LIGHT QUARK MASSES IN QUANTUM CHROMODYNAMICS ^{†)}
AND CHIRAL SYMMETRY BREAKING

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ABSTRACT

We derive model independent lower bounds for the sums of effective quark masses $\bar{m}_u + \bar{m}_d$ and $\bar{m}_u + \bar{m}_s$. The bounds follow from the combination of the spectral representation properties of the hadronic axial currents two-point functions and their behaviour in the deep euclidean region (known from a perturbative QCD calculation to two loops and the leading non-perturbative contribution). The bounds incorporate PCAC in the Nambu-Goldstone version. If we define the invariant masses $\hat{m}$ by

$$\bar{m}_1 = \hat{m}_1 \frac{1}{2} (\log Q^2/\Lambda^2)^{2\gamma_1/\beta_1},$$

and $\langle F^2 \rangle$ is the vacuum expectation value of

$$F^2 = \int_a F_{(a)}^{\mu\nu} F_{\mu\nu}(a),$$

we find, e.g.,

$$\hat{m}_u + \hat{m}_d \geq \sqrt{\frac{2\pi}{3}} \cdot \frac{8f_\pi m_\pi^2}{3\langle\alpha_s F^2\rangle^{\frac{1}{2}}};$$

with the value $\langle\alpha_s F^2\rangle \approx 0.04 \text{ GeV}^2$, recently suggested by various analysis, this gives

$$\hat{m}_u + \hat{m}_d \geq 30 \text{ MeV}$$

The corresponding bounds on $\hat{m}_u + \hat{m}_s$ are obtained replacing $m_\pi^2 f_\pi$ by $m_K^2 f_K$. The PCAC relation can be inverted, and we get upper bounds on the spontaneous masses, $\hat{\mu}$:

$$\hat{\mu} \leq 170 \text{ MeV},$$

where $\hat{\mu}$ is defined by

$$\langle\bar{\psi}\psi\rangle(Q^2) = (\frac{1}{2} \log Q^2/\Lambda^2)^d \hat{\mu}^3, \quad d = 12/(33 - 2n_f).$$

^{†)} This is a revised and expanded version of the section concerning light quark masses in the preprint "Quark Masses and Perturbative QCD" by S. Narison, E. de Rafael and F.J. Yndurain, CPT preprint 80/p.1186 March 1980, (unpublished).

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1. INTRODUCTION

We propose to look at the question of light quark masses from the point of view of the operator product expansion at short distances¹⁾ in the two-point function

$$\psi_5(q^2) = i \int d^4x e^{iq \cdot x} \langle 0 | T (\partial_\mu A^\mu(x)) \partial_\nu A_\nu(0)^+ | 0 \rangle, \quad (1.1)$$

where $\partial_\mu A^\mu(x)$ denotes the divergence of the axial current with the quantum numbers of π^+ or K^+ . We shall assume that the underlying dynamics of the strong interactions is governed by the Lagrangian of quantum chromodynamics²⁾

$$\begin{aligned} \mathcal{L}_{\text{QCD}} = & -\frac{1}{4} F_{\mu\nu}^{(a)} F_{(a)}^{\mu\nu} + i \sum_{j=1}^n \bar{\psi}_j \gamma^\mu D_\mu \psi_j \\ & - \sum_{j=1}^n m_j \bar{\psi}_j \psi_j + \text{gauge fixing} + \text{ghost terms}, \end{aligned} \quad (1.2)$$

where $F_{\mu\nu}^{(a)}(x)$ $a = 1, 2, \dots, 8$ are the Yang-Mills field strengths constructed from the gluon fields $W_\mu^{(a)}$,

$$F_{\mu\nu}^{(a)} = \partial_\mu W_\nu^{(a)} - \partial_\nu W_\mu^{(a)} + g f_{abc} W_\mu^{(b)} W_\nu^{(c)}, \quad (1.3)$$

and $(D_\mu)_{\alpha\beta}$ the covariant derivative acting on the quark colour components $\alpha, \beta = \text{blue, red and yellow}$,

$$D_{\alpha\beta}^\mu = \delta_{\alpha\beta} \partial^\mu - i \frac{1}{2} \lambda_{\alpha\beta}^{(a)} W_{(a)}^\mu. \quad (1.4)$$

The matrices $\lambda_{\alpha\beta}^{(a)}$ are the eight 3×3 Gell-Mann matrices and f_{abc} the structure constants of the colour $SU(3)$ algebra. The parameters of the theory are the gauge coupling constant g and the quark masses m_j ($j = \text{up, down, strange, charm, ...}$) of the various quark flavours, n in total. In this framework, the flavour non-singlet currents of the algebra of currents^{*)} of Gell-Mann are generated by $SU(n) \times SU(n)$ global gauge transformations of the QCD, Lagrangian, e.g.,

*) See, e.g., Ref. 3) where the original references can also be found.

$$A_\mu^a(x) = \bar{\psi}_d(x) \gamma^\mu \gamma_5 \psi_u(x) \quad (1.5)$$

where a trace over the colour degree of freedom of the quark fields is understood. In the presence of the quark mass terms in the QCD Lagrangian, the global $SU(n) \times SU(n)$ chiral symmetry is broken and the non-singlet axial currents are not conserved

$$\partial_\mu A_\mu^a(x) = (m_i + m_j) \bar{\psi}_i(x) i \gamma_5 \psi_j(x). \quad (1.6)$$

This is the way that quark masses appear in the two-point function in Eq. (1).

Because of the expected confinement property of QCD, quark masses (unlike lepton masses) are not directly measurable and we can only have access to them via their observed bound states, (i.e., the hadrons), and their interactions. This explains the diversity of quark mass values (in particular for the up and down quarks) which one can find in the literature^{*)}. In most cases, this diversity corresponds to different definitions: constituent quarks⁵⁾, current algebra quarks⁶⁾, MIT bag quarks⁷⁾, etc ... The main difficulty in comparing different definitions comes from the fact that most of them appeal to the long distance behaviour of QCD of which we still have very little quantitative understanding.

There have been various attempts to relate quark masses, defined via a specific renormalization prescription in perturbative QCD, to low energy parameters like hadron masses and coupling constants. One possible method is that of the finite energy sum rules discussed in Refs 8) and 9); another, the magic moments¹⁰⁾ of Shifman, Vainshtein and Zakharov¹¹⁾; or some other version of the duality concept^{**)}.

There is a good agreement between these methods in the determination of the charm quark mass; but it is our belief that nothing clear and definite has yet come out for the absolute scale of the lighter quarks.

In this paper we discuss how to obtain rigorous lower bounds for the combination of light quark masses

$$\hat{m}_u + \hat{m}_d, \quad \hat{m}_u + \hat{m}_s.$$

*) For a recent review see Refs 4).

**) See, e.g., Ref. 10) where a complete list of references can be found.

These are the scale invariant masses of the dimensional renormalization scheme¹²⁾, which at the one-loop level are related to the running mass $\hat{m}(Q^2)$ via the expression^{*)}

$$\bar{m}(Q^2) = \frac{\hat{m}}{(\frac{1}{2} \log Q^2/\Lambda^2)^{-2/\beta}} \quad (1.7)$$

where $\beta_1 = -11/2 + n/3$; n is the number of flavours; and Λ the invariant scale associated to the QCD coupling constant. These masses have the virtue of having ratios equal to those of the corresponding bare masses for which we have some information from PCAC. The bounds are obtained by combining the positivity properties of the spectral representation of the two-point function $\psi_5(q^2)$ in Eq. (1.1), with an explicit calculation at the two-loop level of the function $\psi_5(q^2)$ and their successive derivatives in the deep euclidean region $-q^2 = Q^2 \gg \Lambda^2$. The calculation of $\psi_5(q^2)$ includes both perturbative and non-perturbative terms. This is where the operator product expansion becomes relevant. The leading non-perturbative effects then appear parametrized in terms of the physical vacuum expectation values of $\bar{\psi}\psi$ and $F^{\mu\nu}F_{\mu\nu}$ operators,

$$m \langle \bar{\psi}\psi \rangle \quad \text{and} \quad \alpha_s \langle F^{\mu\nu}F_{\mu\nu} \rangle$$

with appropriate coefficients which are explicitly evaluated.

As we shall see, it is crucial to incorporate terms of the type $m\langle\bar{\psi}\psi\rangle$ if we want the bounds for $\hat{m}_u + \hat{m}_d$ to be consistent with the Nambu-Goldstone realization of PCAC^{6),14)}. This is precisely the reason why we choose to work with the function ψ_5 in Eq. (1.1), instead of the non-transverse invariant function $D^2(q^2)$ associated to the two-point function

$$\begin{aligned} \Pi_5^{\mu\nu}(q) &= i \int d^4x e^{iq \cdot x} \langle 0 | T A^\mu(x) A^\nu(0)^+ | 0 \rangle \\ &= (-g^{\mu\nu} q^2 + q^\mu q^\nu) \Pi_5(q^2) + g^{\mu\nu} D_5(q^2). \end{aligned} \quad (1.8)$$

The next section gives a detailed discussion of this question.

*) See, e.g., Ref. 13).

The bulk of the paper is contained in the next two sections, except for the technical details of the calculations which can be found in the Appendices. The results are discussed in Section 4.

2. CURRENT ALGEBRA, PCAC AND QCD

There is a familiar current algebra Ward identity between the two-functions $\psi_5(q^2)$ and $\Pi_5^{\mu\nu}(q)$ defined in Eqs (1.1) and (1.8) in the introduction:

$$\begin{aligned} i q_\mu q_\nu \Pi_5^{\mu\nu}(q) &= q^2 D_5(q^2) = \psi_5(q^2) \\ &- q_\nu \int d^4x e^{iq \cdot x} \delta(x^0) \langle 0 | [A^0(x), A^\nu(0)^+] | 0 \rangle \\ &+ i \int d^4x e^{-iq \cdot x} \delta(x^0) \langle 0 | [\partial_\mu A^\mu(0), A^0(x)^+] | 0 \rangle. \end{aligned} \quad (2.1)$$

For the sake of definiteness, unless otherwise stated, $A(x)$ will stand from now onwards for the isospin axial current

$$A^\mu(x) = \bar{\psi}_d(x) \gamma^\mu \gamma_5 \psi_u(x). \quad (2.2)$$

At $q = 0$, the identity in Eq. (2.1) reduces to

$$\psi_5(0) = -i(m_u + m_d) \langle 0 | [\bar{\psi}_d(0) i \gamma_5 \psi_u(0), Q_5^+] | 0 \rangle \quad (2.3)$$

where Q_5 is the axial charge generator

$$Q_5 = \int d\vec{x} A^0(\vec{x}, 0). \quad (2.4)$$

In the Nambu-Goldstone realization of chiral symmetry, this charge does not annihilate the physical vacuum, and we get

$$\psi_5(0) = -(m_u + m_d) \langle 0 | \bar{\psi}_d(0) \psi_d(0) + \bar{\psi}_u(0) \psi_u(0) | 0 \rangle. \quad (2.5)$$

On the other hand, the operator version of PCAC states that

$$\partial_\mu A^\mu(x) = \sqrt{2} f_\pi m_\pi^2 \phi_\pi(x), \quad (2.6)$$

where ϕ_π stands for the interpolating π^+ field; and f_π is the fundamental pion decay constant determined from $\pi \rightarrow \mu\nu$ decay, $f_\pi \approx 93.3$ MeV. Inserting Eq. (2.6) in the definition of $\psi_5(q^2)$ in Eq. (1.1), we obtain the PCAC result

$$\begin{aligned} \psi_5(q^2) \Big|_{\text{PCAC}} &= 2 f_\pi^2 m_\pi^2 i \int d^4x e^{iq \cdot x} \langle 0 | T \phi(x) \phi(0)^\dagger | 0 \rangle \\ &= \frac{2 f_\pi^2 m_\pi^4}{-q^2 + m_\pi^2}, \quad q \rightarrow 0, \end{aligned} \quad (2.7)$$

and from the comparison between Eqs (2.5) and (2.7) we get the well-known PCAC relation

$$(m_u + m_d) \langle \bar{\psi}_u \psi_u + \bar{\psi}_d \psi_d \rangle = -2 f_\pi^2 m_\pi^2. \quad (2.8)$$

In the Nambu-Goldstone realization of chiral symmetry, both $\langle \bar{\psi}\psi \rangle$ and f_π are non-zero, and the pion appears in a massless Goldstone particle. From Eq. (2.8) it then follows that in the chiral limit the up and down quark masses must vanish as the pion mass squared.

From the point of view of QCD, Eq. (2.8) as derived above stands for bare quantities. In the dimensional renormalization scheme, the renormalization of the composite operator $\bar{\psi}\psi$ and the renormalization of the mass compensate each other exactly; therefore Eq. (2.8), as it stands, is also valid for renormalized quantities in the minimal subtraction scheme (MS scheme).

It is instructive to examine the current algebra Ward identity written in Eq. (2.1) at the one-loop level in QCD perturbation theory. In fact, here, the one-loop level corresponds to the zeroth order QCD perturbation theory since no gluons are involved, i.e., to the free quark model. The relevant quark loop diagrams are shown in Fig. 1. The identity in question, in $n = 4 - \epsilon$ dimensions, reads as follows^{*)}

^{*)} To the reader worried about γ_5 manipulations we recommend the paper by Trueman in Ref. 15).

$$\begin{aligned}
 & -3i \int \frac{d^n p}{(2\pi)^n} \text{Tr} \left\{ \not{p} \gamma_5 \frac{i}{\not{p}-m_u} \not{p} \gamma_5 \frac{i}{\not{p}-q-m_d} \right\} \\
 & = (m_u + m_d)^2 (-3i) \int \frac{d^n p}{(2\pi)^n} \text{Tr} \left\{ \gamma_5 \frac{i}{\not{p}-m_u} \gamma_5 \frac{i}{\not{p}-q-m_d} \right\} \\
 & + (m_u + m_d) (-3i) \int \frac{d^n p}{(2\pi)^n} \text{Tr} \left\{ \frac{i}{\not{p}-q-m_d} - \frac{i}{\not{p}-m_u} \right\}.
 \end{aligned} \tag{2.9}$$

The term in the left-hand side is the lowest order expression for $q^2 \cdot D_5(q^2)$. The first term in the right-hand side is the corresponding lowest order expression for $\psi_5(q^2)$. The interesting term is the last one in the right-hand side. It gives a q^2 independent contribution of higher order to the chiral symmetry breaking. More precisely we find,

$$\begin{aligned}
 q^2 D_5(q^2) &= \psi_5(q^2) + \frac{3}{4\pi^2} (m_u + m_d) \left\{ \left(\frac{2}{\epsilon} + \log 4\pi - \gamma_E + 1 \right) (m_u^3 + m_d^3) \right. \\
 &\quad \left. - \left(m_u^3 \log \frac{m_u^2}{\nu^2} + m_d^3 \log \frac{m_d^2}{\nu^2} \right) \right\},
 \end{aligned} \tag{2.10}$$

where γ_E is the Euler constant ($\gamma_E = 0.577 \dots$), and

$$\begin{aligned}
 D_5(q^2) &= \frac{3}{8\pi^2} (m_u + m_d)^2 \left(\frac{2}{\epsilon} + \log 4\pi - \gamma_E \right) \\
 &- \frac{3}{4\pi^2} \int_0^1 dx \left[m_u^2 x + m_d^2 (1-x) + m_u m_d \right] \log \frac{x m_u^2 + (1-x) m_d^2 - x(1-x) q^2}{\nu^2}.
 \end{aligned} \tag{2.11}$$

There is an arbitrary mass scale ν which appears because of the dimensional regularization we have used. In fact, there is also an over-all $(\nu^2)^{-\epsilon/2}$ factor which has been reabsorbed in the definition of a dimensional external coupling (e.g., the weak coupling constant). The identity in Eq. (2.10) show that even in perturbation theory, it is only the leading chiral symmetry breaking terms in

$q^2 D_5(q^2)$ and $\psi_5(q^2)$ which are equal. The non-leading terms contribute differently to $q^2 D_5(q^2)$ and $\psi_5(q^2)$, their difference at that order being precisely

$$\begin{aligned} \psi_5(0) \Big|_{\text{pert}} &= -\frac{3}{4\pi^2} (m_u + m_d) \left\{ \left(\frac{2}{\epsilon} + \log 4\pi - \gamma_E + 1 \right) (m_u^3 + m_d^3) \right. \\ &\quad \left. - \left(m_u^3 \log \frac{m_u^2}{\nu^2} + m_d^3 \log \frac{m_d^2}{\nu^2} \right) \right\}. \end{aligned} \quad (2.12)$$

On the other hand $\psi_5(q^2)$ and $q^2 D_5(q^2)$ have the same absorptive part which can be easily evaluated if we remember that the argument of the log in the right-hand side of Eq. (2.11) has a small imaginary part [i.e., with $R^2 = -q^2 \times (1-x) + m_u^2 x + m_d^2(1-x)$, $\log(R^2 - i\epsilon) = \log|R^2| - i\pi \Theta(-R^2)$]. This way we obtain the well-known result

$$\begin{aligned} \text{Im } \psi_5(t) &= t \text{ Im } D_5(t) \\ &= \frac{3}{8\pi^2} (m_u + m_d)^2 t \left(1 - \frac{(m_d - m_u)^2}{t} \right) \lambda^{1/2} \left(t, \frac{m_u^2}{t}, \frac{m_d^2}{t} \right) \theta(t - (m_u + m_d)^2). \end{aligned} \quad (2.13)$$

Let us now discuss the relevance of the previous remarks to the question of quark masses. From the explicit expression of $D_5(q^2)$ in Eq. (2.11) it is clear that we can get rid of the dependence in the external renormalization if we work with the quantity ($Q^2 \equiv -q^2$)

$$\phi(Q^2) = \frac{\partial}{\partial q^2} D_5(q^2), \quad (2.14)$$

instead of $D_5(q^2)$ itself. By contrast $\psi_5(q^2)$ requires two derivatives to get rid of the $1/\epsilon$ terms. Perturbatively, the two-functions have the same leading behaviour at large Q^2

$$\begin{aligned} \phi(Q^2) &= \frac{3}{8\pi^2} \cdot \frac{(m_u + m_d)^2}{Q^2} \left\{ 1 - \frac{2}{m_u + m_d} \left(\frac{m_u^3}{Q^2} \log \frac{Q^2}{m_u^2} \right. \right. \\ &\quad \left. \left. + \frac{m_d^3}{Q^2} \log \frac{Q^2}{m_d^2} \right) + O\left(\frac{m^4}{Q^4}\right) \right\}, \end{aligned} \quad (2.15)$$

and

$$\begin{aligned}\psi_5''(Q^2) &= \frac{\partial^2 \psi}{(\partial q^2)^2} \\ &= \frac{3}{8\pi^2} \cdot \frac{(m_u+m_d)^2}{Q^2} \left\{ 1 - \frac{m_u^2+m_d^2 + (m_u-m_d)^2}{Q^2} + O\left(\frac{m^4}{Q^4} \log \frac{Q^2}{\mu^2}\right) \right\},\end{aligned}\quad (2.16)$$

though they differ in their next-to-leading behaviour, as explicitly exhibited above. They obey the following dispersion relations

$$\phi(Q^2) = \frac{1}{\pi} \int_{(m_u+m_d)^2}^{\infty} dt \frac{1}{(t+Q^2)^2 t} \operatorname{Im} \psi_5(t) \quad (2.17)$$

and

$$\psi_5''(Q^2) = \frac{2}{\pi} \int_{(m_u+m_d)^2}^{\infty} dt \frac{1}{(t+Q^2)^3} \operatorname{Im} \psi_5(t). \quad (2.18)$$

Eventually, the connection between QCD and hadronic physical observables will be made via the identification at "sufficiently large Q^2 " of these integrals with the corresponding hadronic integrals, i.e., asymptotically

$$\phi(Q^2) = \frac{1}{\pi} \int_{m_\pi^2}^{\infty} dt \frac{1}{(t+Q^2)^2 t} \operatorname{Im} \psi_5^{(H)}(t) \quad (2.19)$$

and

$$\psi_5''(Q^2) = \frac{2}{\pi} \int_{m_\pi^2}^{\infty} dt \frac{1}{(t+Q^2)^3} \operatorname{Im} \psi_5^{(H)}(t), \quad (2.20)$$

where $(1/\pi) \text{Im } \psi_5^{(H)}(t)$ denotes the hadronic absorptive amplitude given by the expression

$$\begin{aligned} \text{Im } \psi_5^{(H)}(t) = & \frac{1}{2} \sum_{\pi} \langle 0 | \partial_{\mu} A^{\mu}(0) | \pi \rangle \langle \pi | \partial_{\nu} A^{\nu}(0)^{\dagger} | 0 \rangle \\ & \times (2\pi)^4 \delta(q - p_{\pi}), \end{aligned} \quad (2.21)$$

with a summation extended to all possible hadron states with the quantum numbers of the π^+ . The pion itself gives a $\delta(t - m_{\pi}^2)$ contribution to the dispersion integrals above which can be evaluated explicitly. Therefore, at sufficiently large Q^2 , one would expect from Eqs (2.15) and (2.19) that

$$\frac{3}{8\pi^2} \cdot \frac{(m_u + m_d)^2}{Q^2} = \frac{2f_{\pi}^2 m_{\pi}^2}{(Q^2 + m_{\pi}^2)^2} + \frac{1}{\pi} \int_{m_{\pi}^2}^{\infty} dt \frac{1}{(t + Q^2)^2 t} \text{Im } \psi^{(H)}(t) \quad (2.22)$$

and from Eqs (2.16) and (2.20), that

$$\frac{3}{8\pi^2} \cdot \frac{(m_u + m_d)^2}{Q^2} = \frac{4f_{\pi}^2 m_{\pi}^4}{(Q^2 + m_{\pi}^2)^3} + \frac{1}{\pi} \int_{m_{\pi}^2}^{\infty} dt \frac{2}{(t + Q^2)^3} \text{Im } \psi^{(H)}(t). \quad (2.23)$$

Since $\text{Im } \psi_5^{(H)}(t)$ is a positive semi-definite function, it follows from these equations that their expected asymptotic behaviour should obey the inequality

$$m_u + m_d > \frac{4\pi}{\sqrt{3}} f_{\pi} m_{\pi} \frac{1}{Q^2} \quad (2.24)$$

from Eq. (2.22), and

$$m_u + m_d > 4\sqrt{\frac{2}{3}} \frac{\pi f_{\pi} m_{\pi}^2}{Q^2} \quad (2.25)$$

from Eq. (2.23).

In the absence of any information about non-perturbative effects it is clear that Eq. (2.24) is a much better bound than Eq. (2.25) and it is then tempting to work with the function $\phi(Q^2)$ in Eq. (2.14) instead of $\psi_5''(Q^2)$. However, the lower bound in Eq. (2.25) has the virtue of being compatible with the PCAC constraint in Eq. (2.8), while the same is not obvious for the bound in Eq. (2.24): the bound for $m_u + m_d$ in Eq. (2.24) is linear in m_π , not quadratic as the PCAC constraint requires. This is the reason why in this paper we choose to work with the function $\psi_5''(Q^2)$. To justify this choice more precisely we shall conclude this section with an analysis of the possible leading non-perturbative contributions to $\psi_5(q^2)$ and $D_5(q^2)$.

For $\psi_5(q^2)$, the operator product expansion at short distances gives the following contributions

$$\begin{aligned} \psi_5(q^2) = & \frac{3}{8\pi^2} (m_u + m_d)^2 \left\{ Q^2 \log \frac{Q^2}{\mu^2} + O(m^2 \log \frac{Q^2}{\mu^2}) + O(\alpha_s) \right. \\ & + (A_1 m_u + A_2 m_d) \frac{\langle \bar{\psi}_u \psi_u \rangle}{Q^2} + (A_1 m_d + A_2 m_u) \frac{\langle \bar{\psi}_d \psi_d \rangle}{Q^2} \\ & \left. + B \alpha_s \frac{\langle F_{(a)}^{\mu\nu}(0) F_{\mu\nu}^{(a)}(0) \rangle}{Q^2} + O\left(\frac{M^4}{Q^4}\right) \right\}. \end{aligned} \quad (2.26)$$

The first line represents the perturbative contribution, the second and third lines are the leading non-perturbative contributions of order $1/Q^2$ which are symbolically depicted in the diagrams of Fig. 2. The explicit expressions for the coefficients A_1 , A_2 and B are given in the next section. The corresponding expansion for $D_5(q^2)$ is

$$\begin{aligned} D(q^2) = & \frac{3}{8\pi^2} \left\{ (m_u + m_d)^2 \log \frac{Q^2}{\mu^2} + O\left(\frac{m^4}{Q^4} \log \frac{Q^2}{\mu^2}\right) + O(\alpha_s) \right. \\ & + (M_1 m_u + M_2 m_d) \frac{\langle \bar{\psi}_u \psi_u \rangle}{Q^2} + (M_1 m_d + M_2 m_u) \frac{\langle \bar{\psi}_d \psi_d \rangle}{Q^2} \\ & \left. + N \alpha_s \frac{\langle F_{(a)}^{\mu\nu}(0) F_{\mu\nu}^{(a)}(0) \rangle}{Q^2} + O(M^4/Q^4) \right\}, \end{aligned} \quad (2.27)$$

with M_1, M_2 and N calculable coefficients^{*)}. Notice that the leading non-perturbative contributions behave as $1/Q^2$ for both $\psi_5(q^2)$ and $D_5(q^2)$. However, the Ward identity in Eq. (2.1) at large Q^2 requires that

$$-Q^2 D_5(q^2) = \psi_5(q^2) - \psi_5(0). \quad (2.28)$$

Since the non-perturbative $\psi_5(0)$ is known [see Eq. (2.5)], the coefficients M_1 and M_2 are then determined to be

$$M_1 = M_2 = -1 \quad (2.29)$$

and furthermore we must have

$$N = \frac{(m_u + m_d)^2}{Q^2} B, \quad (2.30)$$

i.e., the contribution of the operator $F^{\mu\nu}F_{\mu\nu}$ to $D_5(q^2)$ is non-leading.

We can now rewrite Eq. (2.22) with the leading non-perturbative effects incorporated. Then we have

$$\begin{aligned} \frac{3}{8\pi^2} \cdot \frac{(m_u + m_d)^2}{Q^2} &= \frac{2f_\pi^2 m_\pi^2}{(Q^2 + m_\pi^2)^2} + \frac{(m_u + m_d) \langle \bar{\psi}_u \psi_u + \bar{\psi}_d \psi_d \rangle}{Q^4} \\ &+ \frac{1}{\pi} \int_0^\infty dt \frac{1}{9m_\pi^2 (t + Q^2)^2 t} \operatorname{Im} \psi_5^{(H)}(t). \end{aligned} \quad (2.31)$$

^{*)} It is important to realize that the combinations $m\langle\bar{\psi}\psi\rangle$ and $\alpha_s\langle F\cdot F\rangle$ are not renormalized. This is why a v (later, Q^2) dependence need not be specified for these quantities. (The $\bar{\psi}\psi$ requires a proper definition of the limit $\psi(\xi)\psi(0)$, $\xi \rightarrow 0$, which can be done in the usual way.)

If we now use the PCAC estimate of $(m_u + m_d) \langle \bar{\psi}_u \psi_u + \bar{\psi}_d \psi_d \rangle$ [see Eq. (2.8)], we can see that it exactly cancels the $2f_\pi^2 m_\pi^2 / Q^4$ contribution from the pion pole. In other words: there is no Q^2 value, however large, at which the perturbative sum rule Eq. (2.22) is applicable if, at the same time, we wish to be consistent with the Nambu-Goldstone realization of PCAC.

3. THE FUNCTION $\psi_5(q^2)$ IN QCD

The lowest order expression for $\psi_5(q^2)$ dimensionally renormalized, can be easily obtained from the quark loop diagram in Fig. 1. We get

$$\begin{aligned} \psi_5(q^2) \Big|_{\text{lowest order}} &= \frac{3}{8\pi^2} (m_u + m_d)^2 \left\{ Q^2 \log \frac{Q^2}{\nu^2} \right. \\ &\quad \left. + [m_u^2 + m_d^2 + (m_u - m_d)^2] \log \frac{Q^2}{\nu^2} + O\left(\frac{\nu^4}{Q^2} \log \frac{Q^2}{\nu^2}\right) \right\}. \end{aligned} \quad (3.1)$$

There are perturbative and non-perturbative corrections to that expression. The perturbative corrections of order α_s come from the gluon exchange diagrams shown in Fig. 3. The details of their calculation are reported in Appendix A. The result, in the $\overline{\text{MS}}$ -scheme, when added to $\psi_5(q^2)$ (lowest order) gives the two-loop perturbative contribution to $\psi_5(q^2)$, i.e.,

$$\begin{aligned} \psi_5(q^2) \Big|_{\text{pert.}} &= \psi_5(q^2) \Big|_{\text{lowest order}} \\ &\quad + \frac{3}{8\pi^2} (m_u + m_d)^2 \frac{\alpha_s}{\pi} Q^2 \left\{ -\log^2 \frac{Q^2}{\nu^2} + \frac{17}{3} \log \frac{Q^2}{\nu^2} + \text{constant} \right\}. \end{aligned} \quad (3.2)$$

There are two sources of leading non-perturbative terms. Those symbolically represented by the diagrams in Fig. 2a are relatively easy to evaluate. They can be estimated with standard techniques, as in Ref. 11a), and give the following contribution:

$$\psi_5(q^2) \Big|_{\text{non-pert.}}^{\bar{\psi}\psi} = -\frac{(m_u + m_d)^2}{Q^2} \left\{ \left(m_d - \frac{m_u}{2}\right) \langle \bar{\psi}_u \psi_u \rangle + \left(m_u - \frac{m_d}{2}\right) \langle \bar{\psi}_d \psi_d \rangle \right\}. \quad (3.3a)$$

The vacuum expectation value of the operator $F_{(a)}^{\mu\nu} F_{\mu\nu(a)}$ also gives a leading non-perturbative contribution of order $1/Q^2$ via the diagrams shown in Fig. 2. We find

$$\psi_5 \Big|_{\text{non-pert}}^{F^2} = \frac{(m_u + m_d)^2}{Q^2} \cdot \frac{\alpha_s}{8\pi} \langle F^2 \rangle \quad (3.3b)$$

where the expression $\langle F^2 \rangle$ is short for $\sum_a \langle F_{\mu\nu(a)}^{\mu\nu} F_{\mu\nu(a)}^{\mu\nu} \rangle_0$.

We have already mentioned in the previous section that the quantity of interest for our purposes is the second derivative with respect to q^2 of $\psi_5(q^2)$. In general $\psi_5''(Q^2)$ is a function

$$\psi_5''(Q^2) = F_5(Q^2, m_u^2, m_d^2, v^2, \alpha_s) \quad (3.4)$$

of $Q^2 \equiv -q^2$, the renormalized quark masses $m_u(v)$ and $m_d(v)$; the renormalized QCD coupling constant $g(v)$, $\alpha_s = g^2(v)/4\pi$; and v an arbitrary mass scale introduced via renormalization. As already mentioned we have chosen the minimal renormalization scheme of 't Hooft¹²⁾, with $\log 4\pi - \gamma_E$ terms absorbed in the definition of the renormalized coupling constant (i.e., the so-called $\overline{\text{MS}}$ -scheme^{*}). In that scheme $F(Q^2)$ obeys a simple renormalization group equation

$$\left\{ -\frac{\partial}{\partial \lambda} + \beta \alpha_s \frac{\partial}{\partial \alpha_s} - \sum_{u,d} (1 + \gamma) x_i \frac{\partial}{\partial x_i} \right\} F_5 = 0, \quad (3.5)$$

where

$$\lambda = \frac{1}{2} \log \frac{Q^2}{v^2} \quad (3.6a)$$

and

$$x_i = \frac{m_i(v)}{v}. \quad (3.6b)$$

^{*}) This renormalization scheme has been suggested, independently, by various authors. See, e.g., Refs 16)

The functions $\beta(\alpha_s)$ and $\gamma(\alpha_s)$ are respectively associated to the coupling constant renormalization and the mass renormalization (which in the minimal renormalization scheme is the same for all the quark flavours)

$$\beta(\alpha_s) = \beta_1 \frac{\alpha_s}{\pi} + \beta_2 \left(\frac{\alpha_s}{\pi} \right)^2 + \dots, \quad (3.7)$$

$$\gamma(\alpha_s) = \gamma_1 \frac{\alpha_s}{\pi} + \gamma_2 \left(\frac{\alpha_s}{\pi} \right)^2 + \dots; \quad (3.8)$$

with ($N = \#$ of colours; $n = \#$ of flavours). We have,

$$\beta_1 = \frac{1}{6} (-11N + 2n), \quad (3.9a)$$

$$\beta_2 = \frac{-17}{3} \left(\frac{N}{2} \right)^2 + \frac{1}{2} \cdot \frac{N^2-1}{2N} \cdot \frac{n}{2} + \frac{5Nn}{12} \quad (3.9b)$$

and *)

$$\gamma_1 = \frac{3}{2} \cdot \frac{N^2-1}{2N} \quad (3.10a)$$

$$\gamma_2 = \frac{3}{16} \left(\frac{N^2-1}{2N} \right)^2 + \frac{97}{48} \cdot \frac{N^2-1}{4} - \frac{5n(N^2-1)}{48N} \quad (3.10b)$$

The explicit expression for the function

$$F_5(Q^2, m_s^2(\nu), m_d^2(\nu), \alpha_s(\nu); \nu)$$

up to two-loops in perturbative QCD and with the leading non-perturbative contributions included, is then the following:

*) For γ_2 we have used the result of a recent calculation by R. Tarrach, Ref. 17)

$$\begin{aligned}
 F_5 = & \frac{3}{8\pi^2} \cdot \frac{(m_u + m_d)^2}{Q^2} \left\{ 1 - \frac{m_u^2 + m_d^2 + (m_u - m_d)^2}{Q^2} + O\left(\frac{m^4}{Q^4} \log \frac{Q^2}{m^2}\right) \right. \\
 & + \frac{\alpha_s(\nu)}{\pi} \left[-2 \log \frac{Q^2}{\nu^2} + \frac{17}{3} - 2 + O\left(\frac{m^2}{Q^2} \log \frac{Q^2}{m^2}\right) \right. \\
 & - \frac{16\pi^2}{3Q^4} \left[\left(m_d - \frac{m_u}{2}\right) \langle \bar{\psi}_u \psi_u \rangle + \left(m_u - \frac{m_d}{2}\right) \langle \bar{\psi}_d \psi_d \rangle \right] \\
 & \left. \left. + \frac{2\pi}{3} \cdot \frac{\alpha_s(\nu) \langle F^2 \rangle(\nu)}{Q^4} + O\left(\frac{M^6}{Q^6}\right) \right\}. \right.
 \end{aligned} \tag{3.11}$$

The first two terms in the right-hand side of (3.11) correspond to the lowest order contribution with next-to-leading mass corrections. The second set is the perturbative α_s correction, and the penultimate term is the leading non-perturbative correction induced by $\langle \bar{\psi}\psi \rangle \neq 0$. The last term is the leading non-perturbative correction induced by $\alpha_s \langle F^2 \rangle \neq 0$.

With the information given above, the solution to the renormalization group equation, Eq. (3.5), at the two-loop level, is, dropping higher order terms,

$$\begin{aligned}
 F_5 = & \frac{3}{8\pi^2} \cdot \frac{[\bar{m}_u(Q^2) + \bar{m}_d(Q^2)]^2}{Q^2} \left\{ 1 - 2 \frac{\bar{m}_u^2(Q^2) + \bar{m}_d^2(Q^2) - \bar{m}_u(Q^2)\bar{m}_d(Q^2)}{Q^2} \right. \\
 & + \frac{11}{3} \cdot \frac{\bar{\alpha}_s(Q^2)}{\pi} - \frac{16\pi^2}{3Q^4} \left[\left(\bar{m}_d - \frac{\bar{m}_u}{2}\right) \langle \bar{\psi}_u \psi_u \rangle + \left(\bar{m}_u - \frac{\bar{m}_d}{2}\right) \langle \bar{\psi}_d \psi_d \rangle \right] \\
 & \left. + \frac{2\pi}{3} \cdot \frac{\bar{\alpha}_s \langle F^2 \rangle}{Q^4} \right\}.
 \end{aligned} \tag{3.12}$$

where $\bar{\alpha}_s(Q^2)$ denotes the QCD running coupling constant

$$\bar{\alpha}_s(Q^2) = \frac{\pi}{-\beta_1 \log Q^2/\Lambda^2}, \quad (3.13)$$

and $\bar{m}_i(Q^2)$ i = up, down, the QCD running masses at the two-loop level^{*})

$$\bar{m}_i(Q^2) = \frac{\hat{m}_i}{\left(\frac{1}{2} \log Q^2/\Lambda^2\right)^{\gamma_1/\beta_1}} \left\{ 1 - \frac{\gamma_1 \beta_2}{\beta_1^2} \cdot \frac{\log \log Q^2/\Lambda^2}{\frac{1}{2} \log Q^2/\Lambda^2} + \frac{1}{\beta_1^2} \left(\gamma_2 - \frac{\gamma_1 \beta_2}{\beta_1} \right) \frac{1}{\frac{1}{2} \log Q^2/\Lambda^2} \right\}. \quad (3.14)$$

We are now in the position to write down the improved inequality which replaces the zeroth-order inequality given in Eq. (2.25):

$$\begin{aligned} \bar{m}_u(Q^2) + \bar{m}_d(Q^2) &> 4\pi \sqrt{\frac{2}{3}} \frac{f_\pi m_\pi^2}{Q^2} \left| 1 - \frac{3}{2} \frac{m_\pi^2}{Q^2} \right. \\ &+ \frac{\bar{m}_u^2 + \bar{m}_d^2 - \bar{m}_u \bar{m}_d}{Q^2} - \frac{11}{6} \cdot \frac{\bar{\alpha}_s(Q^2)}{\pi} \\ &\left. + \frac{8\pi^2}{3Q^4} \left[\left(\bar{m}_d - \frac{\bar{m}_d}{2} \right) \langle \bar{\psi}_u \psi_u \rangle + \left(\bar{m}_u - \frac{\bar{m}_d}{2} \right) \langle \bar{\psi}_d \psi_d \rangle \right] - \frac{\pi}{3} \cdot \frac{\bar{\alpha}_s \langle F^2 \rangle}{Q^4} \right\}. \end{aligned} \quad (3.15)$$

^{*}) The renormalization of the combinations of operators $m \langle \bar{\psi} \psi \rangle$ and $\alpha_s \langle F^2 \rangle$ has been used also.

As we shall see in the next section, this is only the simplest example of a whole set of inequalities which can be derived from Eqs (2.20), (3.5) and (3.11).

4. QUESTION OF OPTIMAL INEQUALITIES

We shall follow the method first discussed in Ref. 9a) in connection with the total $e^+e^- \rightarrow \text{hadrons}$ cross-section. Differentiating Eq. (3.12) N times with respect to Q^2 and separating the pole contribution from the continuum, we get the following expression, after multiplication by appropriate factors of $g_{\pi\pi}^2 + Q^2$:

$$F_5^{(N)}(Q^2) - 4f_\pi^2 \kappa_\pi^4 \frac{(g_{\pi\pi}^2 + Q^2)^N}{(\kappa_\pi^2 + Q^2)^{N+3}} = \Sigma_N(Q^2) \quad (4.1)$$

$$= \int_{g_{\pi\pi}^2}^{\infty} dt \frac{1}{(t+Q^2)^3} \cdot \left(\frac{g_{\pi\pi}^2 + Q^2}{t+Q^2} \right)^N \frac{2 \operatorname{Im} \psi_5^{(H)}(t)}{\pi}$$

where

$$F_5^{(N)}(Q^2) = \frac{2(-1)^N}{(N+2)!} \left(g_{\pi\pi}^2 + Q^2 \right)^N \frac{\partial^N}{(\partial Q^2)^N} F_5(Q^2). \quad (4.2)$$

With the change of variable

$$x = \frac{g_{\pi\pi}^2 + Q^2}{t + Q^2} \quad (4.3)$$

the integral $\sum_N$ can be written in the form

$$\sum_N (Q^2) = \int_0^1 dx \, x^N \rho(x, Q^2, m_\pi^2) \quad (4.4)$$

where

$$\rho(x, Q^2, m_\pi^2) = \frac{x}{(g_{m_\pi^2} + Q^2)^2} \cdot \frac{2}{\pi} \operatorname{Im} \psi_5 \left(t = \frac{g_{m_\pi^2} + (1-x)Q^2}{x} \right), \quad (4.5)$$

and we are confronted with a typical moment problem because the positivity of $\operatorname{Im} \psi_5(t)$ implies the positivity of ρ ,

$$\rho(x, Q^2, m_\pi^2) \geq 0 \quad (4.6)$$

A necessary and sufficient condition for $\rho \geq 0$ in Eq. (4.4) is that all the matrices (in the indices N and M) $\sum_{N+M}$ and $\sum_{N+M} - \sum_{N+M+1}$ for all $N, M = 0, 1, 2, \dots$ be positive semi-definite. In particular this implies

$$\sum_N (Q^2) > 0, \quad N = 0, 1, 2, \dots \quad (4.7)$$

and

$$\sum_{N-1} (Q^2) \sum_{N+1} (Q^2) > [\sum_N (Q^2)]^2, \quad N = 1, 2, 3, \dots \quad (4.8)$$

The inequality given in Eq. (3.15) is nothing but the requirement that $\sum_0(Q^2) \geq 0$. From now on we shall call Eq. (4.7) the N^{th} -linear constraint and Eq. (4.8) the N^{th} -quadratic constraint.

In order to use these constraints we must evaluate the function $F_5^{(N)}(Q^2)$ defined by Eq. (4.2). Each $F_5^{(N)}(Q^2)$ obeys a renormalization group equation of the type

$$\left\{ -\frac{\partial}{\partial \lambda} + \beta \alpha_s \frac{\partial}{\partial \alpha_s} - \sum_{u,d} (1+\gamma) x_i \frac{\partial}{\partial x_i} \right\} F_5^{(N)} = 0; \quad (4.9)$$

but the boundary conditions change with N . To evaluate these we have to take the N^{th} -derivative of $F_5(Q^2, m_u^2(v), m_d^2(v), v^2; \alpha_s(v))$ given in Eq. (3.11) and then scale the result at $v^2 = Q^2$. The result one obtains is the following:

$$\begin{aligned} F_5^{(N)}(Q^2) = & \frac{2}{(N+1)(N+2)} \cdot \frac{3}{8\pi^2} \cdot \frac{(\hat{m}_u + \hat{m}_d)^2}{Q^2} \cdot \frac{1}{(\log Q/\Lambda)^d} \cdot \left(\frac{g_{\pi\pi}^2 + Q^2}{Q^2} \right)^N \\ & \times \left\{ 1 - (N+1) \frac{\bar{m}_u^2 + \bar{m}_d^2 + (\bar{m}_u - \bar{m}_d)^2}{Q^2} \right. \\ & + \frac{\bar{\alpha}_s(Q^2)}{\pi} \left[\frac{11}{3} + \frac{\gamma_1 \beta_2}{\beta_1^2} \log \log \frac{Q^2}{\Lambda^2} - \left(\gamma_2 - \frac{\gamma_1 \beta_2}{\beta_1} \right) \frac{1}{\beta_1} + 2 S_1(N) \right] \\ & + \left(\frac{\bar{\alpha}_s(Q^2)}{\pi} \right)^2 \left[\frac{17+n}{6} S_1(N) + \left(4 + \frac{33-2n}{12} \right) (S_1(N)^2 - S_2(N)) \right] \\ & - \frac{16\pi^2}{3} \cdot \frac{(N+1)(N+2)}{2Q^4} \left[(\bar{m}_d - \frac{\pi_a}{2}) \langle \bar{\psi}_u \psi_u \rangle + (\bar{m}_u - \frac{\pi_d}{2}) \langle \bar{\psi}_d \psi_d \rangle \right] \\ & \left. + \frac{2\pi}{3} \cdot \frac{(N+1)(N+2)}{2} \cdot \frac{\alpha_s \langle F^2 \rangle}{Q^4} \right\}; \\ d = -2\gamma_1/\beta_1 = \frac{12}{33-2n}, \end{aligned} \quad (4.10)$$

and where

$$S_l(N) = \sum_{k=0}^{\infty} \left\{ \frac{\Gamma(k+1)}{\Gamma(k+l+1)} - \frac{\Gamma(k+N+1)}{\Gamma(k+N+l+1)} \right\}, \quad l=1,2. \quad (4.11)$$

For large N ,

$$\begin{aligned} S_1(N) &\simeq \log N + \gamma_E + O(1/N), \\ S_2(N) &\simeq \frac{\pi^2}{6} + O(1/N). \end{aligned} \quad (4.12)$$

The evaluation of the terms in S_1, S_2 in (4.10) as well as of the behaviour (4.12) is given in Appendix B. These terms appear from the successive derivatives of the term $\alpha_s(v) (1/Q^2) (\log Q^2)$ in Eq. (3.11); and they play an important role in the limitation of the number of derivatives permissible at a given Q^2 .

4a. The linear constraint

This is the statement that

$$\sum_N (Q^2) > 0 \quad \text{for} \quad N = 0, 1, 2, \dots$$

With $\sum_N (Q^2)$ defined in Eq. (4.1) and the calculated expression for $\sum_5^{(N)} (Q^2)$ given in Eq. (4.10), the linear constraint gives the following set of inequalities for $\hat{m}_u + \hat{m}_d$. [The $\hat{m}$ are the renormalization group invariant masses, at the two-loop level, see Eq. (3.14).]

$$\begin{aligned} \hat{m}_u + \hat{m}_d &> \sqrt{\frac{(N+1)(N+3)}{3}} \cdot \frac{4\pi f_\pi^2 m_\pi^2}{Q^2} \cdot (\log Q/\Lambda)^d \\ &\times \left\{ 1 - \frac{9N}{2} \cdot \frac{m_\pi^2}{Q^2} + \frac{N+1}{2} \cdot \frac{\bar{m}_u^2 + \bar{m}_d^2 + (\bar{m}_u - \bar{m}_d)^2}{Q^2} \right. \\ &\quad - \frac{\bar{\alpha}_s(Q^2)}{\pi} [S_1(N) + K(Q^2)] \\ &\quad - \frac{1}{2} \left(\frac{\bar{\alpha}_s(Q^2)}{\pi} \right)^2 \left[\frac{17+n}{6} S_1(N) + \left(4 + \frac{33-2n}{12} \right) (S_1(N)^2 - S_2(N)) \right] \\ &\quad \left. - \frac{(N+1)(N+2)}{2 Q^4} \left[\frac{4\pi^2 m_\pi^2 f_\pi^2}{3} + \frac{\pi}{3} \alpha_s \langle F^2 \rangle \right] \right\} \end{aligned} \quad (4.13)$$

where, for two flavours

$$K(Q^2) = 2.24 - (0.41) \log \log Q^2/\Lambda^2.$$

and we have profited from the PCAC relation to eliminate $m\langle\bar{\psi}\psi\rangle$ in favour of $m_\pi^2 f_\pi^2$.

4b. The quadratic constraint

This is the positivity requirement

$$\sum_{N-1}(Q^2) \sum_{N+1}(Q^2) > \sum_N (Q^2)^2, \quad N=1, 2, 3, \dots$$

With $\sum_N(Q^2)$ defined in Eq. (4.1) and the general expression for $F_5^{(N)}(Q^2)$ given in Eq. (4.10), this constraint gives the following set of inequalities for $\hat{m}_u + \hat{m}_d$:

$$\begin{aligned} \hat{m}_u + \hat{m}_d &\geq \sqrt{\frac{(N+1)(N+2)(N^2+3N+6)}{3}} \cdot \frac{4\pi f_\pi^2 \Lambda_\pi^2 (\log Q/\Lambda)^2}{Q^2} \\ &\times \left\{ 1 - \frac{9N m_\pi^2}{2Q^2} + (N+1) \frac{\bar{m}_u^2 + \bar{m}_d^2 - \bar{m}_u \bar{m}_d}{Q^2} \right. \\ &- \frac{\bar{\alpha}_s}{\pi} [S_1(N) + K(Q^2)] \\ &- \frac{1}{2} \left(\frac{\bar{\alpha}_s}{\pi} \right)^2 \left[\frac{17+N}{6} S_1(N) + \left(4 + \frac{1}{2} \right) (S_1(N)^2 - S_2(N)) \right] \\ &- \frac{(N+1)(N+2)(N^2+3N+6)}{2Q^4} \left[\frac{4\pi^2 m_\pi^2 f_\pi^2}{3} + \frac{\pi}{3} \bar{\alpha}_s \langle F^2 \rangle \right] \Big\}. \end{aligned} \quad (4.14)$$

4c. Optimum bounds

Let us discuss the linear inequality for simplicity; everything that we say for it can be translated without difficulty to the quadratic one. Also, to simplify the discussion we will work to leading order in chiral symmetry-breaking,

and for large N with neglect of terms $O(1/N)$, $O(1/\log N)$. Then, (4.8) simplifies to

$$\hat{m}_u + \hat{m}_d \geq \frac{4\pi f_\pi m_\pi^2}{\sqrt{3}} \cdot \frac{N}{Q^2} \left(\log \frac{Q}{\Lambda} \right)^d \left\{ 1 - d \frac{\log N}{\log Q^2/\Lambda^2} - \left(2d^2 + \frac{1}{2}d \right) \left(\frac{\log N}{\log Q^2/\Lambda^2} \right)^2 - \left(\frac{N}{Q^2} \right)^2 \frac{\pi}{6} \bar{\alpha}_s \langle F^2 \rangle \right\}. \quad (4.15)$$

Suppose we chose $N = x Q^2/\Lambda^2$, with x a small but fixed number. Then, the right-hand side of (4.10) would become

$$\frac{4\pi f_\pi m_\pi^2}{\sqrt{3} \Lambda^2} \times \left(\log \frac{Q}{\Lambda} \right)^d \left\{ 1 - \frac{3}{2}d - 2d^2 \right\},$$

i.e., it would increase without bounds with Q^2 , which is preposterous. In fact, what happens is that with this choice the first $O(\log N/\log Q^2/\Lambda^2)$ correction is $d = 12/29$, while the $O(\log^2 N/\log^2 Q^2/\Lambda^2)$ one is $2d^2 + d/2 = (106/58)d$, i.e., larger than the leading one. Note that this invalidates the calculations of Ref. 11c)*). These authors use a method similar to ours, but neglect the $S_1(N)$ $S_1(N)^2$ corrections. When taken into account, one sees that their bound, at $Q^2 \approx 10$, $N \approx 6$, gets leading (in $\log N/\log Q^2/\Lambda^2$) corrections of $\sim 50\%$, and second order ones of $\sim 90\%$.

In fact, we have to restrict the Q^2 , N value so that corrections do not increase with the order. A possible requirement is to relate N , Q^2 by demanding that, precisely

$$\left(2d^2 + \frac{1}{2}d \right) \frac{\log N(Q^2)}{\log Q^2/\Lambda^2} \lesssim d,$$

so the corrections in the right-hand side of (4.15) become

$$-d \frac{\log N(Q^2)}{\log Q^2/\Lambda^2} \left\{ 1 + d + \dots \right\}.$$

Any such procedure is of course arbitrary, and depends upon what one considers to be "reasonably small" corrections. Because of this there is perhaps a better way to proceed. Let $f(d, N, Q^2)$ denote the function in the right-hand side of (4.15). One may expand it in powers of d :

*) For the light quark masses.

$$f(d, N, Q^2) = f(0, N, Q^2) \{ 1 + df_1(0, N, Q^2) + d^2 f_2(0, N, Q^2) + \dots \},$$

where the main point is that $f(0, N, Q^2)$ is such that the troublesome factor $(\frac{1}{2} \log Q^2/\Lambda^2)^d$ has disappeared:

$$f(0, N, Q^2) = \frac{4\pi f_\pi m_\pi^2}{\sqrt{3}} \cdot \frac{N}{Q^2} \left\{ 1 - \left(\frac{N}{Q^2} \right)^2 \frac{\pi}{6} \langle \bar{\alpha}_s F^2 \rangle \right\}.$$

To this approximation, we may obtain the explicit best bound,

$$\hat{m}_u + \hat{m}_d \geq \sqrt{\frac{2\pi}{3}} \cdot \frac{8f_\pi m_\pi^2}{3 \langle \bar{\alpha}_s F^2 \rangle^{1/2}}; \quad (4.16)$$

it corresponds to

$$\frac{Q^2}{N} = \left\{ \frac{\pi \langle \bar{\alpha}_s F^2 \rangle}{2} \right\}^{1/2}. \quad (4.17)$$

The relative corrections for this are df_1 , with

$$f_1(0, N, Q^2) = \log \log \frac{Q}{\Lambda} - \frac{\log N}{\log Q^2/\Lambda^2} - \frac{1}{2} \left(\frac{\log N}{\log Q^2/\Lambda^2} \right)^2.$$

With, e.g.,

$$\Lambda = 0.45 \text{ GeV}, \quad \langle \bar{\alpha}_s F^2 \rangle^{1/2} = 0.2 \text{ GeV}^2, \quad Q^2 = 20 \text{ GeV}^2$$

we find $df_1(0, N, Q^2) \approx (-0.7)d$. Moreover, the d^2 correction is

$$\left\{ -2 \left(\frac{\log N}{\log Q^2/\Lambda^2} \right)^2 + \frac{1}{2} \log \log \frac{Q}{\Lambda} \right\} d^2 = -(0.9)d,$$

i.e., still small. Actually, the corrections are much smaller for the quadratic bound. Here the optimal leading $f(0, N, Q^2)$ is still the same, but the corrections are to be evaluated at

$$\frac{Q^2}{N^2} = \left\{ \frac{\pi \langle \bar{\alpha}_s F^2 \rangle}{2} \right\}^{1/2} \quad (4.18)$$

instead of (4.17) (note the difference: Q^2/N^2 instead of Q^2/N). With this, and for the same values of Λ , $\langle \alpha_s F^2 \rangle$, Q^2 , we find the corrections

$$-(0.35) d, \quad -(0.16) d^2,$$

i.e., the estimate of f with $f(0, N, Q^2)$ should be good to within 20% of accuracy.

An important feature of the bound is that the leading $O(d^0)$ result, Eq. (4.13) is independent of Λ ; the dependence on Λ only enters through the $O(d)$, $O(d^2)$ terms, and is very slight.

5. CONCLUSIONS AND OUTLOOK

With the input value^{11a)}

$$\bar{\alpha}_s \langle F^2 \rangle = 0.04 \text{ GeV}^2 \quad (5.1)$$

we obtain an optimal lower bound for the sum of renormalization group invariant masses $\hat{m}_u + \hat{m}_d$, at the two-loop level and taking into account the $O(d)$, $O(d^2)$ corrections:

$$\hat{m}_u + \hat{m}_d \geq (30 \pm 6) \text{ MeV}. \quad (5.2)$$

We have allowed for very generous errors, $O(d^3)$, $O([\alpha_s \langle F^2 \rangle / Q^4]^2)$. This bound corresponds to values for the running masses at $Q = 2 \text{ GeV}$.

$$\bar{m}_u + \bar{m}_d \Big|_{Q=2 \text{ GeV}} \geq (25 \pm 5) \text{ MeV}, \quad \Lambda = 0.45 \quad (5.3a)$$

and

$$\bar{m}_u + \bar{m}_d \Big|_{Q=2 \text{ GeV}} \geq (20 \pm 4) \text{ MeV}, \quad \Lambda = 0.1. \quad (5.3b)$$

These values are larger than the so-called current algebra masses⁶⁾, $(m_u + m_d)_{\text{C.A.}} = 11 \text{ MeV}$. However, in the absence of a clear argument to relate the $\hat{m}$'s to the current algebra masses, it is difficult to give much significance to this discrepancy.

We can also obtain lower bounds for the combination $\hat{m}_u + \hat{m}_s$, provided we accept the extension of the PCAC estimate in Eq. (2.8) to the SU(3) strangeness changing current, i.e.,

$$(\hat{m}_u + \hat{m}_s) \langle \bar{\psi}_u \psi_u + \bar{\psi}_s \psi_s \rangle = -2f_K^2 m_K^2.$$

Since experimentally $f_\pi \approx f_K$, it seems also reasonable to advocate SU(3) symmetry to assume $\langle \bar{u}u \rangle \approx \langle \bar{s}s \rangle$. Then, with the same input value for $-\alpha_s \langle F \cdot F \rangle$ as in Eq. (5.1), we obtain

$$\hat{m}_u + \hat{m}_s \geq (510 \pm 100) \text{ MeV} \quad (5.4)$$

which corresponds to the running masses

$$\bar{m}_u + \bar{m}_s \Big|_{Q=2 \text{ GeV}} \geq (430 \pm 90) \text{ MeV}, \quad \Lambda = 0.45, \quad (5.5a)$$

$$\bar{m}_u + \bar{m}_s \Big|_{Q=2 \text{ GeV}} \geq (320 \pm 60) \text{ MeV}, \quad \Lambda = 0.1. \quad (5.5b)$$

Again, these are values higher than the current algebra mass value $m_{\text{S.C.A.}} = 150 \text{ MeV}$.

It is not surprising that the ratios of our bounds are consistent with the ratio of the current algebra masses. This is due to the fact that our bounds incorporate PCAC and the SU(3) limit relation $\langle \bar{u}u \rangle \approx \langle \bar{d}d \rangle \approx \langle \bar{s}s \rangle$. Actually,

if we accept the PCAC equality, say Eq. (2.8), it may be easily seen that our lower bounds on perturbative masses imply upper bounds in spontaneous masses. To see this, assume SU(2) invariance of the $\langle \bar{\psi}_i \psi_i \rangle$, and write¹⁵⁾

$$\langle \bar{\psi} \psi \rangle|_{Q^2} = \left(\log \frac{Q}{\Lambda} \right)^d \hat{\mu}^3; \quad (5.6)$$

equation (2.8) then becomes a relation for the spontaneous mass $\hat{\mu}$:

$$\hat{\mu} = \left(\frac{f_\pi^2 m_\pi^2}{\hat{m}_u + \hat{m}_d} \right)^{1/3}. \quad (5.7)$$

We find, using (4.13)

$$\hat{\mu} \leq \left(\frac{3}{2\pi} \right)^{1/6} \frac{(3f_\pi)^{1/3} \langle \bar{\alpha}_s F^2 \rangle^{1/6}}{2}. \quad (5.8)$$

Numerically, this gives

$$\hat{\mu} \leq (170 \pm 35) \text{ MeV}. \quad (5.9)$$

One feature of our results that we find very interesting is that we have shown that the proportionality factor in the PCAC relation $m_u + m_d \sim m_\pi^2$ is in fact $f_\pi^2 \langle \bar{\alpha}_s F^2 \rangle^{1/2}$. Spontaneous masses are related to $(f_\pi^2 \langle \bar{\alpha}_s F^2 \rangle)^{1/6}$.

The derivation of inequalities of the type discussed here for heavy quarks is interesting in connection with the prediction of the f_F coupling and the f_D coupling which eventually will be determined from $F \rightarrow \mu\nu$ and $D \rightarrow \mu\nu$ decays. It is clear that in this case we cannot rely on PCAC, or on SU(4) symmetry (which would predict $f_D = f_F = f_K = f_\pi$). Lower bounds, based on the relation given in Eq. (2.19), has been given in Ref. 19) with the results

$$f_D \leq 815 \text{ MeV}, \quad f_F \leq 920 \text{ MeV}.$$

These are probably over-estimated. As already pointed out in Ref. 19), it is likely that for heavy quarks one may be able to do a QCD expansion, not in $\alpha_s(Q^2/\Lambda^2)$ but on $\bar{\alpha}_s(M/\Lambda^2)$, in which case the bounds above could be significantly improved. This question is under investigation at present.

Finally, we wish to point out that lower bounds for the light quark systems given above can probably be improved with the additional information provided by the current algebra estimate of the multi-pion contribution to the absorptive amplitude in Eq. (2.21). This is another question we are investigating at the moment.

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APPENDIX A

TWO-LOOP CALCULATION OF THE QCD AXIAL CURRENT TWO-POINT FUNCTION

In order to obtain the α_s correction to the result in Eq. (3.1) we have to consider the two-loop diagrams shown in Fig. 3. We shall be concerned with the leading chiral symmetry breaking contribution only, i.e., terms of order $(m_i + m_j)^2$ in the quark masses. We have

$$\psi_5(q^2)_i^j = -i(m_i + m_j)^2 \int d^4x e^{iq \cdot x} \langle 0 | T \bar{\psi}_j(x) \gamma_5 \psi_i(x) \bar{\psi}_i(0) \gamma_5 \psi_j(0) | 0 \rangle. \quad (A.1)$$

We shall discuss separately the contributions to $\psi_5(q^2)$ from the quark self-energy diagrams (Figs 3a,b) and from the gluon exchange diagram (Fig. 3c).

i) Quark self-energy contributions

With the routing of momenta shown in Figs 3a,b, we can write

$$\begin{aligned} \psi_{SE} = & (m_i^0 + m_j^0)^2 (-3i) \int \frac{d^4p}{(2\pi)^4} \left\{ \text{Tr} \left[\gamma_5 \frac{1}{p} \Sigma(p) \frac{1}{p} \gamma_5 \frac{1}{p-q} \right] \right. \\ & \left. + \text{Tr} \left[\gamma_5 \frac{1}{p} \gamma_5 \frac{1}{p-q} \Sigma(p-q) \frac{1}{p-q} \right] \right\} \end{aligned} \quad (A.2)$$

where

$$\Sigma(p) = p \Sigma(p^2, \epsilon).$$

In the Feynman gauge

$$\Sigma(p^2, \epsilon) = \frac{g^2}{v\epsilon} \cdot \frac{N^2 - 1}{2N} \cdot \frac{(4\pi)^\epsilon \Gamma(\epsilon/2)}{16\pi^2} \int_0^1 dx (-2x + \epsilon x) \left(\frac{v^2}{-x(1-x)p^2} \right)^{\epsilon/2}. \quad (A.3)$$

We use dimensional regularization ($n = 4 - \epsilon$) with $\text{tr } 1 = 4$ (not $2^{n/2}$).

The factor 3 in Eq. (A.2) comes from the colour trace. The quantities $\overset{0}{m}_i, \overset{0}{m}_j$ and $\overset{0}{g}$ are all bare parameters. After the trace operation in Eq. (A.2) we obtain

$$\psi_{SE} = (m_i^0 + m_j^0)^2 12i \int \frac{d^n p}{(2\pi)^n} \cdot \frac{p \cdot (p-q)}{p^2 (p-q)^2} \{ \Sigma(p^2) + \Sigma((p-q)^2) \} \quad (A.4)$$

It is then useful to combine denominators using the formula

$$\frac{1}{(p^2)^{4+\epsilon/2} (p-q)^2} = \left(1 + \frac{\epsilon}{2}\right) \int_0^1 dy y^{\epsilon/2} \frac{1}{[(p-l)^2 - R^2]^{2+\epsilon/2}} \quad (A.5)$$

where

$$l = (1-y)q, \quad R^2 = -y(1-y)q^2. \quad (A.6)$$

We are then left with two-parametric integral

$$\begin{aligned} \psi_{SE} &= (m_i^0 + m_j^0)^2 \frac{1}{4\pi^2} (g^0 y^{-\epsilon/2})^2 \frac{(N^2-1)3\lambda}{2N} \\ &\times \left(\frac{2}{\epsilon} + \log 4\pi - \gamma_E \right) \int_0^1 dx (-2x + \epsilon x) \left(\frac{-y^2}{x(1-x)} \right)^{\epsilon/2} \left(1 + \frac{\epsilon}{2}\right) \\ &\times \int_0^1 dy [y^{\epsilon/2} + (1-y)^{\epsilon/2}] \{ I(1, 2+\epsilon/2) - y(1-y)q^2 I(0, 2+\epsilon/2) \}, \end{aligned} \quad (A.7)$$

with

$$\begin{aligned} I(r, 2 + \frac{\epsilon}{2}) &= i (-1)^{r+\epsilon/2} \frac{(4\pi)^{\epsilon/2}}{16\pi^2} \\ &\times \frac{\Gamma(r+2-\epsilon/2) \Gamma(-r+\epsilon)}{\Gamma(2-\epsilon/2) \Gamma(2+\epsilon/2)} (R^2)^{r-\epsilon} \end{aligned} \quad (A.8)$$

After integration over x and y , we get for q^2 space-like

$$\begin{aligned} \psi_{SE} &= v^{-\epsilon} (m_i^0 + m_j^0)^2 \frac{3q^2}{32\pi^4} (g^0 v^{-\epsilon/2})^2 \frac{N^2-1}{2N} \\ &\times \left\{ -\frac{1}{\epsilon^2} - \frac{1}{\epsilon} (\log 4\pi - \gamma_E) - \frac{9}{4\epsilon} + \text{constant} \right\} \left(\frac{v^2}{-q^2} \right)^\epsilon. \end{aligned} \quad (A.9)$$

ii) The gluon exchange contribution

With the routing of momenta shown in Fig. 3c, we can write in the Feynman gauge

$$\begin{aligned} \psi_{GE} &= (m_i^0 + m_j^0)^2 (-3i) \int \frac{d^n k_1}{(2\pi)^n} \int \frac{d^n k_2}{(2\pi)^n} \cdot \frac{1}{(k_1 - k_2)^2} (g^0)^2 \frac{N^2-1}{2N} \\ &\times \text{Tr} \left\{ \gamma_5 \frac{1}{k_1} \gamma^\alpha \frac{1}{k_2} \gamma_5 \frac{1}{k_2 - q} \gamma_\alpha \frac{1}{k_1 - q} \right\} \\ &= 3(g^0)^2 \frac{N^2-1}{2N} (m_i^0 + m_j^0)^2 \int \frac{d^n k_1}{(2\pi)^n} \int \frac{d^n k_2}{(2\pi)^n} \\ &\times \frac{4 \left\{ (4-\epsilon)(k_1^2 - k_1 \cdot q)(k_2^2 - k_2 \cdot q) - \epsilon [q^\mu k_1 \cdot k_2 - (k_1 \cdot q)(k_2 \cdot q)] \right\}}{k_1^2 k_2^2 (k_1 - k_2)^2 (k_1 - q)^2 (k_2 - q)^2}. \end{aligned} \quad (A.10)$$

This integral can be simplified to the following expression

$$\begin{aligned} \psi_{GE} &= (m_i^0 + m_j^0)^2 3(g^0)^2 \frac{N^2-1}{2N} \left[4q^4 I - 16q^2 J \right. \\ &\quad \left. + 2\epsilon q^2 K^2 + 8(1-\frac{\epsilon}{2}) L \right], \end{aligned} \quad (A.11)$$

where I, J, K are the following integrals:

$$I \equiv \int \frac{d^n k_1}{(2\pi)^n} \int \frac{d^n k_2}{(2\pi)^n} \cdot \frac{1}{k_1^2 k_2^2 (k_1 - k_2)^2 (k_1 - q)^2 (k_2 - q)^2}; \quad (A.12)$$

$$J \equiv \int \frac{d^n k_1}{(2\pi)^n} \cdot \frac{1}{k_1^2 (k_1 - q)^2} \int \frac{d^n k_2}{(2\pi)^n} \cdot \frac{1}{(k_1 - k_2)^2 (k_2 - q)^2}; \quad (A.13)$$

$$K \equiv \int \frac{d^n k}{(2\pi)^n} \cdot \frac{1}{k^2 (k - q)^2}; \quad (A.14)$$

$$L \equiv \int \frac{d^n k}{(2\pi)^n} \cdot \frac{1}{k_1^2} \int \frac{d^n k_2}{(2\pi)^n} \cdot \frac{1}{(k_1 - k_2)^2 (k_2 - q)^2}. \quad (A.15)$$

The integral I is convergent. For q spacelike we find

$$I = (v^2)^{-\epsilon} \left(\frac{1}{16\pi^2} \right)^2 \frac{1}{-q^2} \zeta(3) \left(\frac{v^2}{-q^2} \right)^\epsilon \quad (A.16)$$

where $\zeta(3)$ is the Rieman ζ function of argument 3 ($\zeta(3) = 1.202 \dots$). The other integrals can be easily done. For q spacelike we find

$$J = -(v^2)^{-\epsilon} \left(\frac{1}{16\pi^2} \right)^2 \left[\frac{2}{\epsilon^2} + \frac{2}{\epsilon} (\log 4\pi - \gamma_E) + \frac{5}{\epsilon} + \text{constant} \right] \left(\frac{v^2}{-q^2} \right)^\epsilon; \quad (A.17)$$

$$K^2 = -(v^2)^{-\epsilon} \left(\frac{1}{16\pi^2} \right)^2 \left[\frac{4}{\epsilon^2} + \frac{4}{\epsilon} (\log 4\pi - \gamma_E) + \frac{8}{\epsilon} + \text{constant} \right] \left(\frac{v^2}{-q^2} \right)^\epsilon; \quad (A.18)$$

and

$$L = (v^2)^{-\epsilon} \left(\frac{1}{16\pi^2} \right)^2 \left[\frac{1}{2\epsilon} + \text{constant} \right] \left(\frac{v^2}{-q^2} \right)^\epsilon. \quad (\text{A.19})$$

Inserting these results in Eq. (A.11), we finally obtain

$$\begin{aligned} \psi_{GE} &= (v^2)^{-\epsilon/2} (m_i^0 + m_j^0)^2 q^2 \frac{3}{32\pi^4} \left(\frac{g^0}{v^{\epsilon/2}} \right)^2 \frac{N^2 - 1}{2N} \\ &\times \left(\frac{4}{\epsilon^2} + \frac{4}{\epsilon} (\log 4\pi - \gamma_E) + \frac{19}{2} \cdot \frac{1}{\epsilon} + \text{constant} \right) \left(\frac{v^2}{-q^2} \right)^\epsilon. \end{aligned} \quad (\text{A.20})$$

iii) Mass renormalization

The final expression for $\psi_{5 \text{ bare}}(q^2)$ from the lowest order contribution and the sum of quark-self energy corrections [Eq. (A.9)] and gluon exchange correction [Eq. (A.20)] is (with $N = 3$)

$$\begin{aligned} \psi_{5 \text{ bare}} &= (v^2)^{-\epsilon/2} (m_i^0 + m_j^0)^2 \frac{3g^2}{8\pi^2} \left\{ \frac{2}{\epsilon} + \log 4\pi - \gamma_E + 2 \right. \\ &- \log \frac{-q^2}{v^2} - \frac{\epsilon}{2} (\log 4\pi - \gamma_E + 2) \log \frac{-q^2}{v^2} + \frac{\epsilon}{4} \log^2 \frac{-q^2}{v^2} \\ &\left. + \frac{(g^0 v^{-\epsilon/2})^2}{4\pi^2} \left[\frac{4}{\epsilon^2} + \frac{4}{\epsilon} (\log 4\pi - \gamma_E) + \frac{29}{3\epsilon} + \text{constant} \right] \left(\frac{v^2}{-q^2} \right)^\epsilon \right\}. \end{aligned} \quad (\text{A.21})$$

To this order we simply have $g^0 v^{-\epsilon/2} = g$, the renormalized coupling constant, and $\alpha_s = g^2/4\pi$. On the other hand, the bare masses, when expanded in terms of renormalized parameters, in the ϵ renormalization scheme (also called minimal subtraction scheme), give

$$m_i^0 = m_i \left\{ 1 + \frac{-2}{\epsilon} \cdot \frac{\alpha_s}{\pi} + O(\alpha_s^2) \right\}. \quad (\text{A.22})$$

When incorporated in Eq. (A.21), and expanding $(v^2/-q^2)^\epsilon$ to the required order, we finally obtain

$$\begin{aligned} \psi_{5 \text{ bare}} = & (v^2)^{-\epsilon/2} (m_i + m_j)^2 \frac{3q^2}{8\pi^2} \left\{ \frac{2}{\epsilon} - \log \frac{-q^2}{v^2} + \text{constant} \right. \\ & + \frac{\alpha_s}{\pi} \left[-\frac{4}{\epsilon^2} + \frac{5}{3\epsilon} + \log \frac{-q^2}{v^2} - 2(\log 4\pi - \gamma_E) \log \frac{-q^2}{v^2} \right. \\ & \left. \left. - \frac{17}{3} \log \frac{-q^2}{v^2} + \text{constant} \right] \right\}. \end{aligned} \quad (\text{A.23})$$

The renormalized $\psi_5(q^2)$ is obtained by subtracting from $(v^2)^{\epsilon/2} \psi_{5 \text{ bare}}$ its poles in powers of $2/\epsilon - \gamma_E + \log 4\pi$, i.e.,

$$\begin{aligned} \psi_5(q^2) = & (m_i + m_j)^2 \frac{3q^2}{8\pi^2} \left\{ -\log \frac{-q^2}{v^2} \right\} \\ & \times \left\{ 1 + \frac{\alpha_s}{\pi} \left[-\log \frac{-q^2}{v^2} + \frac{17}{3} \right] \right\}. \end{aligned} \quad (\text{A.24})$$

This is the final expression for $\psi_5(q^2)$, renormalized in the modified minimal subtraction scheme ($\overline{\text{MS}}$ -scheme), Eq. (3.2).

APPENDIX B

We consider the basic equation for the second derivative of ψ_5 , before improving with the renormalization group:

$$\begin{aligned} \psi_{5 \text{ pert}}'' &= \frac{3}{8\pi^2 Q^2} (m_u + m_d)^2 \left\{ 1 + \frac{\alpha_s(\nu)}{\pi} \left[-2 \log \frac{Q^2}{\nu^2} \right] \right. \\ &+ \left(\frac{\alpha_s(\nu)}{\pi} \right)^2 \left[\left(4 + \frac{33-2n}{12} \right) \log^2 \frac{Q^2}{\nu^2} - \frac{17+n}{6} \log \frac{Q^2}{\nu^2} \right] \\ &\left. + \frac{\alpha_s(\nu)}{\pi} \times \text{constant} + \left(\frac{\alpha_s(\nu)}{\pi} \right)^2 \times \text{constant} \right\}. \end{aligned} \quad (\text{B.1})$$

The terms in $((\alpha_s(\nu)/\pi) \times \text{constant})$ have been calculated in Appendix A, and are taken into account in Eq. (3.11); the terms in $((\alpha_s(\nu)/\pi)^2 \times \text{constant})$ will be neglected. To get the renormalization group improved $F_5^{(N)}$ of Eq. (4.10) we have to differentiate N times (B.1) with respect to Q , and afterwards set $Q^2 = \nu^2$, $\alpha_s \rightarrow \bar{\alpha}$, $m \rightarrow \bar{m}$. We see from (B.1) that this involves the derivatives of the following functions:

$$\frac{1}{x}, \quad \log x, \quad \frac{\log x}{x}, \quad \frac{\log^2 x}{x},$$

with $x = Q^2/\nu^2$. For the first two we have, for $N \geq 1$,

$$\frac{\partial^N}{\partial x^N} \left(\frac{1}{x} \right) = (-1)^N \frac{N!}{x^{N+1}}; \quad \frac{\partial^N}{\partial x^N} \log x = (-1)^{N-1} \frac{(N-1)!}{x^N}. \quad (\text{B.2})$$

Using (B.2),

$$\begin{aligned} \frac{\partial^N}{\partial x^N} \left(\frac{\log x}{x} \right) &= \sum_{k=0}^N \binom{N}{k} \left(\frac{\partial^{N-k}}{\partial x^{N-k}} \cdot \frac{1}{x} \right) \frac{\partial^k}{\partial x^k} \log x \\ &= (-1)^N \frac{N!}{x^{N+1}} \left(\log x - \sum_{k=1}^N \frac{1}{k} \right). \end{aligned} \quad (\text{B.3})$$

The functions $S_\ell(N) = \sum_{k=1}^N k^{-\ell}$ may be rewritten for $N = \text{integer} \geq 1$ as

$$S_\ell(N) = \sum_{j=0}^{\infty} \left\{ \frac{\Gamma(j+1)}{\Gamma(j+\ell+1)} - \frac{\Gamma(j+N+1)}{\Gamma(j+\ell+N+1)} \right\}; \quad (\text{B.4})$$

this expression, however, allow us to continue the $S_\ell(N)$ to arbitrary N . Note that $S_\ell(N=0) = 0$, so we may rewrite (B.3) as

$$\frac{\partial^N}{\partial x^N} \cdot \frac{\log x}{x} = (-1)^N \frac{N!}{x^{N+1}} (\log x - S_1(N)) \quad (\text{B.5})$$

where, with S_1 given by (B.4), the expression is valid for arbitrary N . When setting $Q^2 = v^2$, the term $\log x$ drops; and thus we obtain the $S_1(N)$ terms of Eq. (4.10). The term in $S_1^2 - S_2$ is slightly more complicated. It involves the derivatives of $(\log^2 x)/x$. We have, for $N \geq 1$, and using (B.2) and (B.5),

$$\begin{aligned} \frac{\partial^N}{\partial x^N} \left(\frac{\log^2 x}{x} \right) &= \sum_{k=0}^N \binom{N}{k} \left(\frac{\partial^k}{\partial x^k} \log x \right) \frac{\partial^{N-k}}{\partial x^{N-k}} \cdot \frac{\log x}{x} \\ &= (\log x) \{ \log x - S_1(N) \} (-1)^N \frac{N!}{x^{N+1}} + (-1)^{N-1} \frac{(N-1)!}{x^{N+1}} \log x \\ &\quad + \sum_{k=1}^{N-1} \binom{N}{k} (-1)^{k-1} \frac{(k-1)!}{x^k} (-1)^{N-k} \frac{(N-k)!}{x^{N-k+1}} \{ \log x - S_1(N-k) \} \\ &= (-1)^N \frac{N!}{x^{N+1}} \{ \log x - 2S_1(N) \} \log x \\ &\quad + \frac{(-1)^N N!}{x^{N+1}} \sum_{k=1}^{N-1} \frac{S_1(N-k)}{k}. \end{aligned}$$

We finally have to use the identity

$$\sum_{k=1}^{N-1} \frac{S_1(N-k)}{k} = [S_1(N)]^2 - S_2(N),$$

so, taking advantage of (B.4) to get

$$S_0(0) = 0, \quad S_1(1)^2 - S_2(1) = 0,$$

we finally find

$$\begin{aligned} \frac{\partial^N}{\partial x^N} \left(\frac{\log^2 x}{x} \right) &= \frac{(-1)^N N!}{x^{N+1}} \left\{ [\log x - 2S_1(N)] \log x \right. \\ &\quad \left. + S_1(N)^2 - S_2(N) \right\}, \end{aligned} \quad (\text{B.6})$$

from which the corresponding term in (4.10) may be obtained immediately.

At large N , the expansions of the S_ℓ have been discussed in Ref. 20); they are easily obtained from (B.4).

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FIGURE CAPTIONS

- Fig. 1 : Zero order diagram for ψ_5 , D_5 .
- Fig. 2 : Non-perturbative contributions to ψ_5 , D_5 ,
- Fig. 3 : Gluon corrections to ψ_5 , D_5 .
- Fig. 4 : The running masses as functions of Q , for two typical values of Λ .

Fig. 1

Fig. 2

Fig. 3

Fig. 4a