilde{F}|\eta\rangle} \right]^2 \frac{p_\pi^3}{p_\eta^3}, \quad (68)$$

where p_π (p_η) is the momentum of the π (η). Similarly,

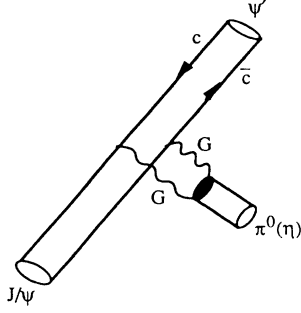


FIG. 2. A two-gluon transition amplitude in the heavy-quark multipole expansion.

for pseudoscalar 3π emission one can extract the 3π amplitude of $F\bar{F}$. (We hope to return to a more detailed presentation of the phenomenology of this mode, as well as a calculation of the chiral loops for its amplitude, in the future.) The use of $\Upsilon' \rightarrow \Upsilon M$ ($M = \pi^0, \eta^0, 3\pi$) would, of course, be the most reliable from the standpoint of the heavy-quark expansion. Comparison with results of $\psi' \rightarrow J/\psi M$ could allow an experimental determination of the accuracy of the multipole expansion. Unfortunately, data on all of these reactions does not yet exist. Only $\psi' \rightarrow J/\psi \pi^0$ and $\psi' \rightarrow J/\psi \eta^0$ have been measured.

In this section, we have described a method to measure, in principle, ratios of quark masses in a way which is free from the ambiguity of the reparametrization transformation. The heavy-quark multipole expansion is a rigorous approximation scheme in QCD (much like the chiral expansion itself). Its validity can, in principle, be checked experimentally, such that extraction of the $F\bar{F}$ matrix elements would constitute a true measurement in our sense of the word. Theoretically, the key new ingredient is the use of a $U(1)_A$ probe which is not invariant under reparametrization.

VI. ESTIMATE OF QUARK MASSES AT SECOND ORDER

Our full measurement scheme is not yet practical. The available data come from ψ' decays, in particular, the ratio

$$\frac{\Gamma(\psi' \rightarrow J/\psi + \pi^0)}{\Gamma(\psi' \rightarrow J/\psi + \eta^0)} = (3.6 \pm 0.9) \times 10^{-2}. \quad (69)$$

From this we extract

$$r_{F\bar{F}} = \frac{\langle 0 | F\bar{F} | \pi^0 \rangle}{\langle 0 | F\bar{F} | \eta^0 \rangle} = 0.0430 \pm 0.0055. \quad (70)$$

We would like to use this to obtain the quark mass ratio.

The presence of the unmeasured constant L_{14} in Eq. (65) prevents us from obtaining completely model-independent results. However, experience with other low-energy constants [19,20] allows us to give an estimate of L_{14} . The parameter L_{14} describes the energy dependence of $F\bar{F}$ matrix elements,

$$\langle 0 | F\bar{F} | M(p) \rangle \propto 1 + \frac{4L_{14}}{F^2} p^2 + \dots \quad (71)$$

This energy dependence is governed by the physical intermediate states (besides the Goldstone modes) that couple to $F\bar{F}$. A check of the data tables reveals that the lightest such state is η' at 960 MeV, and that other pseudoscalars and multibody states lie above 1.4 GeV. We then expect that

$$0 \leq \frac{4L_{14}}{F^2} \leq \frac{1}{m_{\eta'}^2}. \quad (72)$$

This same result can be expressed more formally by writing a sum rule (see Refs. [7,19]) involving L_{14} ,

$$\int \frac{ds}{s-p^2} \rho_{PF}(s) = \frac{F^2 B_0}{2} \left[1 + \frac{4L_{14}}{F^2} p^2 + \dots \right], \quad (73)$$

where

$$\rho_{PF}(s) = i \int d^4x e^{ip \cdot (x-y)} \langle 0 | \bar{\psi} \gamma_5 \psi(x) F\bar{F}(y) | 0 \rangle.$$

Single-particle saturation then also yields Eq. (72). The main point is that the sum rule receives contributions from fairly high values of s and, hence, the parameter L_{14} is expected to be small.

Collecting the experimental ingredients needed to evaluate Eq. (65), we obtain

$$\frac{m_d - m_u}{m_d + m_u} \frac{m_s + \hat{m}}{m_s - \hat{m}} = 0.59 \pm 0.07 \pm 0.08, \quad (74)$$

where the first uncertainty is experimental and the second is theoretical, corresponding to

$$L_{14} = \frac{F_\pi^2}{8m_{\eta'}^2} \pm \frac{F_\pi^2}{8m_{\eta'}^2}. \quad (75)$$

This theoretical uncertainty should be understood rather as a range than as a 63% confidence limit of a Gaussian distributed fluctuation.

Because $\hat{m}/m_s \ll 1$, this ratio is sensitive only to m_u/m_d . Solving for this quantity, we obtain

$$\frac{m_u}{m_d} = 0.30 \pm 0.05 \pm 0.05, \quad (76)$$

somewhat below the lowest-order measurement, or the estimate of Eq. (32). It seems securely away from the point $m_u = 0$, thus again disfavoring this option to solve the strong CP problem.

Previous estimates of the above combination of masses have relied on the K^0-K^+ mass difference, where the electromagnetic effects need to be subtracted off in order to reveal the $u-d$ quark mass difference. As originally calculated by Gasser and Leutwyler, the effects of quark masses are given by

$$\frac{m_K^2}{m_\pi^2} \frac{(m_{K^0}^2 - m_{K^+}^2)_{\text{QM}}}{m_K^2 - m_\pi^2} = \left[\frac{m_d - m_u}{m_d + m_u} \frac{m_s + \hat{m}}{m_s - \hat{m}} \right] \{ 1 + 2\Delta_m \}, \quad (77)$$

where

$$\begin{aligned}\Delta_m &= 1 - \frac{F_K^2}{F_\pi^2} - \delta_{\text{GMO}} - \frac{32L_7}{F_\pi^2} (m_K^2 - m_\pi^2) \\ &= -0.43 - 0.82 \left[\frac{L_7}{10^{-3}} \right].\end{aligned}\quad (78)$$

At lowest order, Dashen's theorem yields 0.29 for the left-hand side of Eq. (77), while a direct calculation of the electromagnetic mass difference using pseudoscalar and vector intermediate states of the electromagnetic mass difference [21] yields a value of 0.41. When combined with our value of the quark mass ratio, Eq. (74), these estimates correspond to

$$\Delta_m = -0.25, \quad L_7 = -0.22 \times 10^{-3}$$

and

$$\Delta_m = -0.15, \quad L_7 = -0.34 \times 10^{-3},$$

respectively. These are close to the value of $L_7 = -0.4 \times 10^{-3}$ suggested by Leutwyler [7].

Our determination of the quark mass ratio has crucially relied on the work of Voloshin and Zakharov which uses the heavy-quark expansion to relate $\psi' \rightarrow J/\psi\pi^0(\eta)$ to matrix elements of $F\bar{F}$. Without this knowledge, the $\psi' \rightarrow J/\psi\pi^0(\eta)$ amplitudes would have been parametrized as a general pseudoscalar effective Lagrangian using only SU(3) symmetry, as in Eq. (38) (the η^0 would be replaced by a bilinear of ψ and ψ'). This would then have exhibited the SU(3) reparametrization invariance. However, the extra input that the important operator is $F\bar{F}$ removes the reparametrization invariance and singles out particular forms for the matrix elements, those of Eq. (64). How well should this procedure be expected to work? Subleading operators in the heavy-quark multipole expansion will enter at the level of (μ/m_c) where μ is a typical hadronic scale. [Perhaps $(m_\rho/m_\psi) \sim 0.25$ is a reasonable estimate of this suppression.] However, all operators in the multipole expansion yield the same ratios in Eq. (64) to first order in the masses [22]; the first-order analysis is universal. The effect of subleading operators in the multipole expansion only influences the chiral coefficients determined at order E^4 (i.e., M_0^2). Within chiral SU(3), effects at order E^4 are typically suppressed compared to order E^2 by a factor of 30%. Thus, the subleading multipole corrections to the ratio of matrix elements would be expected to enter at the level of $30\% \times (\mu/m_c)$ [$\approx 7\%$]. Since the present experimental uncertainty in the amplitude ratio is 13%, the subleading corrections are probably smaller than the experimental error bars. We note, however, that if the ratio can be measured in ρ decay, we will be able to confirm experimentally the absence or presence of subleading heavy-quark mass effects.

VII. CONCLUSIONS

The analysis of quark masses at next to leading order in the chiral expansion has proven to be subtle. If the experimental analysis is restricted to chiral SU(3), as has been the case up to the present work, there is a continu-

ous family of quark mass matrices that leads to identical physics. We have shown how $U(1)_A$ transformations may single out a unique mass matrix. By using chiral symmetry and the heavy-quark multipole expansion [10,11] for transitions of b, c quarks, we have been able to give a procedure for a model-independent measurement of the light-quark mass ratio.

Although present data do not allow a complete measurement, the remaining model dependence, contained in the unknown (but measurable) parameter L_{14} , is estimated to be small. By bounding this constant, we have been able to extract the quark mass ratio given in Eq. (74). This value differs somewhat from previous estimates, but is not consistent with $m_u = 0$. An important consideration is that the present estimate is the first which arises from experimental observables which do not have the reparametrization ambiguity.

Some directions for further work are indicated. Experimental measurements of $\Upsilon' \rightarrow \Upsilon\pi^0(\eta^0)$ would remove uncertainties due to the heavy-quark expansion. Theoretical and experimental studies of the 3π transition would remove the last remaining source of model dependence. Next-to-leading-order calculations of electromagnetic contributions to the $K^+ - K^-$ mass difference are needed. These developments could help considerably in the extraction of quark masses.

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APPENDIX A: SURVEY OF FIRST-ORDER MEASUREMENTS OF QUARK MASSES

Our information on quark masses comes from several sources of varying quality. In this appendix we take a tour through these measurements under the common assumption that we are working to first order in the mass. Recall our distinction between "measurement" and "model" given in the Introduction. In this division, there are only three true sources of measurements: (1) π, K, η masses [\hat{m}/m_s and $(m_d - m_u)/m_s$], (2) $\psi' \rightarrow J/\psi\pi^0(\eta^0)$ [$(m_d - m_u)/(m_s - \hat{m})$], and (3) $\eta \rightarrow 3\pi$ decay [$(m_d - m_u)/m_s$], where there is reason to suspect the utility of the third of these. In addition, there are more model-dependent sources: (4) $\pi N\sigma$ term (\hat{m}/m_s), (5) other hadron masses [$(m_d - m_u)/m_s$], and (6) $\rho - \omega$ splitting [$(m_d - m_u)/m_s$]. These results are summarized in Table I, but in some cases the caveats discussed below may be

TABLE I. Lowest-order measures of quark masses. See the text for a fuller discussion.

	$\frac{\hat{m}}{m_s}$	$\frac{m_d - m_u}{m_s - \hat{m}}$
MEASUREMENTS		
π, K, η masses	$\frac{1}{26}$	$\frac{1}{43}$
$\psi' \rightarrow J/\psi + \pi^0(\eta)$		$\frac{1}{30 \pm 4}$
$\eta \rightarrow \pi^+ \pi^- \pi^0$ (i) strict lowest order		$\frac{1}{21}$
(ii) with final-state interactions		$\frac{1}{32 \pm 5}$
MODELS		
σ term	$\frac{1}{15}(1-y)$	
Hadron masses		$\frac{1}{67} \rightarrow \frac{1}{20}$

more important than the numerical values.

(1) π, K, η masses. This method is surveyed in the main text. It yields our only true measurement of \hat{m}/m_s . The measurement of $(m_d - m_u)/m_s$ uses Dashen's theorem [23] to subtract out the electromagnetic contribution to the $K^0 - K^+$ mass difference. In an effective-Lagrangian framework, Dashen's theorem follows from the $(\mathbf{8}_L, \mathbf{1}_R) + (\mathbf{1}_L, \mathbf{8}_R)$ transformation property of the electromagnetic current. The only symmetry-allowed Lagrangian which does not vanish in the chiral limit is then

$$\mathcal{L}_{\text{em}} = \alpha c_1 \text{Tr}(QUQU^\dagger). \quad (\text{A1})$$

Because of the factors of Q , the effective Lagrangian does not involve the neutral mesons at all, and the π^+ and K^+ matrix elements are identical, leading to Dashen's theorem. Corrections to this result would occur through operators at next order in the energy expansion, such that

$$\mathcal{L}'_{\text{em}} = \frac{\alpha c_1}{\Lambda^2} \text{Tr}(Q^2 \partial_\mu U \partial^\mu U^\dagger), \quad (\text{A2})$$

whose matrix elements would be of order αm_π^2 or αm_K^2 . The effects of such next-order corrections have not yet been analyzed in chiral perturbation theory.

(2) $\psi' \rightarrow J/\psi \pi^0, \psi' \rightarrow J/\psi \eta^0$. Since both ψ' and J/ψ are isoscalar and SU(3) scalar, these two decays violate isospin and SU(3) symmetry, respectively. Their ratio is then a measure of $(m_d - m_u)/(m_s - \hat{m})$. When working to first order, we do not need to involve the QCD multipole expansion described in the text. Rather, the result is a prediction of the symmetry alone [22] and the ratio follows directly from degenerate perturbation theory

$$R = \frac{\Gamma(\psi' \rightarrow J/\psi \pi^0)}{\Gamma(\psi' \rightarrow J/\psi \eta^0)} = \frac{27}{16} \left[\frac{m_d - m_u}{m_s - \hat{m}} \right] \left[\frac{p_\pi}{p_\eta} \right]^3, \quad (\text{A3})$$

where p_π (p_η) is the pion (eta) momentum.

There exists the possibility of electromagnetic contributions to this transition. However, it can be shown rigorously to be suppressed. There is no chiral operator of order E^0 (E is energy) with the right symmetry properties. Equivalently, the matrix element vanishes in the soft-pion limit using the soft-pion theorems because the axial charge Q_5^3 commutes with the electromagnetic current. One might worry that the presence of the heavy charmed quark mass might make corrections to the soft-pion limit more important than usual. However, if anything, it seems to suppress any correction [23–25]. Modifications on the pion side, as in Fig. 3(a), are similar to corrections to Dashen's theorem in meson masses. Of the diagrams which feel the presence of the charmed quark, Fig. 3(b) is forbidden by the pion quark numbers, Fig. 3(c) is forbidden by color, Fig. 3(d) is forbidden by C invariance, leaving Fig. 3(e) as the leading correction of this class. However, it can be shown to be suppressed by the QCD multipole expansion. The diagram of Fig. 3(e) vanishes with respect to Fig. 2 as $m_c \rightarrow \infty$, and has a nominal suppression of order $\alpha_s(m_c)/(\mu/m_c)$, where μ is a typical hadronic scale. In summary, we expect the electromagnetic effects to be as suppressed here as they are in the meson masses, and, hence, the measurement here is on the same footing as the more familiar measurement from $m_{K^0} - m_{K^+}$.

The experimental measurement

$$R = 0.036 \pm 0.009 \quad (\text{A4})$$

implies a mass value

$$\frac{m_d - m_u}{m_s - \hat{m}} = 0.033 \pm 0.004. \quad (\text{A5})$$

This is somewhat larger than Eq. (1), but with a difference which can be attributed to the presence of higher-order effects.

(3) $\eta \rightarrow 3\pi$ decay. This decay is forbidden in the SU(2) limit, and, hence, can only take place through quark mass

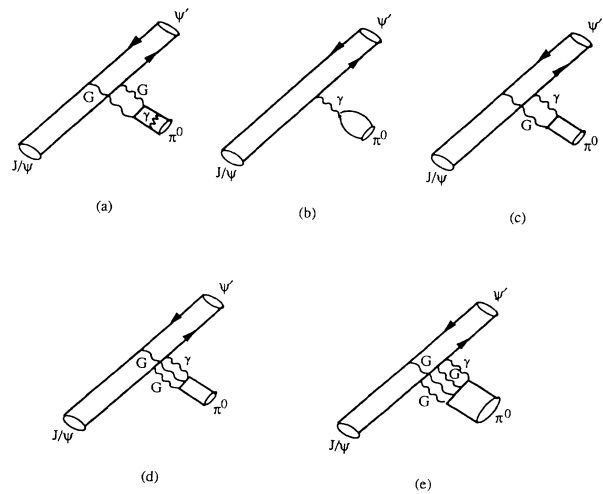


FIG. 3. Possible electromagnetic corrections in $\psi' \rightarrow J/\psi \pi^0(\eta^0)$. As described in the text, most of these diagrams vanish.

differences and electromagnetism. However, the effect of electromagnetism vanishes at lowest order in the chiral expansion as originally shown by Sutherland. In an effective Lagrangian framework, this again follows from a calculation using Eq. (11). Thus, the decay provides a technically valid first-order measurement of $m_d - m_u$. The amplitude is

$$M(\eta \rightarrow \pi^+ \pi^- \pi^0) = \frac{(m_d - m_u)B_0}{3\sqrt{3}F_\pi} \left[1 + \frac{3(s - s_0)}{m_\eta^2 - m_\pi^2} \right] \quad (\text{A6})$$

with $s = (p_\eta - p_0)^2$ and $s_0 = (m_\eta^2 + 3m_\pi^2)/3$. This leads to a decay rate at lowest order

$$\Gamma_0 = 125 \text{ keV} \left[\frac{m_d - m_u}{m_s - \hat{m}} \right]^2. \quad (\text{A7})$$

From the experimental decay rate, $\Gamma = 0.028 \pm 0.03 \text{ keV}$, we extract

$$\frac{m_d - m_u}{m_s - \hat{m}} = 0.047 = \frac{1}{21}. \quad (\text{A8})$$

However, there are known final-state interactions in the various $\pi\pi$ subchannels which have been neglected above. These can lead to an enhancement of the rate, and it is perhaps not quite fair to neglect these. An alternate procedure could be to calculate the effect of final-state interactions, and also η - η' mixing, using chiral perturbation theory to next order, while at the same time continuing to treat $(m_u - m_d)$ as a first-order parameter. This can be done using the result of Ref. [2], with the result

$$\Gamma_{\text{fsi}} = (300 \pm 95) \text{ keV} \left[\frac{m_u - m_d}{m_s - \hat{m}} \right]^2, \quad (\text{A9})$$

where the error is an estimate of the uncertainty in the theoretical evaluation. This results in

$$\frac{m_d - m_u}{m_s - \hat{m}} = 0.031 \pm 0.005 = \frac{1}{32 \pm 5}. \quad (\text{A10})$$

We feel that this latter value is a more realistic estimate than is Eq. (A8), but the difference between the two indicates the sizable uncertainties in this evaluation.

(4) The sigma term. In πN scattering at very low ener-

gy, one can use chiral symmetry plus dispersion techniques to extract the matrix element

$$\begin{aligned} \sigma &= \langle P | \hat{m}(\bar{u}u + \bar{d}d) | P \rangle \\ &\approx 45 \text{ MeV}, \end{aligned} \quad (\text{A11})$$

where the numerical value corresponds to the most recent evaluation of Ref. [26]. In addition, hyperon masses, when treated to first order, yield the following matrix element:

$$\langle P | (m_s - \hat{m})(\bar{u}u + \bar{d}d - 2\bar{s}s) | P \rangle = \frac{3}{2}(m_\Xi - m_N). \quad (\text{A12})$$

Although the operators in (A11) and (A12) are not identical, we can form the measure of mass

$$\frac{\hat{m}}{m_s - \hat{m}} = \frac{2\sigma}{3(m_\Xi - m_N)}(1-y) = \frac{1}{14.4}(1-y), \quad (\text{A13})$$

where

$$y \equiv \frac{2\langle P | \bar{s}s | P \rangle}{\langle P | \bar{u}u + \bar{d}d | P \rangle}. \quad (\text{A14})$$

Because of the dependence on the $\bar{s}s$ matrix element (i.e., y), this is not a full first-order measurement of the mass ratio. However, for modest values of y and if first order is sufficient, we have

$$y = 0, 0.2, 0.4, \quad (\text{A15})$$

$$\frac{\hat{m}}{m_s} = \frac{1}{15}, \frac{1}{18}, \frac{1}{24},$$

which indicates a reasonable range for this mass ratio.

(5) Other hadron masses. There are a limited number of results on hadron mass splittings which can be derived from symmetry considerations alone. For example, to first order the $I=2$ splitting

$$\begin{aligned} m_{\Sigma^+} + m_{\Sigma^-} - 2m_{\Sigma^0} &= 1.7 \pm 0.1 \text{ MeV}, \\ m_{\rho^+} - m_{\rho^0} &= -0.3 \pm 2.2 \text{ MeV}, \end{aligned} \quad (\text{A16})$$

are due to electromagnetism alone. In addition, both electromagnetism and quark masses satisfy the Coleman-Glashow relation

$$\begin{aligned} m_{\Sigma^+} - m_{\Sigma^-} + m_n - m_p + m_{\Xi^-} - m_{\Xi^0} &= 0 \\ &= 0.4 \pm 0.6 \text{ MeV (expt)}. \end{aligned} \quad (\text{A17})$$

For the quark masses this follows from the SU(3)-octet property of mass differences, while for electromagnetism it can be simply obtained from the U -spin singlet character of the interaction.

Unfortunately, we cannot use a symmetry argument to isolate the quark mass differences. There is the first-order relation

$$\frac{m_d - m_u}{m_s - \hat{m}} = \frac{(m_n - m_p)_{\text{QM}}}{m_\Xi - m_\Sigma}, \quad (\text{A18})$$

where $(m_n - m_p)_{\text{QM}}$ is the quark mass contribution to the n - p mass difference,

$$m_n - m_p = (m_n - m_p)_{\text{QM}} + (m_n - m_p)_{\text{EM}}. \quad (\text{A19})$$

Unlike in the π, K system, the electromagnetic effect cannot be subtracted using symmetry. There is a method for calculating the electromagnetic splitting which is, in principle, rigorous, using the Cottingham formula [26,27]. An interesting feature emerges from this calculation. The electromagnetic shift diverges, due to self-energy diagrams, and this divergence needs to be absorbed into renormalized values of $m_d - m_u$. This is to be expected, but a similar renormalization was *not* needed in the mesons at lowest order. This raises the possibility that different meanings of masses may occur in mesons and baryons. The precise value of the quark mass depends on the renormalization prescription used to specify the remaining finite renormalization in the Cottingham formula (see the first reference in Ref. [3]). If one disregards the high-energy contributions, the Born contribution to the Cottingham result yields $(m_n - m_p)_{\text{EM}} = -0.76 \pm 0.30$ MeV and thus

$$(m_n - m_p)_{\text{QM}} = 2.05 \pm 0.30, \quad (\text{A20})$$

$$\frac{m_d - m_u}{m_s - \hat{m}} = 0.017 \pm 0.03 = \frac{1}{57 \pm 9}.$$

A similar estimate can be obtained in a quark model if the effect of photon exchange is represented by

$$H_{\text{EM}} = \sum_{i \neq j} \left[Q_i Q_j C + \frac{Q_i Q_j}{M_i M_j} H \mathbf{S}_i \cdot \mathbf{S}_j \right] \quad (\text{A21})$$

representing the Coulomb energy (C) and hyperfine interaction (H). Independent of the values of the parameters C, H , one has

$$(m_n - m_p)_{\text{EM}} = \frac{-1}{3} (m_{\Sigma^+} + m_{\Sigma^-} - 2m_{\Sigma^0})$$

$$= -0.57 \pm 0.03 \text{ MeV} \quad (\text{A22})$$

consistent with the Cottingham estimate. This yields

$$\frac{m_d - m_u}{m_s - \hat{m}} = 0.015 = \frac{1}{67} \quad (\text{A23})$$

instead of Eq. (A20). However, the model dependence becomes evident if one uses the same model on the $K^{*0} - K^{*+}$ mass difference. Neglecting the constituent mass difference in the hyperfine portion, one has

$$(m_{K^{*0}} - m_{K^{*+}})_{\text{EM}} = -\frac{2}{3} (m_{\rho^+} - m_{\rho^0}) = 0.2 \pm 1.5 \text{ MeV}, \quad (\text{A24})$$

$$\frac{m_d - m_u}{m_s - \hat{m}} = \frac{(m_{K^{*0}} - m_{K^{*+}})_{\text{QM}}}{(m_{K^*} - m_{\rho})} = 0.053 \pm 0.016 = \frac{1}{19 \pm 8},$$

which is not at all consistent. We conclude that, although hadron masses contain information on $m_d - m_u$, one must become more confident about the models used to extract the electromagnetic contribution.

(6) $\rho - \omega$ mixing. Because ω is a mixture of SU(3) singlet and octet, SU(3) cannot be used to analyze the mixing of ρ and ω . Rather, quark model/Okuba-Zweig-Iizuka (OZI) rule motivations must be used. The quark mass contribution to the mixing is driven by

$$M_{\rho\omega} = \langle \rho | m_u \bar{u}u + m_d \bar{d}d | \omega \rangle$$

$$= \frac{(m_u - m_d)}{2} \langle \rho | \bar{u}u - \bar{d}d | \omega \rangle, \quad (\text{A25})$$

while mass splittings are governed by

$$M_{K^*} - m_{\rho} = \langle K^* | m_u \bar{u}u + m_d \bar{d}d + m_s \bar{s}s | K^* \rangle$$

$$- \langle \rho | m_u \bar{u}u + m_d \bar{d}d + m_s \bar{s}s | \rho \rangle$$

$$= -\frac{(m_s - \hat{m})}{3} [\langle K^* | \bar{u}u + \bar{d}d - 2\bar{s}s | K^* \rangle$$

$$- \langle \rho | \bar{u}u + \bar{d}d - 2\bar{s}s | \rho \rangle]. \quad (\text{A26})$$

The quark model says that the matrix elements are related such that

$$\frac{m_d - m_u}{m_s - \hat{m}} = \frac{-M_{\rho\omega}}{M_{K^*} - m_{\rho}}. \quad (\text{A27})$$

There can be electromagnetic contributions to $M_{\rho\omega}$. One known contribution is due to $\rho \leftrightarrow \gamma \leftrightarrow \omega$, which contributes 0.4 MeV to $M_{\rho\omega}$. Subtracting this off [27], analysis of $\omega - \rho$ mixing would yield

$$M_{\rho\omega} = -2.6 \text{ MeV}, \quad (\text{A28})$$

$$\frac{m_d - m_u}{m_s - \hat{m}} = 0.023 = \frac{1}{44}.$$

APPENDIX B: $U(1)_A$ TRANSFORMATION WITH A SINGLET FIELD

In this appendix we review and generalize the construction due to Gasser and Leutwyler of the Lagrangian containing an SU(3)-singlet pseudoscalar field ϕ_0 . The goal is to verify that the couplings of the singlet field do not contain new information that might allow one to overcome the reparametrization ambiguity without using the θ dependence. We need to allow U(1) transformations in the matrix U . For this we add a singlet coordinate ϕ_0

$$\tilde{U} \equiv \exp \left\{ i \frac{\tau \cdot \phi}{F} \right\} \exp \left\{ \frac{i \phi_0}{3} \right\} = U \exp \left\{ \frac{i \phi_0}{3} \right\}. \quad (\text{B1})$$

Note that we need not identify ϕ_0 with a single meson field, such as η' . In practice, we will integrate out ϕ_0 before applying the resulting Lagrangian. The important feature is the transformation of the fields under chiral rotations, i.e.,

$$\tilde{U} \rightarrow \tilde{L} \tilde{U} \tilde{R}^\dagger, \quad (\text{B2})$$

where now \tilde{L} and \tilde{R} may include $U(1)_A$ transformations. In particular, for a pure $U(1)_A$ rotation of Eq. (47), we have

$$\tilde{U} \rightarrow e^{i\alpha} \tilde{U} e^{i\alpha}, \quad (\text{B3})$$

which amounts to

$$\phi_0 \rightarrow \phi_0 + 6\alpha . \quad (\text{B4})$$

At the same time, θ will be modified to

$$\theta \rightarrow \theta - 6\alpha . \quad (\text{B5})$$

These rules lead to the crucial observation that

$$\theta + \phi_0 = \theta - i \text{Tr} \ln \tilde{U} \quad (\text{B6})$$

is not modified by a chiral $U(1)_A$ transformation.

The effective Lagrangian is the most general invariant combination of the fields θ_0 , \tilde{U} , and QCD parameters $\{\theta, m_i\}$. There is now the possibility of a Lagrangian at order E^0 , i.e.,

$$\mathcal{L}_0 = -V_0(\theta + \phi_0) , \quad (\text{B7})$$

where $V_0(\theta + \phi_0)$ is an arbitrary function of the invariant combination $\theta + \phi_0$. At order E^2 , we have the generalization of \mathcal{L}_2 , i.e.,

$$\begin{aligned} \mathcal{L}_2 = & \frac{F^2}{4} V_1(\theta + \phi_0) \text{Tr}(D_\mu \tilde{U} D^\mu \tilde{U}^\dagger) + \frac{F^2}{4} [V_2(\theta + \phi_0) \text{Tr}(\chi \tilde{U}^\dagger) + V_2^*(\theta + \phi_0) \text{Tr}(\tilde{U} \chi^\dagger)] \\ & + \frac{1}{2} V_3(\theta + \phi_0) \partial_\mu \phi_0 \partial^\mu \theta + \frac{1}{2} V_4(\theta + \phi_0) \partial_\mu \theta \partial^\mu \theta + \frac{1}{2} V_5(\theta + \phi_0) \partial_\mu \phi_0 \partial^\mu \phi_0 , \end{aligned} \quad (\text{B8})$$

where $V_i(\theta + \phi_0)$ are again arbitrary functions. This construction was first given by Gasser and Leutwyler [2]. Finally, the generalization of \mathcal{L}_4 is given by

$$\begin{aligned} \mathcal{L}_4 = & K_1 [\text{Tr}(D_\mu \tilde{U} D^\mu \tilde{U}^\dagger)]^2 + K_2 \text{Tr}(D_\mu \tilde{U} D_\nu \tilde{U}^\dagger) \text{Tr}(D^\mu \tilde{U} D^\nu \tilde{U}^\dagger) + K_3 \text{Tr}(D^\mu \tilde{U} D_\mu \tilde{U}^\dagger D^\nu \tilde{U} D_\nu \tilde{U}^\dagger) \\ & + [K_4 \text{Tr}(\chi^\dagger \tilde{U}) + K_4^* \text{Tr}(\chi \tilde{U}^\dagger)] \text{Tr}(D_\mu \tilde{U} D^\mu \tilde{U}^\dagger) + K_5 \text{Tr}(D_\mu \tilde{U} D^\mu \tilde{U}^\dagger \tilde{U} \chi^\dagger) + K_5^* \text{Tr}(D_\mu \tilde{U} D^\mu \tilde{U}^\dagger \chi \tilde{U}^\dagger) \\ & + K_6 \text{Tr}(\tilde{U} \chi^\dagger) \text{Tr}(\tilde{U} \chi^\dagger) + K_6^* \text{Tr}(\chi \tilde{U}^\dagger) \text{Tr}(\chi \tilde{U}^\dagger) + K_7 \text{Tr}(\chi \tilde{U}^\dagger) \text{Tr}(\tilde{U} \chi^\dagger) + K_8 \text{Tr}(\chi^\dagger \tilde{U} \chi^\dagger \tilde{U}) + K_8^* \text{Tr}(\chi \tilde{U}^\dagger \chi \tilde{U}^\dagger) \\ & - iK_9 \text{Tr}(L_{\mu\nu} D^\mu \tilde{U} D^\nu \tilde{U}^\dagger) - iK_9^* \text{Tr}(R_{\mu\nu} D^\mu \tilde{U} D^\nu \tilde{U}^\dagger) + K_{10} \text{Tr}(\tilde{U}^\dagger L_{\mu\nu} \tilde{U} R_{\mu\nu}) , \end{aligned} \quad (\text{B9})$$

plus terms with derivatives of θ . Here $K_i = K_i(\theta + \phi_0)$, and K_1, K_2, K_3, K_7 , and K_{10} are real. If one identifies ϕ_0 with the η' field, the dependence on $\theta + \phi_0$ is equivalent to the ‘‘soft η' ’’ theorems of Witten [16] where the η' matrix elements are related to derivatives of the vacuum energy with respect to θ .

At this stage we can explore the reparametrization transformation of Sec. II. We find that it exists in a modified form, i.e., Eq. (23) is replaced by

$$\begin{aligned} \chi & \rightarrow \chi + \lambda [\det \chi^\dagger] \chi \frac{1}{\chi^\dagger \chi} e^{-i\theta} , \\ M & \rightarrow M^{(\lambda)} = M + 2\lambda \det M M^{-1} e^{-i\theta} . \end{aligned} \quad (\text{B10})$$

The use of the Cayley-Hamilton relation then allows one to maintain the same physical observables as long as we modify

$$K_6(\theta + \phi_0) \rightarrow K_6(\theta + \phi_0) - \frac{\lambda}{2} V_2(\theta + \phi_0) e^{-i(\theta + \phi_0)} , \quad (\text{B11})$$

$$K_8(\theta + \phi_0) \rightarrow K_8(\theta + \phi_0) + \frac{\lambda}{2} V_2(\theta + \phi_0) e^{-i(\theta + \phi_0)} .$$

If we neglect θ and ϕ_0 , this is just the previous reparametrization change. However, in the presence of θ and ϕ_0 , it is a nontrivial extension, preserving the general form of the Lagrangian. The argument about the invariance of the resulting physics is similar to that of Sec. II. The parameters in V_i, K_i are arbitrary and must be determined phenomenologically. One can start with a mass matrix M and determine the V_i, K_i , or one may use $M^{(\lambda)}$ and find a different set of parameters [related to the original basis by Eq. (B11)], resulting in the same observables if θ is not involved.

We can see from this construction that, if $\theta=0$, matrix elements involving ϕ_0 do not help in resolving the quark mass ambiguity. With $\theta=0$, the previous transformation is fully present in all matrix elements. In practice, therefore, we have gained nothing for our purpose by including ϕ_0 . In addition, all singlet fields are too heavy for the reliable use of the chiral energy expansion. Therefore, it is preferable to integrate ϕ_0 out of the theory and concentrate on the low-energy particles. This is accomplished by defining a new field $\tilde{\phi}_0 = \theta + \phi_0$ and integrating out $\tilde{\phi}_0$. It is easy to verify that this leads to a Lagrangian of the form described in Sec. IV.

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