Pure QCD Bounds and Estimates for Light Quark Masses

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Abstract

We consider bounds on light quark masses that follow from positivity of the pseudoscalar correlator spectral function plus the assumption that perturbative QCD is valid for the correlator and its derivatives up to order $N$ for momenta $t \geq \hat{t}$. We find that the bounds vary a lot depending on the assumed value of $\hat{t}$ and even, if it is too small ($\hat{t} \simeq 1.5, 1.6, 2.1 \text{ GeV}^2$ for respectively $N = 0, 1, 2$), that there is incompatibility between the assumption of validity of perturbative QCD and positivity. This allows us to establish a criterion for the values of $\hat{t}$ admissible, and to get upper and lower bounds for $m_s$ and upper bounds for $m_d + m_u$, $m_d - m_u$.

The upper bounds are not particularly interesting, but the lower ones are very tight; specifically we find

$$240 \text{ MeV} \leq m_s; \quad 16 \text{ MeV} \leq m_d + m_u$$

if we assume perturbative QCD to give a valid description of the correlator for $t \geq 2.2 \text{ GeV}^2$; or, if it only holds for $t \geq 4.5 \text{ GeV}^2$ then

$$150 \text{ MeV} \leq m_s; \quad 10 \text{ MeV} \leq m_d + m_u.$$ 

Here the masses are running masses defined at 1 GeV. We also show reasonable models where the bounds are saturated. The results suggest that some of the current estimates of the light quark masses are less precise than ordinarily claimed.

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§1. Introduction
Quark masses cannot be measured directly because of confinement, so indirect methods have to be devised to estimate them. In particular, light quark \((u, d, s)\) masses can only be obtained either from lattice simulations\(^1\) or via QCD sum rules, which is the method that will be used in this paper. The advantage of this method is twofold: first, one can check, using perturbation theory, the validity of the calculations and, secondly, one may use very general properties of spectral functions to get bounds which will only depend on QCD. This second feature is what will be of interest for us here.

The use of QCD sum rules for getting light quark masses, or QCD bounds, goes back to refs. 2, 3 and, especially, ref. 4. Since then a large number of determinations of the masses have been made. Among these, we may quote those in refs. 5, 6 as very comprehensive ones, and refs. 7, 8, 9 as recent determinations employing increasingly precise QCD calculations\(^{10,11}\) which have been becoming available. Quoting from refs. 7, 9 one has

\[
m_u + m_d = 12 \pm 2.5 \text{ MeV} = 171 \pm 15 \text{ MeV} \tag{1.1}
\]

and the masses refer to the \(\overline{\text{MS}}\) masses, defined at 1 GeV\(^2\). The first value comes from ref. 7, that for \(m_s\) from ref. 9.

In the present paper we will contend that the errors quoted in Eq. (1.1) are excessively optimistic as indeed a large contribution to the estimates comes not from QCD but from low energy models. That this is so, that the errors must be underestimated, follows from the fact that, as we will show, bounds using only perturbative QCD, in a region where it should be applicable, can be obtained which are hardly compatible with (1.1). What is more, we will construct explicit, simple models incorporating perturbative QCD and positivities that show that the largest source of uncertainty is the value of the momentum at which one assumes a perturbative calculation to produce a good approximation. In fact, the determinations of the light quark masses do indeed depend to an important extent on low energy models, and the implicit assumption of when the perturbative expression takes over.

§2. Derivation of the bounds
We will follow ref. 4 and define the correlator,

\[
\Psi_{5}^{12}(t) = i \int d^4 x \langle \text{vac} | T \partial^\mu A_{\mu}^{12}(x) \partial^\nu A_{\nu}^{12}(0) | \text{vac} \rangle, \tag{2.1}
\]

\(t = -q^2\) and \(|\text{vac}\rangle\) the physical vacuum. The axial current is

\[
A_{\mu}^{12}(x) = \bar{q}_1(x) \gamma_\mu \gamma_5 q_2(x), \tag{2.2}
\]

and the indices 1,2 refer to quark flavours, of which we will consider various pairings among the \(u, d, s\). The second derivative with respect to \(t\) of the correlator \(F_{5}^{12}(t) = \partial^2 \Psi_{5}^{12}(t)/\partial t^2\) satisfies a dispersion relation of the form

\[
F_{5}^{12}(t) = \int_0^\infty ds \frac{1}{(s + t)^3} \frac{2 \text{Im} \Psi_{5}^{12}(s)}{\pi}. \tag{2.3}
\]

Because one can write the spectral function as

\[
\text{Im} \Psi_{5}^{12}(s) = \frac{\pi}{2} \sum_I |\langle \text{vac} | \partial^\mu A_{\mu}^{12}(0) | I \rangle|^2 (2\pi)^4 \delta_4(q - p_I), \tag{2.4}
\]

it follows that \(\text{Im} \Psi_{5}^{12}(s) \geq 0\): it is this positiveness that will allow us to derive quite general bounds.

For sufficiently large \(t\) perturbative QCD is applicable to calculate \(\Psi_{5}^{12}(t)\). To leading order in \(\alpha_s\) and \(m_i\) we have (\(N_c\)=number of colours =3)

\[
F_{5}^{12}(t) = \frac{N_c}{8 \pi^2} \frac{[m_1(t) + m_2(t)]^2}{t}, t \gg A^2, \tag{2.5a}
\]

and, for the imaginary part,

\[
\text{Im} \Psi_{5}^{12}(s) = \frac{N_c}{8 \pi} s \frac{[m_1(s) + m_2(s)]^2}{s \gg A^2}. \tag{2.5b}
\]
It is very important, to get tight, reliable bounds, to use the information contained in both equations (2.4a,b). This is achieved by working with the function

\[ \varphi_{12}(t) = F_5^{12}(t) - \int_t^\infty ds \frac{2 \text{Im} \Psi_5^{12}(s)}{(s+t)^3} \]

\[ = \int_0^t ds \frac{2 \text{Im} \Psi_5^{12}(s)}{(s+t)^3}. \quad (2.6) \]

Using the QCD evaluation (2.5b) for the spectral function Im \( \Psi_5^{12}(s) \) when \( s \geq t \) in (2.6) we now get the perturbative QCD estimate,

\[ \varphi_{12}(t) = \frac{1}{4 \text{LO}} \frac{N_c}{8 \pi^2} \frac{[m_1(t) + m_2(t)]^2}{t}, \quad (2.7) \]

note the factor \( \frac{1}{t} \) gained with respect to Eq. (2.5a). It will also turn out that \( \varphi \) is better than \( F_5 \) in that higher order corrections are smaller for it.

Next we use the operator version of PCAC to write

\[ \partial \cdot A^{12} = \sqrt{2} f_{12} M_{12}^2 \phi_{12}, \quad (2.8) \]

where \( \phi_{12} \) is the field for the pseudoscalar Goldstone boson with decay constant \( f_{12} \) and mass \( M_{12} \): \( \phi_{ud} = \phi_{\pi^+}, \, M_{ud} = M_{\pi^+}, \, \phi_{us} = \phi_{K^+}, \, M_{us} = M_{K^+}, \, \phi_{ds} = \phi_{K^0}, \, M_{ds} = M_{K^0}. \) The contribution of the corresponding one-particle intermediate state to (2.4) is then calculable explicitly and we get,

\[ \varphi_{12}(t) = \frac{4 f_{12}^2 M_{12}^4}{(t + M_{12}^2)^3} + \frac{2}{\pi} \int_{s_0}^t ds \frac{\text{Im} \Psi_{12}^5(s)}{(s+t)^3}; \quad (2.9) \]

\[ s_0 = M_{ud}^2 = 9 M_{\pi}^2 \text{ for } ud \text{ quarks, } s_0 = (M_K + 2 M_\pi)^2 \text{ for the } (u,d)s \text{ states.} \]

Combining (2.9) with (2.7) we get immediately a bound. If we believe that the LO expression (2.7) is a good description of \( \varphi(t) \) for \( t \geq t_0 \) then, because Im \( \Psi_5 \) in (2.9) is positive we get

\[ m_1(t_0) + m_2(t_0) \geq \left\{ \frac{27 \pi^2 f_{12}^2 M_{12}^4}{3 (t_0 + M_{12}^2)^3} \right\}^{\frac{1}{2}}. \quad (2.10) \]

Our task in the coming sections lies in refining (2.10) for the various quark choices.

\section*{§3. Derivatives. Upper and lower bounds on \( m_s \)}

In principle it would appear that one can improve the bound in Eq. (2.10) by considering quantities related to derivatives. We will here consider the \( \varphi^{(N)} \),

\[ \varphi^{(0)}(t) = \int_0^t ds \frac{2 \text{Im} \Psi(s)}{(s+t)^3} \frac{1}{\pi} = \frac{4 f_{12}^2 M_{12}^4}{(t + M_{12}^2)^3} + \int_{s_0}^t ds \frac{2 \text{Im} \Psi(s)}{(s+t)^3} \frac{1}{\pi}; \quad (3.1a) \]

\[ \varphi^{(1)}(t) = 3 \int_0^t ds \frac{2 \text{Im} \Psi(s)}{(s+t)^4} \frac{1}{\pi} = \frac{12 f_{12}^2 M_{12}^4}{(t + M_{12}^2)^4} + 3 \int_{s_0}^t ds \frac{2 \text{Im} \Psi(s)}{(s+t)^4} \frac{1}{\pi}; \quad (3.1a) \]

\[ \varphi^{(2)}(t) = 12 \int_0^t ds \frac{2 \text{Im} \Psi(s)}{(s+t)^5} \frac{1}{\pi} = \frac{48 f_{12}^2 M_{12}^4}{(t + M_{12}^2)^5} + 12 \int_{s_0}^t ds \frac{2 \text{Im} \Psi(s)}{(s+t)^5} \frac{1}{\pi}; \quad (3.1a) \]

and \( \varphi^{(0)} \) coincides with \( \varphi \) as defined above.

We will not consider higher derivatives, of order \( N > 2 \). The QCD NLO (next to leading order) corrections to the LO result grow with \( N \), as \( \log N \) for \( a_s \) corrections, and as powers of \( N \) for the \( O(\text{mass}^2/t^4) \) corrections\(^1\).\(^4\). We may compensate this by taking larger values of \( t \) for larger \( N \), and we are thus faced with a problem of optimization: we have to take sufficiently many derivatives that we get good bounds, but not too many that this is offset by the ensuing growth of \( t \). A very sophisticated optimization method is described in ref. 4; here we will not go that far and will consider only \( N = 0,1,2 \): we prefer to sacrifice optimality for reliability.

\(^1\) We will suppress the indices 12 from \( \varphi_{12} \) etc. when they are superfluous
We start by considering the correlators containing the strange quark, say the quantities \( \varphi^{(N)}_{us}(t) \). These may be calculated in QCD if \( t \) is large enough. We will here keep the LO and NLO terms\(^2\) in \( \alpha_s \) as well as terms of relative order \( m_s^2/t \), \( m_s^4/t^2 \), and the leading (in \( \alpha_s \)) nonperturbative contributions associated with the nonzero condensates

\[
\langle \text{vac} | : \bar{q}(0)q(0) : | \text{vac} \rangle, \quad \langle \text{vac} | : \alpha_s G^2(0) : | \text{vac} \rangle,
\]

and \( q \) are the quark operators for \( u, s \) quarks. The first condensate may be eliminated using PCAC and flavour SU(3) invariance in favour of products of \( f_K, M_K \). Using the results of refs. 4, 10,

\[
\frac{1}{\pi} \text{Im} \psi^{us}_5(s) = \frac{3m^2(s)}{8\pi^2} \left\{ \left[ 1 + \frac{17\alpha_s}{3\pi} \right] s - 2m^2(s) \left[ 1 + \frac{16\alpha_s}{3\pi} \right] \right\},
\]

\[
F^{us}_5(t) = \frac{3}{8\pi^2} \left\{ \frac{m^2(t)}{t} \left[ 1 + \frac{11\alpha_s}{3\pi} \right] - 2m^3(t) \left[ 1 + \frac{28\alpha_s}{3\pi} \right] \right. + \frac{1}{t^3} \left[ \frac{8\pi^2 f^2_K M^2_K}{3} + \frac{2\pi(\alpha_s : G^2 :)}{3} \right] \right\}
\]

and we then have,

\[
\varphi^{(0)}_{us}(t) = \frac{3}{8\pi^2} \left\{ \frac{m^2(t)}{t} \left[ 1 + \left( \frac{3}{4} + 2 \log 2 \right) \frac{\alpha_s}{\pi} \right] - \frac{2m^4(t)}{t^2} \left[ \frac{1}{\pi} + (6 + 4 \log 2) \frac{\alpha_s}{\pi} \right] \right. + \frac{1}{t^3} \left[ \frac{8\pi^2 f^2_K M^2_K}{3} + \frac{2\pi(\alpha_s : G^2 :)}{3} \right] \right\};
\]

\[
\varphi^{(1)}_{us}(t) = \frac{3}{8\pi^2} \left\{ \frac{m^2(t)}{t^2} \left[ \frac{1}{4} + \left( \frac{3}{4} + 2 \log 2 \right) \frac{\alpha_s}{\pi} \right] - \frac{4m^4(t)}{t^3} \left[ \frac{1}{\pi} + \left( \frac{29}{6} + 4 \log 2 \right) \frac{\alpha_s}{\pi} \right] \right. + \frac{3}{t^4} \left[ 8\pi^2 f^2_K M^2_K + 2\pi(\alpha_s : G^2 : ) \right] \right\};
\]

\[
\varphi^{(2)}_{us}(t) = \frac{3}{8\pi^2} \left\{ \frac{m^2(t)}{t^4} \left[ \frac{11}{16} + \left( \frac{187}{48} + \log 2 \right) \frac{\alpha_s}{\pi} \right] - \frac{12m^4(t)}{t^5} \left[ \frac{15}{16} + \left( \frac{29}{3} + 4 \log 2 \right) \frac{\alpha_s}{\pi} \right] \right. + \frac{12}{t^6} \left[ 8\pi^2 f^2_K M^2_K + 2\pi(\alpha_s : G^2 : ) \right] \right\}
\]

with \( m = m_s(t) \) the two loop running mass\(^{12}\)

\[
m(t) = m \left( \frac{1}{2} \log t/A^2 \right)^{-d_m} \left[ 1 - d_1 \log \log t/A^2 + d_2 \frac{1}{\log t/A^2} \right];
\]

\[
d_m = \frac{4}{\beta_0}, \quad d_1 = 8 \frac{51 - \beta_0 n_f}{\beta_0}, \quad d_2 = 8 \frac{3}{\beta_0} \left[ \left( \frac{101}{12} - \frac{5}{2} n_f \right) \beta_0 - 51 + \frac{19}{3} n_f \right], \quad \beta_0 = 11 - \frac{2}{7} n_f.
\]

An extra advantage of using the combination giving the \( \varphi^{(N)}(t) \), and not simply the derivatives \( \partial^N F_5(t)/\partial t^N \), is that, as announced, and as Eqs. (3.2) show, the NLO corrections for the first are substantially smaller than for the last. This will make the calculations based on perturbative QCD more reliable.

As discussed, we may combine Eqs. (3.1), (3.2) to derive bounds on \( m_s \). We do so and rewrite the result as

\[
Am_s^4 - Bm_s^2 + C \leq 0
\]

\(^2\)There are more terms known than the ones we use here\(^{9,11}\). The \( O(\alpha_s) \) corrections to the nonperturbative pieces are known, as is also the \( O(m_s^4) \) term. these are all subleading and of the same order in \( 1/t \) as the nonperturbative contributions we have included. Given the small influence of these terms, and the fact that the more important one, the gluon condensate, is very poorly known, we have thought it superfluous to include them. The NNLO correction to the term quadratic in \( m_s \) is also known; but not that for the \( O(m_s^4) \) one. We have preferred to keep symmetry between the two as, for the \( s \) quark case, they are quite comparable. We have checked that the inclusion of this NNLO correction would not substantially alter our results.
where $A, B, C$ may be read from (3.1, 2); for $\varphi^{(0)}$ and to LO,

$$A = \frac{N_c}{8\pi^2} \frac{6}{4t^2}, \quad B = \frac{N_c}{8\pi^2} \frac{1}{4t}, \quad C = \frac{4f_K^2 M_K^4}{(t + M_K^2)^3}$$

and corresponding expressions to NLO. Obviously, Eq. (3.4) only has a solution if

$$B^2 \geq 4AC \tag{3.5}$$

so, unless this condition is satisfied we find an incompatibility between the validity of the QCD expression and positivity. Defining the critical values $t_N$ those for which we get equality in Eq. (3.5), and the corresponding equations obtained from the various terms in Eqs. (3.2), we get the values

$$t_0 = \begin{cases} 1.76 \text{ GeV}^2 & \text{LO} \\ 1.47 \text{ GeV}^2 & \text{NLO} \\ 1.36 \text{ GeV}^2 & \text{NLO + NP} \end{cases}, \quad t_1 = \begin{cases} 2.09 \text{ GeV}^2 & \text{LO} \\ 1.75 \text{ GeV}^2 & \text{NLO} \\ 1.61 \text{ GeV}^2 & \text{NLO + NP} \end{cases}, \quad t_2 = \begin{cases} 2.46 \text{ GeV}^2 & \text{LO} \\ 2.22 \text{ GeV}^2 & \text{NLO} \\ 2.04 \text{ GeV}^2 & \text{NLO + NP} \end{cases} \tag{3.6}$$

The tag “NP” indicates that we have included the nonperturbative pieces as in Eqs. (3.2); we have taken the following values for the parameters

$$M_K = 495.7 \text{ MeV}, \quad f_K = 115 \text{ MeV}, \quad \Lambda(n_f = 3, 1 \text{ loop}) = 300 \text{ MeV}.$$  

It is interesting to note that the values of the $t_N$ do not change much from LO to NLO to NLO + NP and that they generally decrease from LO to NLO to NLO + NP, as would be expected: one imagines that the NLO expression is valid for smaller values of $t$ than the LO one, and also that including NP effects improves the convergence. The values of $t_N$ found are rather large: comparable to the lower range among those employed in the calculations of e.g. refs. 7, 8, 9. If we assumed that the perturbative QCD expression would be valid as soon as $t = t_N$ (something that cannot be the case) we would have obtained evaluations of $m_s$. These give too large values, such that $m_s(1 \text{ GeV}^2) \approx 450 \text{ MeV}$. What we do is to consider that the QCD evaluation of the $N$th derivative at $t$ is to be trusted if the QCD evaluation of the next derivative $N + 1$ is compatible with positivity. Thus, at LO we can use the zeroth derivative if $t \geq t_1 = 2.09 \text{ GeV}^2$, and the first one if $t \geq t_2 = 2.46 \text{ GeV}^2$. We will refer to the bounds so obtained as optimum, or optimist bounds. Alternatively, we may want to play it safe and require $t \geq 2t_N$. The corresponding bounds are reported in Table I, where we have also included the bounds obtained for $N = 2$ and $t = 6.5 \text{ GeV}^2$.

<table>
<thead>
<tr>
<th></th>
<th>LO</th>
<th>NLO</th>
<th>NLO + NP</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N = 0$:</td>
<td>$t_1$</td>
<td>$295 &lt; m_s &lt; 596$</td>
<td>$240 &lt; m_s &lt; 477$</td>
</tr>
<tr>
<td></td>
<td>$2t_1$</td>
<td>$158 &lt; m_s &lt; 1018$</td>
<td>$142 &lt; m_s &lt; 847$</td>
</tr>
<tr>
<td>$N = 1$:</td>
<td>$t_2$</td>
<td>$308 &lt; m_s &lt; 609$</td>
<td>$234 &lt; m_s &lt; 527$</td>
</tr>
<tr>
<td></td>
<td>$2t_2$</td>
<td>$162 &lt; m_s &lt; 1048$</td>
<td>$140 &lt; m_s &lt; 916$</td>
</tr>
<tr>
<td>$N = 2$:</td>
<td>$t = 6.5$:</td>
<td>$156 &lt; m_s &lt; 1140$</td>
<td>$129 &lt; m_s &lt; 1038$</td>
</tr>
</tbody>
</table>

Table I. Bounds, in MeV, for various values of $t$ on $m_s \equiv m_s(1 \text{ GeV}^2)$.

The bounds are stable from LO to NLO to NLO + NP, and also for the various values of $N$. The upper bound is not very interesting, as it is well above all existing estimates; but the lower one is very tight, as, indeed, it is violated by several of the calculations found in the literature (refs. 1, 8, 9) and is barely compatible with others[5, 6]. We will discuss this in a latter section. For the moment we summarize the lower bounds in the two possibilities,

$$\begin{align*}
\text{Optim. bound:} & \quad 244 \text{ MeV} < m_s \\
\text{Safe bound:} & \quad 149 \text{ MeV} < m_s. \tag{3.7}
\end{align*}$$

§4. Lower bounds on $m_d \pm m_u$
4.1. Lower bound on $m_d + m_u$

The combination $ud$ allows us to derive bounds on $m_d + m_u$. The equations are similar to (3.1, 2) with the replacement $m_s \rightarrow m_d + m_u$, $f_K \rightarrow f_\pi = 95$ MeV and $M_K \rightarrow M_\pi = 137.3$ MeV and, moreover, taking $n_f = 2$, $\Lambda = 350$ MeV. The term in $m^4$ is slightly different, but it is utterly negligible now: for this reason only lower bounds may be obtained. We choose the values of the $t$ at which we calculate the bounds to be the same as those for the $s$ quark case. Specifically, we define throughout this section $t_1 = 1.75$ GeV$^2$, $t_2 = 2.22$ GeV$^2$. Then we have the results in Table II,

<table>
<thead>
<tr>
<th>NLO, $t_1 = 1.75$ GeV$^2$:</th>
<th>$16.3 &lt; m_d + m_u$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N = 0$</td>
<td>$2t_1 = 3.5$ GeV$^2$:</td>
</tr>
<tr>
<td>NLO, $t_2 = 2.2$ GeV$^2$:</td>
<td>$16.7 &lt; m_d + m_u$</td>
</tr>
<tr>
<td>$N = 1$</td>
<td>$2t_2 = 4.5$ GeV$^2$:</td>
</tr>
<tr>
<td>NLO, $N = 2$: $t = 6.5$ GeV$^2$:</td>
<td>$9.0 &lt; m_d + m_u$</td>
</tr>
</tbody>
</table>

Table II. NLO bounds in, MeV, for $m_d + m_u \equiv m_d(1$ GeV$^2) + m_u(1$ GeV$^2)$.

The bounds are also now very stable. We may, as for the $s$ quark case, highlight the best bounds,

$$\begin{align*}
\text{Optim. bound: } & 16.5 \text{ MeV} < m_d + m_u \\
\text{Safe bound: } & 9.8 \text{ MeV} < m_d + m_u.
\end{align*}$$

(4.1)

It may perhaps be remarked that the bounds for the $m_d + m_u$ combination are more reliable than for the $m_s$ case. This is because the NP contributions are much smaller in this case. At the values of $t$ we are considering of just a few percent; and the same is true of $O(m^6)$ ones, still smaller.

4.2. Lower bound on $m_d - m_u$

We now consider the difference between $\varphi_{ds}$ and $\varphi_{us}$. We will still be able to calculate this from QCD, but a rigorous proof of the positivity of

$$\delta \Psi(s) \equiv \Psi^{ds}_S(s) - \Psi^{us}_S$$

is not possible. However, it is very likely that this positivity holds; in fact, it follows in the chiral SU(2) limit provided one assumes that $(m_d - m_u)/m_d \gg (m_d, m_u)/m_s$, an inequality that is amply satisfied in all estimates. Moreover, the positivity of $\delta \Psi(s)$ may be checked experimentally on the Kaon pole, and from QCD at large $s$. So we will assume it.

A second problem now is that we have to subtract, from the pole terms, the electromagnetic contributions to the mass differences, as they are comparable to the masses themselves. We will use for this the chiral dynamics estimate\[13\]

$$M_{K^0}^2 - M_{K^+}^2 = (1.9 \pm 0.5)M_{K^0}^2 - M_{\pi^+}^2$$

so we replace, in the difference of the pole terms,

$$M_{K^0}^4 - M_{K^+}^4 \rightarrow \delta M_{K}^4 \equiv (M_{K^0}^4 - M_{K^+}^4)_{\text{physical}} - (M_{K^0}^4 - M_{K^+}^4)_{\text{c.m.}} = (5.18 \pm 0.48)M_{K}^4.$$

(4.2)

We will furthermore assume that $f_{K^+} = f_{K^0}$. We thus have, from QCD and using the NLO calculations of refs. 4, 10,

$$\begin{align*}
\delta \varphi^{(0)}(t) = & \frac{2N_c\Delta}{8\pi^2t} \left\{ t \left[ 1 + \left( \frac{7}{8} + 2 \log 2 \right) \frac{\alpha_s}{\pi} \right] - m_s^2 t \left( \frac{1}{8} + \left( \frac{7}{8} + 4 \log 2 \right) \frac{\alpha_s}{\pi} \right) \right\}, \\
\delta \varphi^{(1)}(t) = & \frac{6N_c\Delta}{8\pi^2t^2} \left\{ \frac{1}{6} + \left( \frac{7}{8} + \frac{7}{8} \log 2 \right) \frac{\alpha_s}{\pi} \right] - \frac{m_s^2}{t \left( \frac{1}{12} + \left( \frac{7}{8} + \frac{8}{8} \log 2 \right) \frac{\alpha_s}{\pi} \right) \right\},
\end{align*}$$

$$\Delta = m_s(t) [m_d(t) - m_u(t)]$$

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We now get two types of bounds. If we make no assumptions on \(m_s\), we still obtain lower bounds on \(m_d - m_u\); but of course much better bounds are obtained if assuming a reasonable value for the strange quark mass. The results are given in Table III.

\[
\begin{array}{l}
NLO, \quad t_1 : \ 6.22 \pm 0.6 < m_d - m_u \\
N = 0 \quad 2t_1 : \ 2.57 \pm 0.3 < m_d - m_u \\
NLO, \quad t_2 : \ 6.32 \pm 0.6 < m_d - m_u \\
N = 1 \quad 2t_2 : \ 2.52 \pm 0.3 < m_d - m_u \\
\end{array}
\]

Table III. Bounds, in MeV, for \(m_d - m_u \equiv m_d(1 \text{ GeV}^2) - m_u(1 \text{ GeV}^2)\). \(m_s(1 \text{ GeV}^2) = 200\) MeV.

The bounds are also here very stable. If we leave \(m_s\) as a free parameter the bounds deteriorate and we find,

\[
N = 0; \quad t_1 : \ m_d - m_u > 3.37 \text{ MeV}; \quad N = 1; \quad t_2 : \ m_d - m_u > 3.33 \text{ MeV}
\]

and they are obtained with \(m_s \sim 530\) MeV. For the choice \(2t_1, 2t_2\) the bounds decrease to 1 MeV and are attained with \(m_s \sim 800\) MeV. The bounds for \(m_s = 200\) MeV are very tight in the sense that they essentially coincide with the existing estimates\(^5,6\). This poses the problem of the errors, and corrections to the bounds, to which we now turn.

§5. Errors and corrections to the bounds. Estimates of masses

It is not the purpose of this paper to present a new evaluation of light quark masses; but we want to give at least estimates of how much the bounds may be expected to deviate from the true values of these quantities. We will give the detailed calculations for \(m_d + m_u\), for which the methods are more reliable, and at the end present the results corresponding to \(m_s\). Also we will consider the case \(N = 1\), assuming perturbative QCD to be valid above \(\hat{t}\), with \(t = t_2 = 2.2\) GeV\(^2\) and \(\hat{t} = 2t_2 = 4.5\) GeV\(^2\).

Let us rewrite the equations for clarity of reference. From (3.1b) and the equation for \(ud\) analogous to (3.2b) we have, equating the QCD expression and the dispersive representation,

\[
\frac{[m_d(t) + m_u(t)]^2}{2t^2} = \frac{12f_\pi^2M_\pi^4}{(t + M_\pi^2)^4} + \frac{6}{\pi} \int_{s_0}^{t} ds \frac{\Im \Psi_5(s)}{(s + t)^4}, \quad s_0 = 9M_\pi^2.
\]

(We have written the LO expression, but NLO evaluations will be performed throughout this section). If \(\Im \Psi_5(s)\) vanished in the interval \(s_0 \leq s \leq \hat{t}\) then, by putting \(t = \hat{t}\) in Eq. (5.1) the lower bounds would become equalities. So, to determine how tight are the bounds, and to estimate \(m_d + m_u\) we require models for \(\Im \Psi_5(s)\) in that low momentum region.

In the lower end of the interval we may use chiral dynamics to evaluate the contribution of the 3\(\pi\) intermediate state. The calculation is elementary and one finds\(^9\)

\[
\Im \Psi_5(s) = \frac{M_\pi^2}{768\pi^3f_\pi^2},
\]

an approximation that we expect to be valid until the opening of the \(\rho \pi\) threshold, at \(s = s_{\rho \pi} = (M_\rho + M_\pi)^2\). The contribution of (5.2) is minute, and will consequently be neglected. From \(s_{\rho \pi}\) onwards we expect that the continuum of \(\Im \Psi_5(s)\) will be dominated by the \(\rho \pi\) intermediate state as happens e.g. in \(e^+ e^- \rightarrow \text{hadrons}\) annihilations. One could estimate the contribution of this channel with the help of vector meson dominance in the soft limit, which is certainly not a very accurate model. Since we are only interested in an estimate
we will merely interpolate between zero at $s_{\rho\pi}$ and the QCD perturbative value at $\hat{t}$. Thus we consider $\text{Im} \Psi_{5}^{\text{continuum}} \simeq \text{Im} \Psi_{5}^{\text{pert, QCD}}$ and

$$
\frac{1}{\pi} \text{Im} \Psi_{5}^{\pi}(s) = \begin{cases} 
0, s \leq s_{\rho\pi} \\
\frac{3}{8\pi^{2}} \frac{[m_{d}(\hat{t}) + m_{u}(\hat{t})]^{2}}{t - s_{\rho\pi}} s(s - s_{\rho\pi}) \left[1 + \frac{17\alpha_{s}(\hat{t})}{3\pi}\right], s_{\rho\pi} \leq s \leq \hat{t}
\end{cases}
$$

(5.3)

so that $\text{Im} \Psi_{5}^{\pi}(\hat{t}) = \text{Im} \Psi_{5}^{\text{pert, QCD}}(\hat{t})$.

Besides the $\rho\pi$ continuum we have the contribution of the $\pi' = \pi(1300)$ resonance. We may write this as

$$
\frac{6}{\pi} \text{Im} \Psi_{5}^{\pi'}(s) = 12r f_{\pi}^{2} M_{\pi}^{4} \delta(s - M_{\pi}^{2}).
$$

(5.4)

The quantity $r$, ratio between the wave functions at the origin of the $\bar{u}d$ in the $\pi$, $\pi'$, is not known, nor can it be obtained in any direct manner from the $\pi'$ width. In a constituent quark model, $r \sim 0.3$ to 0.5; and similar values are obtained in bag models. In a purely Coulombic model one would get $r = 1/8$. So we allow $r$ to vary in the range 0 $\leq r \leq 0.5$. Anyway, the contribution of the $\pi'$ is rather small.

With all this we write

$$
\frac{6}{\pi} \int_{s_{0}}^{\hat{t}} ds \frac{\text{Im} \Psi_{5}(s)}{(s + t)^{4}} \simeq \frac{12f_{\pi}^{2}M_{\pi}^{4}}{(t + M_{\pi}^{2})^{4}} r + \frac{6}{\pi} \int_{s_{\rho\pi}}^{\hat{t}} ds \frac{\text{Im} \Psi_{5}^{\pi}(s)}{(s + t)^{4}}.
$$

(5.5)

Plugging this into (5.1) with $t = \hat{t} = t_{2}$, $2t_{2}$ we get the estimates reported in Table IV.

<table>
<thead>
<tr>
<th>bound</th>
<th>$r = 0$</th>
<th>$r = 0.25$</th>
<th>$r = 0.5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\hat{t} = t_{2} = 2.2$ GeV$^{2}$</td>
<td>16.7</td>
<td>19.4</td>
<td>19.6</td>
</tr>
<tr>
<td>$\hat{t} = 2t_{2} = 4.5$ GeV$^{2}$</td>
<td>9.8</td>
<td>12.5</td>
<td>12.9</td>
</tr>
</tbody>
</table>

Table IV. Bounds and estimates, in MeV, for $m_{d} + m_{u}$.

As is seen here the main source of error (and a large error it is) comes from the variation of the region $t \geq \hat{t}$ where we believe that perturbative QCD may be applied to evaluate $\text{Im} \Psi_{5}$. On this one has no control. For $e^{+}e^{-} \to$ hadrons we know that the cross section is well described by perturbative QCD from $s \sim 1$ to 2 GeV$^{2}$. If we assume this, then $\hat{t} \sim 2$ GeV$^{2}$ and $m_{d} + m_{u} \sim 20$ MeV. But one may argue that the NLO correction in $e^{+}e^{-} \to$ hadrons is small, $\alpha_{s}/\pi$, while that for $\text{Im} \Psi_{5}$ is large, $17\alpha_{s}/3\pi$. This suggests a latter onset of the perturbative regime for the latter quantity, say at $2t_{2} \sim 4.5$ GeV$^{2}$ and then $m_{d} + m_{u} \sim 13$ MeV.

For $m_{s}$ similar considerations would apply and we get the results summarized in Table V.

<table>
<thead>
<tr>
<th>bound</th>
<th>$r = 0$</th>
<th>$r = 0.25$</th>
<th>$r = 0.5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\hat{t} = t_{2} = 2.2$ GeV$^{2}$</td>
<td>221</td>
<td>242</td>
<td>250</td>
</tr>
<tr>
<td>$\hat{t} = 2t_{2} = 4.5$ GeV$^{2}$</td>
<td>138</td>
<td>169</td>
<td>175</td>
</tr>
</tbody>
</table>

Table V. Bounds and estimates, in MeV, for $m_{s}$.

The estimates take into account NLO and NP corrections. The effective two-body threshold is now given by $K\rho$ or $K^{*}\pi$, with an average mass squared of 1.3 GeV$^{2}$. For the mass of the $K^{*}$ resonance we have guessed $M_{K^{*}} = 1.5$ GeV. Like for $m_{d} + m_{u}$ the resonance contributes little, while a very large variation occurs when we move the region where the onset of the perturbative regime takes place. also in common with the $ud$ case we find that the bound we had obtained are rather tight.

Before finishing this section a few words have to be said to clarify further the meaning of the results reported in Tables IV, V and say a few words comparing them with other derivations. As for the first, we note that our results were obtained by comparing the QCD expression, say for $N = 0$ and the $ud$ case...
\[ F_5^{\text{QCD}}(t), \text{and the dispersive integral, that we may call } F_5^{\text{disp.}}(t), \text{obtained from the model to } s = t \text{ and QCD above it:} \]

\[
F_5^{\text{disp.}}(t) = \frac{4f_2^2M_\pi^4}{(t + M_\pi^2)^3} + \frac{4f_2^2M_\pi^4}{(t + \hat{M}_\rho^2)^3} + \frac{2\int_{\hat{t}}^{t} ds \left( \frac{\text{Im}\Psi_5^{\text{QCD}}(s)}{s + t}\right)^3 + \frac{2\int_{\hat{t}}^{\infty} ds \left( \frac{\text{Im}\Psi_5^{\text{QCD}}(s)}{s + t}\right)^3}{(s + t)^3}}.
\]

The estimates of the Tables correspond to requiring equality at \( \hat{t} \); but of course what is really needed is equality, up to neglected higher order corrections (in our evaluation, \( O(\alpha_s^2) \)), for all \( t \geq \hat{t} \). Equally, as \( t \to \infty \) is guaranteed; so we expect that we will have it for intermediate \( t \) as well. We have checked this numerically for \( N = 0 \), the \( ud \) case with

\[
\hat{t} = 2.2 \text{ GeV}^2, \, r = 0.5, \, m_d + m_u = 19.9 \text{ MeV}.
\]

Here we get, for the ratios \( \rho_0(t) = F_5^{\text{QCD}}(t)/F_5^{\text{disp.}}(t) \), \( \rho_1(t) = F_5^{\text{QCD}}(t)/F_5^{\text{disp.}}(t) \) the values

\[
\begin{array}{c|cccccc}
    t & 2.2 & 4.5 & 8.5 & 30 & 100 & \text{GeV}^2 \\
    \rho_0 & 1.22 & 1.10 & 1.04 & 1.01 & 1.005 & \\
    \rho_1 & 1.06 & 1.03 & 0.96 & 0.93 & 0.94 & \\
\end{array}
\]

i.e., what one would expect\(^3\) for a calculation with an error \( O(\alpha_s^2) \). Actually, virtual equality may be obtained if we replace the rather crude model for \( \text{Im}\Psi_5^{\text{QCD}}(s) \), with a linear threshold (Eq. (5.3)) by a more realistic model, e.g., with a square-root threshold for the \( \rho\pi \) channel.

Lastly, our evaluations show why some other estimates find such small values for the masses. Specifically, considering ref. 9, probably the more complete (from the point of view of perturbative QCD) evaluation of \( m_s \) we see that the very low value for this quantity, \( m_s = 171 \text{ MeV} \), is obtained because the authors there assume that perturbative QCD holds for \( F_5(t) \) for \( t \sim 2 \), \( 3 \text{ GeV}^2 \); but a model is employed for \( \text{Im}\Psi_5(s) \) which is well below the perturbative QCD value up to very large momenta, \( s \sim 6.5 \text{ GeV}^2 \). Furthermore, in the same calculation, we took the perturbative value for \( \text{Im}\Psi_5(s) \) down to 2.2 to 4.5 \text{ GeV}^2 we would get values quite compatible with those reported in Table V, 175 to 250 MeV.

\[ \text{§6. Summary and discussion} \]

The results of this note may be viewed as, first, a set of bounds such that, to go below them would imply that perturbative QCD fails at unreasonably low values of \( t \), say \( t \sim 4 \to 5 \text{ GeV}^2 \): these are the “Safe” bounds of Eqs. (3.7), (4.1). Secondly, we find indications that the actual values may easily be larger (the “Optim.” bounds in the same equations). The evaluations of the last section, Tables IV and V, are to be viewed as “existence proofs” that the bounds can be saturated using reasonable physical assumptions. Putting all together we may draw the conclusion that current estimations of the errors in the evaluations of quark masses are excessively optimistic. We would consider brackets

\[
\begin{align*}
140 \text{ MeV} & \leq m_s \leq 254 \text{ MeV}, \\
10 \text{ MeV} & \leq m_d + m_u \leq 20 \text{ MeV}
\end{align*}
\]

(6.1)

to represent realistic, attainable estimates. For the difference \( m_d - m_u \) the bounds are good only if we restrict \( m_s \). If we assume this to be bounded as in Eq. (6.1), then we find

\[
2 \text{ MeV} \leq m_d - m_u \leq 11 \text{ MeV}
\]

(6.2)
to be a generous, but attainable, bracket.

One may wonder how high one has to put the onset of the perturbative regime if we take values for the quark masses as low as those in some recent lattice and other determinations\(^1,14\). The answer is, impossibly high. Considering for example the \( s \) quark, even if we assume that perturbative QCD is only valid at \( t \geq \hat{t} = 6.5 \text{ GeV}^2 \), and only the use of \( \phi^{(0)} \) is allowed (no derivatives) one still has \( m_s > 110 \text{ MeV} \), and, for \( \hat{t} = 10 \text{ GeV}^2 \), \( m_s > 90 \text{ MeV} \). This assuming that the spectral function vanishes completely below the

---

\(^1\) The fact that the largest error occurs, for \( \rho_0(t) \), at \( t = \hat{t} \) where nominally one should have equality is easily understood if we realize that, to determine the values of \( m_d + m_u \), we have used Eq. (3.2a), which only coincides with \( F_5(t) \) minus the integral \( 2\int_{\hat{t}}^{\infty} ds \left( \frac{\text{Im}\Psi_5^{\text{QCD}}(s)}{\pi(s + t)} \right)^3 \) to corrections \( O(1/\log^2 t/\Lambda^2) \).
corresponding values of \( t \): if we include estimates for the low momentum piece like those in §4 we increase the values of \( m_s \) by at least 25\%. For the combination \( m_d + m_u \) the corresponding bounds are 8 and 7 MeV.

We want finally to say a few words about bounds on the individual \( u, d \) masses, and the connections among the various determinations. In the present work we have only used perturbative QCD and positivity; but more information may be obtained using chiral dynamics evaluations that permit estimates of ratios of quark masses. Using this one may disentangle relations like (6.1, 2). This is what is done in a recent paper by Lelouch, de Rafael and Taron\cite{15}, in which questions similar to the ones raised here are also discussed. This paper, which appeared after the present work was finished, is largely complementary to ours: as stated, chiral dynamics estimations of the mass ratios are included, but the question of the compatibility of perturbative QCD with positivity is not raised.

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References