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TOPOLOGICAL CHARGE SCREENING AND THE 'PROTON SPIN' BEYOND THE CHIRAL LIMIT

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Abstract

The theory of the 'proton spin' effect proposed in our earlier papers is extended to include the chiral $SU(3)$ symmetry breaking and flavour mixing induced by non-vanishing quark masses in QCD. The theoretical basis is the derivation of exact, unified Goldberger-Treiman (GT) relations valid beyond the chiral limit. The observed suppression in the flavour singlet axial charge $a^0(Q^2)$ is explained by an anomalously small value for the slope of the singlet current correlation function $\langle 0|T\ \partial^\mu J^0_{\mu 5}\ \partial^\nu J^0_{\nu 5}|0\rangle$, a consequence of the screening of topological charge in the QCD vacuum. Numerical predictions are obtained by evaluating the current correlation functions using QCD spectral sum rules. The results, $a^0(Q^2) = 0.31 \pm 0.02$ and $\int dx\ g_1^p(x,Q^2) = 0.141 \pm 0.005$ (at $Q^2 = 10\ \mathrm{GeV}^2$), are in good agreement with current experimental data on the polarised proton structure function g_1^p.

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1. Introduction

The 'proton spin' problem, i.e. the question of why the first moment of the flavour singlet component of the polarised proton structure function g_1^p is anomalously suppressed, has inspired an impressive research effort, both theoretical and experimental, for over a decade. (For recent reviews, see e.g. refs.[1,2]. As is well-known, the first moment of g_1^p can be expressed in terms of the axial charges of the proton as follows:

$$\int_0^1 dx\; g_1^p(x;Q^2) \;=\; \frac{1}{12}C_1^{\rm NS}\big(\alpha_s(Q^2)\big)\,\Big(a^3+\frac{1}{3}a^8\Big)+\frac{1}{9}C_1^{\rm S}\big(\alpha_s(Q^2)\big)\;a^0(Q^2) \tag{1.1}$$

Here, $C_1^{\rm NS}$, C_1^S are the appropriate Wilson coefficients arising from the OPE for two electromagnetic currents, while the axial charges are defined from the forward matrix elements

$$\langle p,s|J_{\mu5}^3|p,s\rangle = \frac{1}{2}a^3 s_\mu \qquad \langle p,s|J_{\mu5}^8|p,s\rangle = \frac{1}{2\sqrt{3}}a^8 s_\mu \qquad \langle p,s|J_{\mu5}^0|p,s\rangle = a^0(Q^2)s_\mu \tag{1.2}$$

where $J_{\mu5}^a$ (often denoted A_μ^a) are the axial currents and s_μ is the proton polarisation vector. a^3 and a^8 are known in terms of the F and D coefficients from beta and hyperon decay, so that an experimental determination of the first moment of g_1^p in polarised deep inelastic scattering (DIS) allows a determination of the singlet axial charge $a^0(Q^2)$. The 'proton spin' problem is that it is found experimentally that $a^0(Q^2)$ is strongly suppressed relative to a^8, which would be its expected value if the OZI (Zweig) rule were exact in this channel.

DIS is normally described theoretically using the QCD parton model. In this model, the axial charges are represented (in the AB renormalisation scheme) in terms of moments of parton distributions as follows[3,4]:

$$a^3 = \Delta u - \Delta d \qquad a^8 = \Delta u + \Delta d - 2\Delta s \qquad a^0(Q^2) = \Delta u + \Delta d + \Delta s - n_f\frac{\alpha_s}{2\pi}\Delta g(Q^2) \tag{1.3}$$

In the parton model, the 'proton spin' problem takes the following form. In the naive, or valence quark, parton model we would expect the strange quark and gluon distributions to vanish, i.e. $\Delta s = 0$, $\Delta g(Q^2) = 0$. In that case, $a^0 = a^8$, the OZI prediction. Inserted into eq.(1.1), this gives the Ellis-Jaffe sum rule[5]. However, the observed suppression $a^0(Q^2) < a^8$ can be accommodated in the full QCD parton model by invoking either or both a non-zero polarised strange quark distribution $\Delta s \neq 0$ or a non-zero polarised gluon distribution $\Delta g(Q^2) \neq 0$. An interesting conjecture (in line with the insights of our alternative approach) is that the suppression is primarily due to the gluon distribution[3], although a quantitative prediction would still only follow if $\Delta g(Q^2)$ can be independently measured, either through a precise analysis of the Q^2 dependence of g_1^p [4] or directly through other less inclusive high energy processes such as open charm production. Notice, however, that even in the QCD parton model picture, it is *not* possible to identify $a^0(Q^2)$ with spin[6]. This identification only holds for free quarks, in which case the Q^2 scale dependence (which is related to the $U_A(1)$ axial anomaly) disappears from a^0. As has been emphasised many times[7-9,1], the so-called 'proton spin' problem is not a problem of *spin* – rather, it is a question of understanding the dynamical origin of the OZI violation $a^0(Q^2) < a^8$.

In a series of papers[7,10-12], we have a proposed an alternative, complementary, approach to the 'proton spin' problem which provides both a new physical insight into the origin of the suppression in $a^0(Q^2)$ and a quantitative prediction, which is in good agreement with the current experimental data. In our approach (reviewed in refs.[8,1]), the flavour singlet axial charge $a^0(Q^2)$ is decomposed into the product of an RG-invariant 1PI vertex and a non-perturbative, but target independent, QCD correlation function which we subsequently identify as the first moment of the QCD topological susceptibility $\chi'(0)$, i.e.

$$a^0(Q^2) \quad = \quad \frac{1}{2m_N} 6\ \sqrt{\chi'(0)}\ \hat{\Gamma}_{\eta^0 NN} \tag{1.4}$$

where $\chi'(0) = \frac{d}{dk^2}\chi(k^2)|_{k=0}$ and

$$\chi(k^2) = i\int d^4x\ e^{ikx}\langle 0|T\ Q(x)\ Q(0)|0\rangle \tag{1.5}$$

with $Q = \frac{\alpha_s}{8\pi}\mathrm{tr}G_{\mu\nu}\tilde{G}^{\mu\nu}$ the gluon topological charge density. In the vertex, η^0 denotes the 'OZI Goldstone boson', i.e. the (unphysical) state which would become the Goldstone boson for spontaneously broken $U_A(1)$ in the absence of the anomaly (OZI limit). We now make the key assumption that the RG-invariant vertex obeys the OZI rule, viz. $\hat{\Gamma}_{\eta^0 NN} = \sqrt{2}\ \hat{\Gamma}_{\eta^8 NN}$. Then, comparing with the GT relation for a^8 in the chiral limit, we obtain our prediction:

$$\frac{a^0(Q^2)}{a^8} \quad = \quad \frac{\sqrt{6}}{f_\pi}\ \sqrt{\chi'(0)}\Big|_{Q^2} \tag{1.6}$$

The suppression in $a^0(Q^2)$ simply reflects an anomalously small value of $\chi'(0)$, which we confirmed by an explicit calculation using QCD spectral sum rules[12]. In this picture, the suppression is therefore a target-independent effect, i.e. a generic property of the QCD vacuum rather than a specific property of the proton. Since $a^0(Q^2)$ can be expressed, via the axial $U_A(1)$ anomaly, as the proton matrix element of the topological charge Q, its suppression can be understood as a screening of topological charge in the QCD vacuum. We conclude that the fundamental dynamics underlying the violation of the Ellis-Jaffe sum rule is not to do with quark spin, but instead is a manifestation of topological charge screening by the QCD vacuum.

This 'target-independence' property may in principle be tested directly in experiment, by studying semi-inclusive DIS in which a hadron carrying a large fraction of the target energy is observed in the target fragmentation region. Such experiments should be possible at, e.g. polarised HERA. The details of our proposal are described in refs.[13-15].

Although our previous analysis was restricted to the chiral limit of QCD, it was clear from the derivation that the final result for $a^0(Q^2)$ should only have a weak dependence on the quark masses. Indeed, the cancellation of the explicit quark mass dependence in

$a^0(Q^2)$ was already pointed out in ref.[7]. However, the introduction of quark masses does involve a significant complication in the analysis. The purpose of this paper is therefore to present the generalisation of our theory of the 'proton spin' to QCD beyond the chiral limit.

Underlying our approach to polarised DIS – the 'CPV' method reviewed in some detail in ref.[1] – is the $U_A(1)$ Goldberger-Treiman (GT) relation. The initial insight that the 'proton spin' problem was essentially one of OZI violation and could be understood in terms of an extension of the GT relation to the flavour singlet channel was made by one of us in ref.[7]. The $U_A(1)$ GT relation was subsequently put on a firm field-theoretical basis in refs.[10,11], where the connection with the slope of the topological susceptibility was first established.

The introduction of quark masses complicates the $U_A(1)$ GT analysis in two ways. First, the pure gluon topological susceptibility has to be combined with correlation functions of pseudoscalar operators of the form $\phi_5 = \sum \bar{q}\gamma_5 q$ arising from the extra explicit chiral symmetry breaking terms in the divergence of the axial current. Second, since the quark masses break flavour $SU(3)$, the $U_A(1)$ GT relation is mixed with those for the flavour non-singlet axial charges. In this paper, we present the unified GT relations for the flavour singlet and non-singlet axial charges, expressing them in terms of 1PI vertices and the first moments of the correlation functions of the divergences of the axial currents as follows:

$$G_A^a \;=\; \frac{1}{2m_N}\; F_{ab}\; \hat{\Gamma}_{\eta^b NN} \tag{1.7}$$

where $a = 0, 3, 8$ is the $SU(3)$ flavour index, the axial charges are normalised as

$$G_A^3 = \frac{1}{2}a^3 \qquad G_A^8 = \frac{1}{2\sqrt{3}}a^8 \qquad G_A^0(Q^2) = a^0(Q^2) \tag{1.8}$$

and

$$(FF^T)_{ab} \;=\; \lim_{k=0}\frac{d}{dk^2}\; i\int d^4x\; \langle 0|T\; \partial^\mu J^a_{\mu 5}(x)\; \partial^\nu J^b_{\nu 5}(0)|0\rangle \tag{1.9}$$

It is important to realise that, like the singlet $U_A(1)$ GT relation, these are *exact* relations in QCD field theory. They go beyond the pole-dominance approximation used in the conventional GT relations, replacing the decay constants by current correlation functions and the πNN or ηNN couplings by appropriate 1PI vertex functions.

In the second part of the paper, we make this analysis quantitative by calculating the relevant current correlation functions using QCD spectral sum rules. This confirms the stability of our earlier results[12] to the introduction of quark masses. A very careful analysis is presented, with particular attention given to the inclusion of higher order corrections in α_s or $m_s^2\tau$ and to the stability of the sum rules with respect to the Borel parameter τ. We find that the size of the explicit chiral and $SU(3)$ breaking effects is in line with our theoretical expectations and confirms the validity of the Laplace sum rule method for calculating correlation functions, such as the topological susceptibility, in the flavour singlet channel.

The paper is organised as follows. In section 2, we quote the (anomalous) chiral Ward identities which we need to derive the unified Goldberger-Treiman relations. The derivation itself is presented in section 3. In section 4, we relate these new GT relations to the 'proton spin' sum rule and describe our expectations for the results of a spectral sum rule calculation of the relevant current correlation functions. This is elaborated on in section 5, where the pattern of explicit mass cancellations is exhibited in the framework of an effective lagrangian.

In section 6, we evaluate the current correlation functions (1.9) using the QCD spectral sum rule technique. The presence of quark masses requires a substantially more complicated analysis than we had previously performed in the chiral limit to evaluate the slope of the topological susceptibility. However, the results confirm our earlier conclusions[12]. In section 7, these numerical results are used in the GT relations and our prediction for the 'proton spin' suppression is obtained. Our conclusions from this work are presented in section 8.

Appendix A deals with some technical aspects of the derivation of the unified GT formulae. Their relationship with conventional current algebra and PCAC methods is discussed briefly in Appendix B. The renormalisation group properties of the Green functions and vertices involved in the GT relations are derived in Appendix C. Finally, since both our formal methods and spectral sum rule analysis have been repeatedly criticised in the literature by Ioffe (see e.g. refs.[16,17] and references therein), we explain in Appendix D why these criticisms are not correct and show in detail the errors in refs.[16-20] which lead Ioffe to his false conclusions.

2. Chiral Ward Identities

The derivation of the generalised Goldberger-Treiman relations is based on the chiral Ward identities satisfied by the composite operator propagators and vertex functions. In this section, we derive these in the form which will be most convenient for the applications which follow.

For the propagators, the starting point is the Ward identity for the generating functional $W[V_{\mu 5}^a, V_\mu^a, \theta, S_5^a, S^a]$ of Green functions which are '1PI' with respect to the designated fields (composite operators). Here, $V_{\mu 5}^a, V_\mu^a, \theta, S_5^a, S^a$ are the sources for the composite operators $J_{\mu 5}^a, J_\mu^a, Q, \phi_5^a, \phi^a$ respectively, where

$$J_{\mu 5}^a = \bar{q}\gamma_\mu\gamma_5 T^a q \qquad J_\mu^a = \bar{q}\gamma_\mu T^a q \qquad Q = \frac{\alpha_s}{8\pi}\mathrm{tr}G_{\mu\nu}\tilde{G}^{\mu\nu}$$
$$\phi_5^a = \bar{q}\gamma_5 T^a q \qquad \phi^a = \bar{q}T^a q \tag{2.1}$$

In this notation, $T^i = \frac{1}{2}\lambda^i$ are flavour $SU(n_f)$ generators, and we include the singlet $U_A(1)$ generator $T^0 = \mathbf{1}$ and let the index $a = 0, i$. We will only need to consider fields where i corresponds to a generator in the Cartan sub-algebra, so that $a = 0, 3, 8$ for $n_f = 3$ quark flavours. We define d-symbols by $\{T^a, T^b\} = d_{abc}T^c$. Since this includes the flavour singlet $U(1)$ generator, they are only symmetric on the first two indices. For $n_f = 3$, the explicit values are $d_{000} = d_{033} = d_{088} = 2, d_{330} = d_{880} = 1/3, d_{338} = d_{383} = -d_{888} = 1/\sqrt{3}$. (For further notation and description of the formalism used here, see ref.[11].)

The chiral Ward identities are written in the functional formalism as follows:

$$\partial_\mu \frac{\delta W}{\delta V_{\mu 5}^a} - 2n_f \delta_{a0} \frac{\delta W}{\delta \theta} - d_{adc} m^d \frac{\delta W}{\delta S_5^c} + d_{adc} S^d \frac{\delta W}{\delta S_5^c} - d_{adc} S_5^d \frac{\delta W}{\delta S^c} = 0 \tag{2.2}$$

where we have displayed both the anomalous breaking term for the $U_A(1)$ current and the soft breaking induced by the quark masses. The quark mass matrix is written as $m^a T^a$, so that for $n_f = 3$,

$$\begin{pmatrix} m_u & 0 & 0 \\ 0 & m_d & 0 \\ 0 & 0 & m_s \end{pmatrix} = m^0 \mathbf{1} + m^3 T^3 + m^8 T^8 \tag{2.3}$$

Notice that there are no variation terms for the currents themselves as we have restricted to fields where a is a Cartan sub-algebra index. It is convenient to use a notation where a functional derivative is denoted simply by a subscript. So, also transforming to momentum space, we can rewrite eq.(2.2) compactly as

$$ik_\mu W_{V_{\mu 5}^a} - 2n_f \delta_{a0} W_\theta - d_{adc} m^d W_{S_5^c} + d_{adc} S^d W_{S_5^c} - d_{adc} S_5^d W_{S^c} = 0 \tag{2.4}$$

The Ward identities for composite operator Green functions are derived by taking functional derivatives of this basic identity. We will need the following identities for 2-point functions:

$$\begin{aligned} &ik_\mu W_{V_{\mu 5}^a V_{\nu 5}^b} - 2n_f \delta_{a0} W_{\theta V_{\nu 5}^b} - M_{ac} W_{S_5^c V_{\nu 5}^b} = 0 \\ &ik_\mu W_{V_{\mu 5}^a \theta} - 2n_f \delta_{a0} W_{\theta\theta} - M_{ac} W_{S_5^c \theta} = 0 \\ &ik_\mu W_{V_{\mu 5}^a S_5^b} - 2n_f \delta_{a0} W_{\theta S_5^b} - M_{ac} W_{S_5^c S_5^b} - \Phi_{ab} = 0 \end{aligned} \tag{2.5}$$

where we have introduced the still more compact notation

$$M_{ab} = d_{acb} m^c \qquad\qquad \Phi_{ab} = d_{abc} \langle \phi^c \rangle \tag{2.6}$$

$\langle \phi^c \rangle$ is the VEV $\langle \bar{q} T^c q \rangle$, so that for $n_f = 3$ the condensates may be written as

$$\begin{pmatrix} \langle \bar{u}u \rangle & 0 & 0 \\ 0 & \langle \bar{d}d \rangle & 0 \\ 0 & 0 & \langle \bar{s}s \rangle \end{pmatrix} = \frac{1}{3} \langle \phi^0 \rangle \mathbf{1} + 2 \langle \phi^3 \rangle T^3 + 2 \langle \phi^8 \rangle T^8 \tag{2.7}$$

Notice that with these definitions,

$$\frac{1}{8} \det M = m_u m_d m_s \qquad\qquad \frac{1}{6} \det \Phi = \langle \bar{u}u \rangle \ \langle \bar{d}d \rangle \ \langle \bar{s}s \rangle \tag{2.8}$$

with the obvious generalisation for arbitrary n_f.

Combining the individual equations in (2.5), we find the important identity:

$$k_\mu k_\nu W_{V_{\mu 5}^a V_{\nu 5}^b} - M_{ac} \Phi_{cb} = W_{S_D^a S_D^b} \tag{2.9}$$

where S_D^a is the source for the current divergence operator $D^a = 2n_f\delta_{a0}Q + d_{acd}m^c\phi_5^d$. In conventional notation,

$$
\begin{aligned}
W_{S_D^a S_D^b} &= i\int dx\ e^{ikx}\ \langle 0|T\ D^a(x)\ D^b(0)|0\rangle \\
&= i\int dx\ e^{ikx}\ \langle 0|T\ \partial^\mu J_{\mu 5}^a(x)\ \partial^\nu J_{\nu 5}^b(0)|0\rangle
\end{aligned}
\tag{2.10}
$$

The zero-momentum Ward identities play a special role. These follow immediately from eqs.(2.5) under the assumption that there are no massless particles (in particular, no exact Goldstone bosons) contributing $1/k^2$ poles in the 2-point functions. With this assumption, we find simply

$$
\begin{aligned}
&2n_f\delta_{a0}W_{\theta\theta} + M_{ac}W_{S_5^c\theta} = 0 \\
&2n_f\delta_{a0}W_{\theta S_5^b} + M_{ac}W_{S_5^c S_5^b} + \Phi_{ab} = 0
\end{aligned}
\tag{2.11}
$$

The generating functional for proper vertices, Γ, is defined from W by a partial Legendre transform (Zumino transform[21]), in which the transform is made only on the fields Q, ϕ_5^a, ϕ^a and not on the currents. A number of important results on these transforms are collected in Appendix A. The resulting proper vertices are '1PI' wrt the propagators for these composite operators only. As explained fully in ref.[11], by separating off the particle poles in the propagators, this is the definition which gives the closest identification of these field-theoretic vertices with physical low-energy couplings such as $g_{\pi NN}$ etc.

We therefore define the generating functional $\Gamma[V_{\mu 5}^a, V_\mu^a, Q, \phi_5^a, \phi^a]$ as:

$$
\Gamma[V_{\mu 5}^a, V_\mu^a, Q, \phi_5^a, \phi^a] = W[V_{\mu 5}^a, V_\mu^a, \theta, S_5^a, S^a] - \int dx\ \Big(\theta Q + S_5^a\phi_5^a + S^a\phi^a\Big)
\tag{2.12}
$$

The chiral Ward identities corresponding to eq.(2.4) are therefore:

$$
ik_\mu\Gamma_{V_{\mu 5}^a} - 2n_f\delta_{a0}Q - d_{acd}m^c\phi_5^d + d_{acd}\phi^d\Gamma_{\phi_5^c} - d_{acd}\phi_5^d\Gamma_{\phi^c} = 0
\tag{2.13}
$$

The Ward identities for the 2-point vertices will also be important in the derivation of the GT relations. These follow directly from eq.(2.13):

$$
\begin{aligned}
&ik_\mu\Gamma_{V_{\mu 5}^a V_{\nu 5}^b} + \Phi_{ac}\Gamma_{\phi_5^c V_{\nu 5}^b} = 0 \\
&ik_\mu\Gamma_{V_{\mu 5}^a Q} - 2n_f\delta_{a0} + \Phi_{ac}\Gamma_{\phi_5^c Q} = 0 \\
&ik_\mu\Gamma_{V_{\mu 5}^a \phi_5^b} + \Phi_{ac}\Gamma_{\phi_5^c\phi_5^b} - M_{ab} = 0
\end{aligned}
\tag{2.14}
$$

It is then straightforward to derive the following important identity, analogous to eq.(2.9):

$$
k_\mu k_\nu\Gamma_{V_{\mu 5}^a V_{\nu 5}^b} + M_{ac}\Phi_{cb} = \Phi_{ac}\Gamma_{\phi_5^c\phi_5^d}\Phi_{db}
\tag{2.15}
$$

3. The Goldberger-Treiman Relations

We now present a unified derivation of the Goldberger-Treiman relations for the flavour singlet and non-singlet axial charges.[(1)] The derivation follows the principles of refs.[10,11], extended to include non-zero quark masses and flavour mixing. This allows us to present all the GT relations in terms of a single, unified formula involving the 2-point correlation functions of the divergences of the flavour singlet and non-singlet currents.

The axial charges G_A^a are defined as the form factors in the forward nucleon matrix elements of the axial currents, viz.

$$\langle p,s|J_{\mu 5}^a|p,s\rangle = G_A^a s_\mu \tag{3.1}$$

where p_μ and $s_\mu = \bar{u}(p,s)\gamma_\mu\gamma_5 u(p,s)$ are respectively the momentum and polarisation vector of the nucleon.

To express this matrix element in our composite propagator-vertex formalism, we introduce an interpolating field N and source S_N for the nucleon as in refs.[10,11]. (Notice that this is purely a formal device – there is no dynamics implicit in this manoeuvre.) The matrix element is then just the 3-point function $W_{V_{\mu 5}^a S_N S_N}$ with the external propagators amputated. From eq.(A.8), we can re-express this in terms of the vertex functional Γ as follows:

$$\begin{aligned}\langle p,s|J_{\mu 5}^a|p,s\rangle &= \bar{u}(p,s)\Big[W_{S_N S_N}^{-1}\ W_{V_{\mu 5}^a S_N S_N}\ W_{S_N S_N}^{-1}\Big]u(p,s) \\ &= \bar{u}(p,s)\Big[\Gamma_{V_{\mu 5}^a NN} \ +\ W_{V_{\mu 5}^a \theta}\ \Gamma_{QNN}\ +\ W_{V_{\mu 5}^a S_5^b}\ \Gamma_{\phi_5^b NN}\Big]u(p,s)\end{aligned} \tag{3.2}$$

Since the propagators on the rhs vanish at zero momentum (this requires the absence of any $1/k^2$ poles, which is assured by the $U_A(1)$ anomaly and quark masses), we find simply

$$2m_N G_A^a\ \bar{u}\gamma_5 u = \bar{u}\Big[k_\mu \Gamma_{V_{\mu 5}^a NN}\big|_{k=0}\Big]u \tag{3.3}$$

where m_N is the nucleon mass. The GT relations then follow immediately from the Ward identity (2.13) for Γ. Differentiating wrt the nucleon fields, we find

$$2m_N G_A^a = \Phi_{ab}\hat{\Gamma}_{\phi_5^b NN}\big|_{k=0} \tag{3.4}$$

where for convenience we define $i\bar{u}\ \Gamma_{\phi_5^a NN}\ u = \hat{\Gamma}_{\phi_5^a NN}\ \bar{u}\gamma_5 u$, etc.

(1) Similar generalised GT relations have been presented some time ago, with the same motivation of explaining the 'proton spin' problem, by Efremov, Soffer and Törnqvist[22] using the more conventional PCAC language.

A non-forward version of the GT relation, which was used extensively in refs.[10-12], can be found from eq.(3.2) by using the Ward identities (2.5) for the propagators together with (2.13) for $\Gamma_{V_{\mu 5}^a NN}$. This allows us to write, for all k,

$$2m_N G_A^a(k^2) + k^2 G_P^a(k^2) = -\Big(2n_f\delta_{a0}W_{\theta\theta} + M_{ac}W_{S_5^c\theta}\Big)\hat{\Gamma}_{QNN} \\ -\Big(2n_f\delta_{a0}W_{\theta S_5^b} + M_{ac}W_{S_5^c S_5^b}\Big)\hat{\Gamma}_{\phi_5^b NN} \tag{3.5}$$

$G_P^a(k^2)$ is the pseudoscalar form factor in the non-forward matrix element $\langle p,s|J_{\mu 5}^a|p,s\rangle$, and again has no $1/k^2$ pole for the reasons given above. This expression clearly reduces to eq.(3.4) on using the zero-momentum Ward identities (2.11) for the propagators.

The remaining step to convert eq.(3.4) into the useful form of the GT relations is to normalise the field ϕ_5^a appropriately. Clearly, eq.(3.4) is independent of the normalisation. However, with a suitable choice, the vertices can be made both RG invariant and essentially identical to the physical Goldstone boson couplings $g_{\pi NN}$ etc. To achieve this, we define normalised fields

$$\eta^a = B_{ab}\phi_5^b \tag{3.6}$$

where B is a constant matrix(2) such that

$$\frac{d}{dk^2}\Gamma_{\eta^a\eta^b}\Big|_{k=0} = \delta_{ab} \tag{3.7}$$

This condition ensures that the fields η^a have unit coupling to the Goldstone bosons. The case of the singlet η^0 is of course special, since it is only after mixing with the topological field Q (and then flavour mixing) that it becomes the physical η'. The intricacies of this are discussed fully in ref.[11]. Indeed, this is why it is most convenient to impose the normalisation condition as above on the matrix of 2-point vertices $\Gamma_{\eta^a\eta^b}$, which is the inverse of the pseudoscalar propagator matrix, since this most simply characterises the η^0 before mixing with Q.

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(2) From the Ward identity (in matrix notation)

$$ik_\mu\Gamma_{V_{\mu 5}\eta} + \Phi B^T\ \Gamma_{\eta\eta} - MB^{-1} = 0$$

and writing

$$\Gamma_{V_{\mu 5}\eta} = ik_\mu f(k^2)$$

we find

$$\Gamma_{\eta\eta} = k^2(\Phi B^T)^{-1}f\ +\ (\Phi B^T)^{-1}M\Phi(B\Phi)^{-1}$$

The normalisation condition (3.7) can therefore be applied while keeping B in eq.(3.6) a constant. This determines (see Appendix B for the relation to PCAC)

$$f(0) = \Phi B^T$$

However, it is *not* possible, as in the chiral limit case[11], to impose a normalisation valid for all k, such as $\Gamma_{\eta^a\eta^b} = k^2\delta_{ab} - (m_\eta^2)_{ab}$, by allowing B to be a function of k^2.

The proof that the vertices $\Gamma_{\eta^a NN}$ defined with the fields normalised according to eq.(3.7) are RG invariant now goes through in the same way as shown in the chiral limit in ref.[11]. In Appendix C, we summarise some of the main results for the extension to non-zero quark masses. Ref.[11] also contains a careful description of how our formalism is related to standard current algebra (PCAC). A simple illustration of this is included in Appendix B.

Re-expressing eq.(3.4) in terms of the properly normalised vertices, we have

$$2m_N G_A^a = \Phi_{ac} B_{cb}^T \, \hat{\Gamma}_{\eta^b NN}\big|_{k=0} \tag{3.8}$$

where B is to be determined from the 2-point vertex condition

$$\frac{d}{dk^2}\Gamma_{\phi_5^a \phi_5^b}\big|_{k=0} = B_{ac}^T \, \frac{d}{dk^2}\Gamma_{\eta^c \eta^d}\big|_{k=0} \, B_{db} = B_{ac}^T B_{cb} \tag{3.9}$$

The straightforward approach to finding $\Gamma_{\phi_5^a \phi_5^b}$ is to write it as one component of the inverse of the propagator matrix $W_{\mathcal{S}\mathcal{S}}$ (with $\mathcal{S} = \{\theta, S_5^a\}$). This was the approach used in refs.[10,11] to relate $\Gamma_{\phi_5^0 \phi_5^0}$ to the topological susceptibility $W_{\theta\theta}$. However, inverting this matrix in the multi-flavour case is cumbersome, so here we use an alternative approach.

First, we use the Ward identities (2.14) to express $\Gamma_{\phi_5^a \phi_5^b}$ in terms of $\Gamma_{V_{\mu 5}^a V_{\nu 5}^b}$:

$$\begin{aligned} k_\mu k_\nu \Gamma_{V_{\mu 5}^a V_{\nu 5}^b} &= i k_\nu \Phi_{ac} \, \Gamma_{\phi_5^c V_{\nu 5}^b} \\ &= \Phi_{ac} \, \Gamma_{\phi_5^c \phi_5^d} \, \Phi_{db} \; - \; M_{ac} \Phi_{cb} \end{aligned} \tag{3.10}$$

Then, using the general identity (A.9) for partial Legendre transforms, we relate $\Gamma_{V_{\mu 5}^a V_{\nu 5}^b}$ to the 2-current propagator $W_{V_{\mu 5}^a V_{\nu 5}^b}$:

$$\Gamma_{V_{\mu 5}^a V_{\nu 5}^b} \; = \; W_{V_{\mu 5}^a V_{\nu 5}^b} \; - \; W_{V_{\mu 5}^a \mathcal{S}} \, W_{\mathcal{S}\mathcal{T}}^{-1} \, W_{\mathcal{T} V_{\nu 5}^b} \tag{3.11}$$

where $\mathcal{S}$ and $\mathcal{T}$ represent $\{\theta, S_5^a\}$. Combining with eqs.(2.9) and (2.15) finally yields

$$\Phi_{ac} \, \Gamma_{\phi_5^c \phi_5^d} \, \Phi_{db} \; = \; W_{S_D^a S_D^b} \; + \; k_\mu W_{V_{\mu 5}^a \mathcal{S}} \, W_{\mathcal{S}\mathcal{T}}^{-1} \, W_{\mathcal{T} V_{\nu 5}^b} k_\nu \tag{3.12}$$

and so, in matrix notation,

$$\Phi B^T B \Phi \; = \; \frac{d}{dk^2} W_{S_D S_D}\big|_{k=0} \; + \; \frac{d}{dk^2}\big(k_\mu W_{V_{\mu 5}\mathcal{S}} \, W_{\mathcal{S}\mathcal{T}}^{-1} \, W_{\mathcal{T} V_{\nu 5}} k_\nu\big)\big|_{k=0} \tag{3.13}$$

The argument is almost complete. ΦB^T is precisely the combination we need for the GT relations (3.8), and is related by eq.(3.13) directly to the first moment of the 2-point correlation function (2.10) for the divergences of the currents. This generalises the relation with the topological susceptibility found in refs.[10,11].

It remains to show that the final term in eq.(3.13) vanishes. The first and last factors are of $O(k^2)$, so this will contribute zero unless there is a $1/k^2$ pole in the inverse pseudoscalar propagator matrix $W^{-1}_{\mathcal{ST}}$. As already mentioned, there are no $1/k^2$ poles in the propagators themselves, so all we need show is that the determinant $\Delta(k^2)$ of this propagator matrix is non-vanishing at $k = 0$. This follows from the formula

$$\Delta(0) = W_{\theta\theta}(0)\ (\mathrm{det}M)^{-1}\ \mathrm{det}\Phi \tag{3.14}$$

since $\mathrm{det}M$ and $\mathrm{det}\Phi$ are non-zero (eqs.(2.8)) and $W_{\theta\theta}$ is non-vanishing away from the chiral limit. An elegant proof of eq.(3.14), based on the zero-momentum Ward identities for $W_{\mathcal{ST}}$ is as follows. Define

$$\hat{M} = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & M \end{pmatrix} \qquad\qquad W = \begin{pmatrix} W_{\theta\theta} & W_{\theta S_5^b} \\ W_{S_5^a\theta} & W_{S_5^a S_5^b} \end{pmatrix} \tag{3.15}$$

with $\Delta = \mathrm{det}W$. Then,

$$\begin{aligned} \mathrm{det}M\ \ \Delta &= \mathrm{det}\hat{M}\ \mathrm{det}W \\ &= \begin{vmatrix} W_{\theta\theta} & W_{\theta S_5^b} \\ M_{ac}W_{S_5^c\theta} & M_{ac}W_{S_5^c S_5^b} \end{vmatrix} \end{aligned} \tag{3.16}$$

Using the zero-momentum Ward identities (2.11) and, in the case of the $a = 0$ row taking a linear combination with the first (θ) row, the determinant simplifies, leaving

$$\begin{aligned} \mathrm{det}M\ \ \Delta &= \begin{vmatrix} W_{\theta\theta} & W_{\theta S_5^b} \\ 0 & -\Phi_{ab} \end{vmatrix} \\ &= W_{\theta\theta}\ \mathrm{det}\Phi \end{aligned} \tag{3.17}$$

as required.

This completes the proof of the GT relations. To summarise, we have shown that the flavour singlet and non-singlet axial charges are given by the single, unified relation

$$2m_N G_A^a \ \ = \ \ F_{ab}\ \hat{\Gamma}_{\eta^b NN}\big|_{k=0} \tag{3.18}$$

where $F \equiv \Phi B^T$ is determined from

$$FF^T = \frac{d}{dk^2} W_{S_D S_D}\big|_{k=0} \tag{3.19}$$

that is,

$$F_{ac}F^T_{cb} = \lim_{k=0} \frac{d}{dk^2}\ i \int dx\ e^{ikx}\ \langle 0|T\ \partial^\mu J^a_{\mu 5}(x)\ \partial^\nu J^b_{\nu 5}(0)|0\rangle \tag{3.20}$$

In current algebra terms, the matrix F determined from eq.(3.20) can be identified, subject to the standard PCAC (pole dominance) approximation described in Appendix B, with the pseudo-Goldstone boson decay constants. Under the same PCAC assumptions, the vertices can be identified with the low-energy meson-nucleon coupling constants, i.e. $\hat{\Gamma}_{\eta^3 NN}|_{k=0} = g_{\pi NN}$, etc. It should be emphasised, however, that the relations (3.18) and (3.20) are *exact* – they are neither dependent on this interpretation nor make any PCAC assumption or approximation.

Eq.(3.18) is therefore the natural generalisation of the $U(1)$ GT relation proved in refs.[10,11]. There we showed that, in the chiral limit, the singlet axial charge is given by

$$2m_N G_A^0 = 2n_f \sqrt{\chi'(0)}\, \hat{\Gamma}_{\eta^0 NN}\big|_{k=0} \tag{3.21}$$

where $\chi'(0)$ is the first moment of the topological susceptibility, viz.

$$\chi'(0) = \lim_{k=0} \frac{d}{dk^2}\, i \int dx\, e^{ikx} \langle 0|T\ Q(x)\ Q(0)|0\rangle \tag{3.22}$$

The new formula extends this to include mixing with the flavour non-singlet sector, introducing a matrix structure which replaces the simple square root in eq.(3.21) and generalising the fields in the correlation function to the entire divergence of the current including mass terms as well as the anomaly Q.

3.1 Flavour mixing

The remaining theoretical question related to the unified GT relation (3.18) concerns $SU(3)$ flavour mixing and the extent to which eq.(3.20) determines F.

In the context of PCAC or chiral perturbation theory (incorporating the $1/N_c$ expansion to allow the inclusion of the flavour singlet η' (see ref.[23] and references therein)), the problem of $\eta - \eta'$ mixing is currently receiving renewed attention[23,24]. According to Kaiser and Leutwyler[23], the decay constant matrix in the $a = 0, 8,\ \ \eta - \eta'$ sector is required to contain 4 parameters, viz.

$$\begin{pmatrix} f_{0\eta'} & f_{0\eta} \\ f_{8\eta'} & f_{8\eta} \end{pmatrix} = \begin{pmatrix} f_0 \cos\vartheta_0 & -f_0 \sin\vartheta_0 \\ f_8 \sin\vartheta_8 & f_8 \cos\vartheta_8 \end{pmatrix} \tag{3.23}$$

with $\vartheta_0 \neq \vartheta_8$, in contrast to the previous conventional analysis which assumed $\vartheta_0 = \vartheta_8$. Low-energy theorems[23] yield f_0, f_8 and $\sin(\vartheta_0 - \vartheta_8)$ easily, from the diagonal and off-diagonal combinations $\sum_{P=\eta',\eta} f_{0P} f_{0P}$, $\sum_P f_{8P} f_{8P}$ and $\sum_P f_{0P} f_{8P}$ respectively, but the remaining combination of the mixing angles is harder to identify.

Returning to our result (3.18), (3.20), we find a similar situation. Clearly the relation (3.20) can only determine 3 parameters in F_{ab} (in the a,b = 0,8 sector). However, in general our analysis requires F_{ab} to be characterised by 4 parameters, including a mixing angle undetermined by eq.(3.20).

To see this in more detail, consider the defining equation (3.9) for B, re-expressed in terms of F itself:

$$\Phi_{ac} \frac{d}{dk^2} \Gamma_{\phi_5^c \phi_5^d}\big|_{k=0} \Phi_{db} = F_{ac}\ \frac{d}{dk^2} \Gamma_{\eta^c \eta^d}\big|_{k=0}\ F_{db}^T = F_{ac} F_{cb}^T \tag{3.24}$$

Since the l.h.s. is symmetric, it can be diagonalised by an orthogonal matrix R, i.e.

$$\Phi_{ac}\frac{d}{dk^2}\Gamma_{\phi_5^c\phi_5^d}\big|_{k=0}\Phi_{db} = R^T D^2 R \tag{3.25}$$

where D is diagonal. But since the r.h.s. of eq.(3.24) is unchanged if F is right-multiplied by an independent orthogonal matrix O^T, we find the general solution

$$F = R^T D O \tag{3.26}$$

A convenient parametrisation for F is therefore

$$F = f\begin{pmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix}\sqrt{6}s & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}\cos\phi & \sin\phi\\ -\sin\phi & \cos\phi\end{pmatrix} \tag{3.27}$$

The four parameters are interpreted as an overall scale f which in the PCAC approximation and the limit of exact $SU(3)$ becomes the pion decay constant, an OZI breaking ($s \neq 1$) parameter, an angle θ characterising $SU(3)$ breaking, and finally a mixing angle ϕ for the η^a fields.

We can now check whether any special cases of this general parametrisation are consistent with the RGE (C.10) for F_{ab}. Clearly there is an exact $SU(3)$ limit in which both θ and ϕ are zero, with the RGE being satisfied by $\mathcal{D}s = \gamma s$, $\mathcal{D}f = 0$. The case $\theta = 0$, $\phi \neq 0$ is also RG consistent, with the same solution. (This corresponds to the case $\vartheta_0 = \vartheta_8$ in the parametrisation (3.23).) However, the RGE cannot be satisfied with $\theta \neq 0$ but $\phi = 0$. In the general $SU(3)$ breaking case, therefore, F_{ab} must depend on a mixing angle ϕ which cannot be determined from the condition (3.20).

The consequence of this is that in order to use the full unified GT relation (3.18) to make predictions that include the effect of $SU(3)$ flavour mixing, we would need a further (linear) condition on F beyond eq.(3.20).

Without such an extra condition, we have to neglect flavour mixing. This will produce an uncertainty in our final predictions which we can estimate by defining an $SU(3)$ breaking parameter from the condensates (2.7), viz. $t = \sqrt{6}\langle\phi^8\rangle/\langle\phi^0\rangle$. (The $\sqrt{6}$ factors here and in the definition of s arise because of the different normalisation of the singlet generator: $\mathrm{tr}T^0T^0 = n_f$ whereas $\mathrm{tr}T^iT^j = \frac{1}{2}\delta^{ij}$ for $i,j = 1,\ldots 8$.) Using standard values (6.16) for the condensates, $t \simeq 0.16$. We therefore expect the $SU(3)$ breaking angle $\sin\theta$ to be of $O(t)$ and so omitting flavour mixing effects will produce an uncertainty of $O(10-20\%)$ in our final results.

However, when we evaluate the correlation functions (3.20) using QCD spectral sum rules (section 6), it is in any case difficult to do better, since to incorporate flavour mixing we would have to saturate the spectral functions (below t_c) with the two states η' and η, for both the flavour diagonal and off-diagonal correlators. This would greatly complicate the analysis without significantly improving the accuracy of the final results, so we do not attempt it here. Consequently, our final predictions, presented in section 7, are subject to the approximation of neglecting $SU(3)$ flavour mixing.

4. GT Relations and the Sum Rule for the First Moment of g_1^p

As already quoted in the introduction, the first moment of the polarised proton structure function g_1^p satisfies the following sum rule:

$$
\begin{aligned}
\Gamma_1^p(Q^2) &\equiv \int_0^1 dx\ g_1^p(x;Q^2) \\
&= \frac{1}{12} C_1^{\rm NS}\big(\alpha_s(Q^2)\big)\ \Big(a^3 + \frac{1}{3}a^8\Big) + \frac{1}{9} C_1^{\rm S}\big(\alpha_s(Q^2)\big)\ a^0(Q^2)
\end{aligned}
\tag{4.1}
$$

where the a^a are the axial charges occurring in the GT relations we have just derived:

$$
G_A^3 = \frac{1}{2}a^3 \qquad\qquad G_A^8 = \frac{1}{2\sqrt{3}}a^8 \qquad\qquad G_A^0(Q^2) = a^0(Q^2) \tag{4.2}
$$

The RG scale (Q^2) dependence of $a^0(Q^2)$, due to the anomalous dimension of the singlet axial current, is explicitly displayed.

This sum rule has been analysed using the composite operator propagator-vertex approach to DIS in ref.[12]. Working in the chiral limit, it was shown that

$$
\Gamma^p_{1\,singlet} = \frac{1}{9}\frac{1}{2m_N} 2n_f\ C_1^S\big(\alpha_s(Q^2)\big)\ \sqrt{\chi'(0)}\big|_{Q^2}\ \hat{\Gamma}_{\eta^0 NN} \tag{4.3}
$$

Following refs.[10-12], we now assume that the vertices are well approximated by their OZI values. This is the key assumption that allows us to make a quantitative prediction for Γ_1^p on the basis of a calculation of the topological susceptibility alone. The RG invariance of the vertices is a necessary condition for this assumption to be reasonable. Further phenomenological evidence from $U_A(1)$ current algebra supporting this conjecture is discussed in refs.[10-12].

We therefore assume that $\hat{\Gamma}_{\eta^0 NN}$ satisfies the OZI rule, i.e. $\hat{\Gamma}_{\eta^0 NN} = \sqrt{2}\ \hat{\Gamma}_{\eta^8 NN}$, so that all the OZI breaking in $\Gamma^p_{1\,singlet}$ resides in the topological susceptibility $\sqrt{\chi'(0)}$. Comparing with the standard OZI relation for a^8, we then find that[10,11]

$$
\frac{a^0(Q^2)}{a^8} = \frac{\sqrt{6}}{f_\pi}\ \sqrt{\chi'(0)}\big|_{Q^2} \tag{4.4}
$$

This leads to the following prediction[12] for the 'proton spin' sum rule:

$$
\begin{aligned}
a^0(Q^2 = 10{\rm GeV}^2) &= 0.35 \pm 0.05 \\
\Gamma_1^p(Q^2 = 10{\rm GeV}^2) &= 0.143 \pm 0.005
\end{aligned}
\tag{4.5}
$$

based on our original derivation of $\chi'(0)$ using QCD spectral sum rules[12]:

$$
\sqrt{\chi'(0)}\big|_{Q^2=10{\rm GeV}^2} = (23.2 \pm 2.4)\ {\rm MeV} \tag{4.6}
$$

This is to be compared with the OZI prediction $a^0\big|_{OZI} = a^8 = 0.58 \pm 0.03$ and with the current experimental data from the SMC collaboration[25]:

$$\Gamma_1^p(Q^2 = 10\mathrm{GeV}^2)\big|_{(x>0.003)} \equiv \int_{0.003}^1 dx\ g_1^p(x;Q^2) = 0.141 \pm 0.012 \qquad (4.7a)$$

The result for the entire first moment depends on how the extrapolation to the unmeasured small x region $x < 0.003$ is performed. Using a simple Regge fit, SMC find $\Gamma_1^p = 0.142 \pm 0.017$ from which they deduce $a^0 = 0.34 \pm 0.17$, while using a small x fit using perturbative QCD evolution of the parton distributions[4,26] they find $\Gamma_1^p = 0.130 \pm 0.017$ and $a^0 = 0.22 \pm 0.17$ (all at $Q^2 = 10\mathrm{GeV}^2$).

More recently, SMC have published a further analysis[27] of their data, this time quoting a slightly lower number for the integral over the measured region of x:

$$\Gamma_1^p(Q^2 = 10\mathrm{GeV}^2)\big|_{(x>0.003)} \equiv \int_{0.003}^1 dx\ g_1^p(x;Q^2) = 0.133 \pm 0.009 \qquad (4.7b)$$

Whatever the ultimate resolution of the small x extrapolation, it is encouraging that our prediction (4.5) is in the region now favoured by the data. We would therefore like to test the precision of our result further. An assumption in making this prediction was that the value of a^0 is smooth in the quark masses, so that the chiral limit will be a good approximation, correct up to the usual order of soft $SU(3)$ breaking in ratios of decay constants. The extended version of the GT relations derived in section 3 allow us to test this.

Using the new form (3.18) of the GT relations, we can immediately rewrite the first moment sum rule for g_1^p in the following compact form:

$$\begin{aligned}\Gamma_1^p(Q^2) \equiv \int_0^1 dx\ g_1^p(x,Q^2) &= \frac{1}{9}\frac{1}{2m_N}\ C_1^a\big(\alpha_s(Q^2)\big)\ G_A^a \\ &= \frac{1}{9}\frac{1}{2m_N}\ C_1^a\big(\alpha_s(Q^2)\big)\ F_{ab}\ \hat{\Gamma}_{\eta^b NN} \qquad (4.8)\end{aligned}$$

where we have defined the numerically rescaled Wilson coefficients $C_1^0 = C_1^S$ and $C_1^3 = \sqrt{3}C_1^8 = \frac{3}{2}C_1^{NS}$. All the vertices $\Gamma_{\eta^a NN}$ are RG scale invariant. Apart from the running coupling in the Wilson coefficients, the only Q^2 scale dependence is contained in the singlet components of F_{ab}, according to the RG equation (C.10).

Following the approach of refs.[10-12], we again assume that these RG-invariant vertices are all well approximated by their OZI values. Isospin invariance ensures that the off-diagonal terms in the 2-current correlation functions involving the triplet index 3 vanish, so we need consider only:

$$FF^T = \lim_{k=0}\ \frac{d}{dk^2}\ i \begin{pmatrix} \langle 0|\partial^\mu J^0_{\mu 5}\ \partial^\nu J^0_{\nu 5}|0\rangle & 0 & \langle 0|\partial^\mu J^0_{\mu 5}\ \partial^\nu J^8_{\nu 5}|0\rangle \\ 0 & \langle 0|\partial^\mu J^3_{\mu 5}\ \partial^\nu J^3_{\nu 5}|0\rangle & 0 \\ \langle 0|\partial^\mu J^8_{\mu 5}\ \partial^\nu J^0_{\nu 5}|0\rangle & 0 & \langle 0|\partial^\mu J^8_{\mu 5}\ \partial^\nu J^8_{\nu 5}|0\rangle \end{pmatrix} \qquad (4.9)$$

In section 6, we evaluate these correlators (in the $0,8$ sector) using spectral sum rules. As explained in the last section, we restrict ourselves to single-particle saturation of the appropriate spectral functions, keeping only the η' contribution in the flavour singlet correlator and η in the octet. We do not evaluate the off-diagonal correlator, which is expected to be small due to the approximate cancellation between the decay constants for the η' and η states in the spectral function.

In this approximation of consistently neglecting the $SU(3)$ flavour mixing, and using the OZI relation $\hat{\Gamma}_{\eta^0 NN} = \sqrt{2}\,\hat{\Gamma}_{\eta^8 NN}$, we then identify the 'proton spin' suppression from eq.(4.8) as:

$$\frac{a^0(Q^2)}{a^8} \;\simeq\; \frac{1}{\sqrt{6}}\,\frac{F_{00}}{F_{88}} \tag{4.10}$$

where

$$F_{00} \;\simeq\; \sqrt{\lim_{k=0}\,\frac{d}{dk^2}\; i\langle 0|\partial^\mu J^0_{\mu 5}\;\partial^\nu J^0_{\nu 5}|0\rangle} \tag{4.11}$$

and

$$F_{88} \;\simeq\; \sqrt{\lim_{k=0}\,\frac{d}{dk^2}\; i\langle 0|\partial^\mu J^8_{\mu 5}\;\partial^\nu J^8_{\nu 5}|0\rangle} \tag{4.12}$$

5. Quark Mass Dependence

Before presenting the spectral sum rule analysis in section 6, we give here some analytic arguments based on the Ward identities which suggest that the first moment of the correlation functions (4.9) will have only a weak dependence on the quark masses. The basic reason for this is the identification, up to the standard PCAC pole-dominance assumptions, of F with a decay constant. The explicit dependence on the pseudo-Goldstone boson masses which is present in $W_{S^a_D S^b_D}$ drops out in the first moment.

To see this another way, consider the Ward identity (2.9). Taking the first moment, we see that the explicit dependence on the quark masses m vanishes, leaving

$$FF^T \;=\; \frac{d}{dk^2}W_{S^a_D S^b_D}\big|_{k=0} \;=\; \frac{d}{dk^2}\Big(k^\mu k^\nu W_{V^a_{\mu 5}V^b_{\nu 5}}\Big)\Big|_{k=0} \tag{5.1}$$

The 2-current correlation function can be parametrised as

$$\begin{aligned} W_{V^a_{\mu 5}V^b_{\nu 5}} \;&=\; i\int dx\; e^{ik.x}\;\langle 0|T\;J^a_{\mu 5}(x)\;J^b_{\nu 5}(0)|0\rangle \\ &=\; \Pi^{ab}_T(k^2)\Big(g_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}\Big) \;+\; \Pi^{ab}_L(k^2)\frac{k_\mu k_\nu}{k^2} \end{aligned} \tag{5.2}$$

where $\Pi^{ab}_T(k^2)$, $\Pi^{ab}_L(k^2)$ are dynamical functions which are not determined by the chiral Ward identities. (They are of course related by eqs.(2.5) to other correlation functions.) While $\Pi^{ab}_L(k^2)$ will have poles corresponding to the pseudo-Goldstone bosons coupling to the currents, $\Pi_T^{ab}(k^2)$ is a pole-free function (at least for momenta below the masses of the pseudovector resonances). $\Pi_T^{ab}(0)$ is therefore not expected to have a substantial dependence on the pseudoscalar masses. The absence of a massless pseudoscalar pole in (5.2) requires $\Pi_L^{ab}(0) = \Pi_T^{ab}(0)$, so clearly

$$\frac{d}{dk^2} W_{S_D^a S_D^b}\big|_{k=0} \;=\; \Pi_L^{ab}(0) \;=\; \Pi_T^{ab}(0) \tag{5.3}$$

Although we do not expect a strong mass dependence of the correlation functions (5.1), the individual correlators in the decomposition

$$\begin{aligned}\frac{d}{dk^2} W_{S_D^a S_D^b}\big|_{k=0} \;=\;& 4n_f^2 \delta_{a0}\delta_{b0} \frac{d}{dk^2} W_{\theta\theta}\Big|_{k=0} \;+\; 2n_f \delta_{a0} M_{bd} \frac{d}{dk^2} W_{\theta S_5^d}\Big|_{k=0} \\ &+ 2n_f \delta_{b0} M_{ac} \frac{d}{dk^2} W_{S_5^c \theta}\Big|_{k=0} \;+\; M_{ac} M_{bd} \frac{d}{dk^2} W_{S_5^c S_5^d}\Big|_{k=0}\end{aligned} \tag{5.4}$$

certainly do have an explicit dependence on m. This of course cancels in the sum, although the pattern of cancellations is very intricate.

To illustrate all this, it is instructive to write a simple effective action $\Gamma[Q, \phi_5^a]$ which encodes the information in the zero-momentum chiral Ward identities, and use this to derive explicit expressions for the correlation functions in eq.(5.4).

The zero-momentum Ward identities are

$$\Phi_{ac} \Gamma_{Q\phi_5^c}\Big|_{k=0} = 2n_f \delta_{a0} \qquad\qquad \Phi_{ac} \Gamma_{\phi_5^c \phi_5^b}\Big|_{k=0} = M_{ab} \tag{5.5}$$

The simplest effective action compatible with these identities is

$$\Gamma[Q, \phi_5^a] \;=\; \int dx \;\left[\frac{1}{2a} Q^2 \;+\; 2n_f Q \Phi_{0a}^{-1} \phi_5^a \;+\; \frac{1}{2} \phi_5 \Phi^{-1} f \big(-\partial^2 - \mu^2\big) f \Phi^{-1} \phi_5\right] \tag{5.6}$$

The final term is written in matrix notation. f_{ab} and μ_{ab}^2 are matrices, a and f_{ab} are constant, and μ_{ab}^2 is *defined* by

$$f_{ac}\; \mu_{cd}^2 \; f_{db} \;=\; -M_{ac} \Phi_{cb} \tag{5.7}$$

μ^2 is the pseudo-Goldstone boson mass matrix in the OZI limit of QCD, i.e. neglecting the coupling to the anomaly Q.

It is important to realise that the effective action (5.6) is only an approximation, where the simplest choice of kinetic terms for the fields ϕ_5^a has been made. This corresponds to the pole dominance approximation in standard PCAC (see Appendix B). In this approximation, as we now show, there is strictly no m dependence in (5.1).

The second derivatives of the effective action are

$$\begin{pmatrix} \Gamma_{QQ} & \Gamma_{Q\phi_5^b} \\ \Gamma_{\phi_5^a Q} & \Gamma_{\phi_5^a \phi_5^b} \end{pmatrix} \;=\; \begin{pmatrix} a^{-1} & 2n_f \Phi_{0b}^{-1} \\ 2n_f \Phi_{a0}^{-1} & \Phi^{-1} f \big(k^2 - \mu^2\big) f \Phi^{-1} \end{pmatrix} \tag{5.8}$$

The correlation functions are found by inverting this matrix. We find

$$\begin{aligned}
W_{\theta\theta} &= -a\,\tilde{\Delta}^{-1} \\
W_{\theta S_5^b} &= 2n_f a\,\Delta_{0d}^{-1}\,\Phi_{db} \\
W_{S_5^a\theta} &= 2n_f a\,\Phi_{ac}\,\Big(f\big(k^2-\mu^2\big)f\Big)_{c0}^{-1}\tilde{\Delta}^{-1} \\
W_{S_5^a S_5^b} &= -\Phi_{ac}\,\Delta_{cd}^{-1}\,\Phi_{db}
\end{aligned} \tag{5.9}$$

where

$$\tilde{\Delta} = 1 - 4n_f^2 a\Big(f\big(k^2-\mu^2\big)f\Big)_{00}^{-1} \tag{5.10}$$

and

$$\Delta = f\big(k^2-\mu^2\big)f - 4n_f^2 a\,\hat{I} \tag{5.11}$$

with $\hat{I} = \delta_{a0}\delta_{b0}$. Notice the highly non-trivial μ^2 dependence in all these correlators.(3)

A simple calculation now confirms that (recalling $D^a = 2n_f\delta_{a0}Q + M_{ac}\phi_5^c$) the zero-momentum Ward identity

$$W_{S_D^a S_D^b}\Big|_{k=0} = -M_{ac}\Phi_{cb} \tag{5.12}$$

is satisfied. A slightly trickier calculation also shows that the M and μ^2 terms cancel completely in the first moment and we find

$$\frac{d}{dk^2}W_{S_D^a S_D^b}\Big|_{k=0} = f_{ac}f_{cb} \tag{5.13}$$

In fact, this is required by the key identity (3.9), which shows

$$\frac{d}{dk^2}W_{S_D^a S_D^b}\Big|_{k=0} = \Phi_{ac}\frac{d}{dk^2}\Gamma_{\phi_5^c\phi_5^d}\Big|_{k=0}\Phi_{db} \tag{5.14}$$

The first moment of the correlation function $W_{S_D^a S_D^b}$ is therefore given by the decay constants in the simple effective action (5.6).

Notice however that f_{ab} is only constrained to be a constant by the pole-dominance approximation, *not* by the chiral Ward identities. In general, the f_{ab} appearing in eq.(5.8) could be functions of momentum, i.e. $f_{ab}(k^2)$. In that case, (5.13) is replaced by

$$\begin{aligned}
\frac{d}{dk^2}W_{S_D^a S_D^b}\Big|_{k=0} &= \frac{d}{dk^2}\Big(f\big(k^2-\mu^2\big)f\Big)\Big|_{k=0} \\
&= f^2(0) - f(0)\mu^2 f'(0) - f'(0)\mu^2 f(0)
\end{aligned} \tag{5.15}$$

We see therefore that $\frac{d}{dk^2}W_{S_D^a S_D^b}\Big|_{k=0}$ *can* have a dependence on the quark masses, but only proportional to the derivative $f'(0)$. If, as is consistent with the success of PCAC,

(3) The expressions (5.9) are (in a different notation) identical to those derived in ref.[28] from an effective action or diagrammatic resummation including effects beyond leading order in the $1/N_c$ expansion.

the pole-free dynamical function $f(k^2)$ is slowly-varying in the small-momentum region, then this dependence is relatively weak.

The conclusion of all this is that $FF^T = \frac{d}{dk^2} W_{S_D^a S_D^b}\Big|_{k=0}$ has only a weak residual quark mass dependence proportional to the derivative of a slowly varying dynamical function. The strong, explicit dependence on the quark masses cancels amongst the four individual correlation functions in eq.(5.4).

The same pattern of cancellations is observed if we now write spectral sum rules for $\frac{d}{dk^2} W_{S_D^a S_D^b}\Big|_{k=0}$ using simply the pole-dominance approximation for the propagators given in eq.(5.9). At first sight, we might therefore expect this pattern to be reproduced in the full QCD spectral sum rules described in the next section. In fact that is not so. Of course the sum rules go beyond the pole-dominance approximation, but in addition, for Green functions such as those needed here, which satisfy dispersion relations requiring subtractions, even the sign of the corrections to pole-dominance is not simply determined on general grounds. Nevertheless, as we shall see, the full spectral sum rules do confirm the picture outlined here by showing numerically the relative insensitivity of $\frac{d}{dk^2} W_{S_D^a S_D^b}$ to the strange quark mass.

6. QCD Spectral Sum Rules and Current Correlation Functions

First, we derive the QCD spectral sum rules (for a review, see e.g. ref.[29]) for the flavour-singlet current correlation function

$$\psi_5(k^2) \quad = \quad \Big(\frac{1}{2n_f}\Big)^2 i \int d^4x \; e^{ikx} \langle 0|T \; \partial^\mu J^0_{\mu 5}(x) \; \partial^\nu J^0_{\nu 5}(0) \; |0\rangle \tag{6.1}$$

Recall the anomalous current conservation equation (c.f. eq.(2.2)) is

$$\partial^\mu J^0_{\mu 5} = D^0 = \sum_{q=u,d,s} 2m_q \bar{q}\gamma_5 q + 2n_f Q \tag{6.2}$$

From its analyticity properties and asymptotic behaviour, the correlator obeys the subtracted dispersion relations

$$\frac{1}{k^2}\Big[\psi_5(k^2) - \psi_5(0)\Big] \quad = \quad \int_0^\infty \frac{dt}{t}\frac{1}{(t-k^2-i\epsilon)}\;\frac{1}{\pi}\mathrm{Im}\psi_5(t) \tag{6.3}$$

and

$$\frac{1}{k^4}\Big[\psi_5(k^2) - \psi_5(0) - k^2\psi_5'(0)\Big] \quad = \quad \int_0^\infty \frac{dt}{t^2}\frac{1}{(t-k^2-i\epsilon)}\;\frac{1}{\pi}\mathrm{Im}\psi_5(t) \tag{6.4}$$

From the leading large $K^2 \equiv -k^2 > 0$ behaviour of the correlator, which is $K^4\log(K^2/\mu^2)$, one can deduce that the corresponding derivatives

$$\mathcal{F} = \frac{d^2}{(dK^2)^2}\Big(\frac{\psi_5}{K^2}\Big) \qquad\qquad \mathcal{G} = -\frac{d}{dK^2}\Big(\frac{\psi_5}{K^4}\Big) \tag{6.5}$$

are superconvergent and thus obey the homogeneous RGE:

$$\Big[-\frac{\partial}{\partial t} + \beta\alpha_s\frac{\partial}{\partial\alpha_s} - \sum_i (1+\gamma_m)x_i\frac{\partial}{\partial x_i} - 2\gamma\Big](\mathcal{F};\mathcal{G})(t,\alpha_s,x_i) = 0 \tag{6.6}$$

Here, $x_i \equiv m_i/\mu$ is the ratio of the renormalised quark mass with the $\overline{MS}$-scheme subtraction scale μ, and $t \equiv L/2$ where

$$L \equiv \log(K^2/\mu^2) \tag{6.7}$$

β, γ and γ_m are respectively the QCD β-function, the anomalous dimension for $J^0_{\mu 5}$ and the mass anomalous dimension. The anomalous dimension γ is $O(\alpha_s^2)$, viz.

$$\gamma(\alpha_s) = -\Big(\frac{\alpha_s}{\pi}\Big)^2 \tag{6.8}$$

and does not contribute at the order we consider here. The coefficients of β and γ_m are

$$\beta(\alpha_s) = \sum_{i=1}\beta_i\Big(\frac{\alpha_s}{\pi}\Big)^i \qquad\qquad \gamma_m(\alpha_s) = \sum_{i=1}\gamma_i\Big(\frac{\alpha_s}{\pi}\Big)^i \tag{6.9}$$

where, for three flavours[29],

$$\begin{aligned} &\beta_1 = -9/2 \qquad \beta_2 = -8 \\ &\gamma_1 = 2 \qquad\quad\; \gamma_2 = 91/12 \end{aligned} \tag{6.10}$$

The expression for the running coupling to two-loop accuracy can be parametrised as[29]:

$$a_s(\mu) \equiv \frac{\bar{\alpha}_s(\mu)}{\pi} = a_s^{(0)} \Big[1 - a_s^{(0)} \frac{\beta_2}{\beta_1} \log\log \frac{\mu^2}{\Lambda^2} + O(a_s^2)\Big] \tag{6.11}$$

where

$$a_s^{(0)} \equiv \frac{1}{-\beta_1 \log(\mu/\Lambda)} \tag{6.12}$$

and β_i are the coefficients of the β function given above. We shall use, for three flavours,

$$\Lambda = (375 \pm 75) \text{ MeV} \tag{6.13}$$

from τ decay [30] and LEP[31] data.

The expression for the running quark mass in terms of the invariant mass $\hat{m}_i$ to two-loop accuracy is [(4)][32,29]:

$$\bar{m}_i(\mu) \;=\; \hat{m}_i \; \big(-\beta_1 a_s(\mu)\big)^{-\gamma_1/\beta_1} \Big[1 + \frac{\beta_2}{\beta_1} \Big(\frac{\gamma_1}{\beta_1} - \frac{\gamma_2}{\beta_2}\Big) a_s(\mu) + O(a_s^2)\Big] \tag{6.14}$$

where γ_i are the coefficients of the quark-mass anomalous dimension given above. In this analysis, we shall retain only the strange quark mass and neglect m_u and m_d. We use

$$\bar{m}_s(1 \text{ GeV}) \simeq (197 \pm 29) \text{ MeV} \tag{6.15}$$

from the $e^+e^- \to$ hadrons[33] and τ decay[34] data, and the correlated values of the invariant mass $\hat{m}_s$ and Λ. We shall also use[29]:

$$\langle \bar{s}s \rangle \simeq (0.6 \sim 0.8) \langle \bar{u}u \rangle \qquad \langle \bar{u}u \rangle = -(0.238 \text{ GeV})^3 \tag{6.16}$$

Now, applying the inverse Laplace operator[35]

$$\mathcal{L} \equiv \lim_{K^2, n \to \infty;\; n/K^2 \equiv \tau} (-1)^n \frac{(K^2)^n}{(n-1)!} \frac{\partial^n}{(\partial K^2)^n} \tag{6.17}$$

to the dispersion relations (6.3) and (6.4) gives the sum rules [(5)]

$$\tau^{-3} \mathcal{L}(\mathcal{F}) + \psi_5(0) = \int_0^\infty \frac{dt}{t}\; e^{-t\tau} \frac{1}{\pi} \text{Im}\psi_5(t) \tag{6.18}$$

$$\tau^{-2} \mathcal{L}(\mathcal{G}) - \psi_5(0)\tau + \psi_5'(0) = \int_0^\infty \frac{dt}{t^2}\; e^{-t\tau} \frac{1}{\pi} \text{Im}\psi_5(t) \tag{6.19}$$

---

(4) The truncation of the series at this order is necessary for self-consistency as the quark-quark correlator will be used to $O(\alpha_s)$.

(5) The unsubtracted sum rule, which is independent of $\psi_5(0)$ and $\psi_5'(0)$, is more sensitive to the higher meson states, and thus is more appropriate for studying gluonium parameters[36].

We use the usual duality ansatz for parametrising the spectral function:

$$\frac{1}{\pi}\mathrm{Im}\psi_5(t) \;\simeq\; 2m^4_{\eta'}f^2_{\eta'}\delta\big(t-m^2_{\eta'}\big) \;+\; \theta(t-t_c)\ \text{“QCD continuum”} \tag{6.20}$$

where $f_{\eta'}$ is the RG non-invariant η' ‘decay constant’ (see refs.[11,37]) normalised as

$$\langle 0\ |\partial^\mu J^{(0)}_{\mu 5}|\ \eta'\rangle = 2n_f\ \sqrt{2}\ f_{\eta'}m^2_{\eta'} \tag{6.21}$$

Then, after transferring the QCD continuum contribution to the lhs of eqs.(6.18) and (6.19), we obtain the sum rule:

$$\psi'_5(0) \;=\; \tau^{-2}\Big[-\mathcal{L}(\mathcal{G}_c)+\frac{1}{\tau m^2_{\eta'}}\mathcal{L}(\mathcal{F}_c)\Big]+\psi_5(0)\tau\Big[1+\frac{1}{\tau m^2_{\eta'}}\Big] \tag{6.22}$$

where the index c in $\mathcal{F}_c$ and $\mathcal{G}_c$ indicates that the QCD continuum effect has been transferred into the QCD expression of the correlators[(6)].

Analogously to $\mathcal{F}$ and $\mathcal{G}$, their Laplace transforms also obey an homogeneous RGE [38], where the resummation of the log-terms can be done by subtracting at $\tau = 1/\mu^2$ and introducing the running coupling and masses.

At this point, it is convenient to decompose the full correlation function (6.1) as follows

$$\psi_5(k^2) \;\equiv\; \psi_{gg}(k^2)+2\Big(\frac{m_s}{n_f}\Big)\psi_{qg}(k^2)+\Big(\frac{m_s}{n_f}\Big)^2\psi_{qq}(k^2) \tag{6.23}$$

where

$$\begin{aligned}
\psi_{gg}(k^2) \equiv \chi(k^2) \equiv i\int d^4x\ e^{ikx}\langle 0|T\ Q(x)\ Q(0)|0\rangle \\
\psi_{qg}(k^2) \equiv i\int d^4x\ e^{ikx}\langle 0|T\ Q(x)\ \bar{s}\gamma_5 s(0)\ |0\rangle \\
\psi_{qq}(k^2) \equiv i\int d^4x\ e^{ikx}\langle 0|T\ \bar{s}\gamma_5 s(x)\ \bar{s}\gamma_5 s(0)\ |0\rangle
\end{aligned} \tag{6.24}$$

Here, we have used the expression (6.2) for the divergence of the current and neglected the u and d quark masses.

For the next stage in developing the sum rules, we need the perturbative QCD expressions for these correlators. These have been calculated in the literature. First, the perturbative QCD expression for the gluon-gluon correlator $\psi_{gg}(k^2)$ has been reported in [12] and reads:

$$\psi_{gg}(k^2) = \psi^{PT}_{gg} + \psi^{NP}_{gg}, \tag{6.25}$$

where

$$\begin{aligned}
\psi^{PT}_{gg} &= -\Big(\frac{\alpha_s}{8\pi}\Big)^2\frac{2}{\pi^2}k^4L\Big[1+\Big(\frac{\alpha_s}{\pi}\Big)\Big(\frac{1}{2}\beta_1 L+\frac{83}{4}+...+6\big(3m^2_s+\frac{\pi}{\alpha_s}\lambda^2\big)\frac{1}{k^2}\Big)\Big] \\
\psi^{NP}_{gg} &= -\Big(\frac{\alpha_s}{16\pi^2}\Big)\Big[\Big(1+\frac{1}{2}\beta_1\Big(\frac{\alpha_s}{\pi}\Big)L\Big)\langle\alpha_s G^2\rangle+\frac{2}{K^2}\alpha_s\langle gG^3\rangle\Big]
\end{aligned} \tag{6.26}$$

(6) In the following, we shall omit this index for convenience of notation.

The new corrected coefficient of the perturbative $O(\alpha_s^3)$ term comes from the erratum in [39]. Notice that we have computed the m_s-dependent contribution of $O(\alpha_s^3)$ coming from the 2-loop Feynman diagram with a quark loop inserted on one gluon propagator. This is a new calculation that has not previously been published in the literature.(7)

We have also included the correction due to a tachyonic gluon mass λ, where[40]:

$$\lambda^2 \simeq -(0.43 \pm 0.09)\ \mathrm{GeV}^2 \tag{6.27}$$

in order to take into account the summation of the perturbative series (as a phenomenological alternative to renormalons). A full discussion of the motivation for including this term and its phenomenology is given in ref.[40].

The non-perturbative contributions come from [41] and [42]. Throughout the analysis, we shall use the values of the gluon condensates [43]:

$$\langle \alpha_s G^2 \rangle = (0.07 \pm 0.01)\ \mathrm{GeV}^4 \tag{6.28}$$

and [41]

$$\langle g^3 G^3 \rangle = (1.5 \pm 0.5)\ \mathrm{GeV}^2 \langle \alpha_s G^2 \rangle \tag{6.29}$$

A similar value of $\langle \alpha_s G^2 \rangle$ has been obtained recently from lattice calculations [44].

The QCD expression for the quark-gluon correlator $\psi_{qg}(k^2)$ has been evaluated in [45]. In the $\overline{MS}$-scheme, it reads:

$$\psi_{qg}(k^2) = \psi_{qg}^{PT} + \psi_{qg}^{NP}, \tag{6.30}$$

where

$$\begin{aligned}
\psi_{qg}^{PT} &= \left(\frac{\alpha_s}{\pi}\right)^2 m_s \frac{3}{16\pi^2} k^2 L \left[L - \frac{2}{3}\left(\frac{11}{4} - 3\gamma_E\right)\right] \\
\psi_{qg}^{NP} &= -\left(\frac{\alpha_s}{\pi}\right)^2 \langle \bar{s}s \rangle \frac{L}{2} + \left(\frac{\alpha_s}{\pi}\right) \frac{m_s}{8\pi} \langle \alpha_s G^2 \rangle \frac{L}{k^2} + \left(\frac{\alpha_s}{\pi}\right) \frac{1}{2k^2} \langle g\bar{s}\sigma^{\mu\nu} \frac{\lambda_a}{2} G^a_{\mu\nu} s \rangle
\end{aligned} \tag{6.31}$$

and $\gamma_E = 0.5772\ldots$ is the Euler constant.

Finally, the QCD quark-quark correlator $\psi_{qq}(k^2)$ is known to order $O(\alpha_s^3)$ for the perturbative term [46]. Including the condensates of dimension 6 [35,29], it can be expressed as:

$$\psi_{qq}(K^2 \equiv -k^2) = K^2 \sum_{d=0}^{3} \frac{\psi_{2d}(K^2)}{K^{2d}} \tag{6.32}$$

In the $\overline{MS}$-scheme, the perturbative expression of the renormalised two-point function can be written as:

$$\psi_0(K^2) = \frac{3}{8\pi^2} \sum_{i=0} \left(\frac{\alpha_s}{\pi}\right)^i \sum_{j=0}^{i+1} c_{ij} L^j \tag{6.33}$$

(7) We thank Alexei Pivoravov for checking this result.

where c_{ij} are constant terms from the evaluation of the QCD Feynman diagrams. To $O(\alpha_s^2)$, they read [47,45]:

$$
\begin{aligned}
c_{00} &= -2 \\
c_{10} &= -131/12 \\
c_{20} &= \frac{1}{6}\Big[-17645/24 + (353 - 8n_f)\zeta(3) + (511/18)n_f + (3/4)\zeta(4) - 50\zeta(5)\Big] \\
c_{01} &= 1 \\
c_{11} &= 17/3 \\
c_{12} &= -\frac{1}{2}\gamma_1 c_{01} \\
c_{21} &= 10801/144 - (39/2)\zeta(3) - n_f\Big[65/24 - (2/3)\zeta(3)\Big] \\
c_{22} &= -\frac{1}{4}\Big[c_{11}(-\beta_1 + 2\gamma_1) + 2\gamma_2 c_{01}\Big] \\
c_{23} &= \frac{1}{12}\gamma_1(-\beta_1 + 2\gamma_1)c_{01}
\end{aligned}
\tag{6.34}
$$

where $\zeta(n)$ are the Riemann zeta functions with

$$
\zeta(2) = \frac{\pi^2}{6} \qquad\qquad \zeta(3) = 1.202\ldots \tag{6.35}
$$

Given the approximations and accuracy to which we are working, we only keep the following chiral symmetry breaking and non-perturbative condensate contributions:

$$
\begin{aligned}
\psi_2 &= \frac{3}{8\pi^2}m_s^2\Big[2L + \frac{4}{3}\Big(\frac{\alpha_s}{\pi}\Big)\big(-3L^2 + 2L - 3 + 6\zeta(3)\big)\Big] \\
\psi_4 &= \frac{3}{8\pi^2}m_s^4\big(3 - 2L\big) - m_s\langle\bar{s}s\rangle + \frac{1}{8\pi}\langle\alpha_s G^2\rangle \\
\psi_6 &= -m_s\langle g\bar{s}\sigma^{\mu\nu}\frac{\lambda_a}{2}G^a_{\mu\nu}s\rangle + \frac{112}{27}\pi\rho\alpha_s\langle\bar{s}s\rangle^2
\end{aligned}
\tag{6.36}
$$

The mixed condensate can be parametrised as:

$$
\langle g\bar{s}\sigma^{\mu\nu}\frac{\lambda_a}{2}G^a_{\mu\nu}s\rangle = M_0^2\langle\bar{s}s\rangle \tag{6.37}
$$

where the value of $M_0^2 = (0.8\pm0.1)$ GeV^2 comes from the baryon [48,49] and B^*-B [50] sum rules and $\rho = 2 \sim 3$ [43,51] indicates the deviation from the vacuum saturation estimate of the four-quark operators.

To complete the sum rules, we need the Laplace tranforms of $\mathcal{F}$ and $\mathcal{G}$. These can be obtained from the renormalised QCD expressions above with the help of the generic formulae:

$$
\begin{aligned}
\mathcal{L}\left[\frac{1}{K^{2n}}\right] &= \frac{\tau^n}{\Gamma(n)} \\
\mathcal{L}\left[\frac{L}{K^{2n}}\right] &= \frac{\tau^n}{\Gamma(n)}\Big[L_\tau + \psi(n)\Big] \\
\mathcal{L}\left[\frac{L^2}{K^{2n}}\right] &= \frac{\tau^n}{\gamma(n)}\Big[L_\tau^2 + 2\psi(n)L_\tau + \psi^2(n) - \psi'(n)\Big] \\
\mathcal{L}\left[\frac{L^3}{K^{2n}}\right] &= \frac{\tau^n}{\Gamma(n)}\Big[L_\tau^3 + 3\psi(n)L_\tau^2 + 3\big(\psi^2(n) - \psi'(n)\big)L_\tau + \psi^3(n) - 3\psi(n)\psi'(n) + \psi^{''}(n)\Big]
\end{aligned}
\tag{6.38}
$$

where

$$
\begin{aligned}
L_\tau &\equiv -\log \tau\mu^2 \\
\psi(1) &= -\gamma_E \\
\psi'(1) &= \zeta(2) \\
\psi''(1) &= -2\zeta(3) \\
\psi(n) &= \sum_{j=1}^{n-1}\frac{1}{j} - \gamma_E \\
\psi^{(k)}(n) &= (-1)^k k!\left[\sum_{j=1}^{n-1}\frac{1}{j^{k+1}} - \zeta(k+1)\right] \qquad \text{for } k \geq 1
\end{aligned}
\tag{6.39}
$$

It is then convenient to write the Laplace transforms in the sum rule (6.22) in the notation

$$
\mathcal{L}(\mathcal{F};\mathcal{G}) = \mathcal{L}(\mathcal{F}_{gg};\mathcal{G}_{gg}) + 2\Big(\frac{\bar{m}_s}{n_f}\Big)\mathcal{L}(\mathcal{F}_{qg};\mathcal{G}_{qg}) + \Big(\frac{\bar{m}_s}{n_f}\Big)^2\mathcal{L}(\mathcal{F}_{qq};\mathcal{G}_{qq}) \tag{6.40}
$$

where the indices gg, qg and qq correspond respectively to the gluon-gluon, quark-gluon and quark-quark correlators in eq.(6.24).

6.1 The sum rule for $\chi'(0)$ in the chiral limit

In the chiral limit, $\psi_5'(0)$ reduces to the purely gluonic correlator $\chi'(0)$ evaluated for zero quark mass. This estimate has already been done in our earlier paper [NSV2]. In this case, the chiral Ward identities require $\psi_5(0) = 0$. The Laplace transforms of the gluonic correlator read [12]:

$$
\begin{aligned}
\mathcal{L}(\mathcal{F}_{gg}) = {}& \Big(\frac{\bar{\alpha}_s}{8\pi}\Big)^2\frac{2}{\pi^2}\tau\big(1 - e^{-t_c\tau}(1 + t_c\tau)\big)\left[1 + \Big(\frac{\bar{\alpha}_s}{4\pi}\Big)\Big[83 + 4\beta_1(1-\gamma_E) + 24(3m_s^2 + \frac{\pi}{\bar{\alpha}_s}\lambda^2)\tau\Big]\right] \\
& + \Big(\frac{\bar{\alpha}_s}{8\pi}\Big)\tau^3\left[\frac{1}{2\pi}\langle\alpha_s G^2\rangle + \Big(\frac{\bar{\alpha}_s}{\pi}\Big)\tau\langle gG^3\rangle\right]
\end{aligned}
\tag{6.41}
$$

and

$$\mathcal{L}(\mathcal{G}_{gg}) = \left(\frac{\bar{\alpha}_s}{8\pi}\right)^2 \frac{2}{\pi^2}\tau\left(1-e^{-t_c\tau}\right)\left[1+\left(\frac{\bar{\alpha}_s}{4\pi}\right)\left[83-4\beta_1\gamma_E-24\gamma_E(3m_s^2+\frac{\pi}{\bar{\alpha}_s}\lambda^2)\tau\right]\right]$$
$$-\tau^3\left(\frac{\bar{\alpha}_s}{8\pi}\right)\left[\frac{1}{2\pi}\langle\alpha_s G^2\rangle+\left(\frac{\bar{\alpha}_s}{2\pi}\right)\tau\langle gG^3\rangle\right] \qquad (6.42)$$

Substituting into the Laplace sum rule (6.22), we find the result shown in Fig. 1. This gives a plot of $\sqrt{\chi'(0)}$ versus τ for the optimal value of $t_c = 6$ GeV^2. We observe good stability in the range of τ from 0.2 to 0.5 GeV^{-2}. At the stability points, we find

$$\sqrt{\psi_5'(0)}\Big|_{m_s=0} \equiv \sqrt{\chi'(0)} = (26.4 \pm 4.1)\ \text{MeV} \qquad (6.43)$$

The central value is a little higher than the Laplace sum rule value of (22.3 ± 4.8) MeV obtained in ref.[12] due to the change[39] in the $O(\alpha_s^3)$ perturbative coefficient in eq.(6.26). The different sources of errors are summarised in Table 1.

Since the validity of the spectral sum rules for calculating $\chi'(0)$ has been criticised in the literature by Ioffe[16,17] (see refs.[16-20] and our detailed rebuttal in Appendix D), we should emphasise some features of this derivation.

First, one should notice that the optimization of the sum rule is obtained at the scale $\tau^{-1} = (2-5)$ GeV^2, which is relatively high compared to the scale of ordinary mesons of the order of $m_\rho^2 \simeq 0.6$ GeV^2. This result is in agreement with the expectation [41,40] that the scale of the $U(1)$ channel (gluonium) is relatively high compared with the flavour non-singlet (meson) scale. At the optimisation scale we therefore expect (and find) that higher dimension condensates (including 'instanton' effects[18,52]) are strongly suppressed. This is contrary to the claims in ref.[19], where τ^{-1} is taken at the too low value of 1 GeV^2.

Second, the apparently large perturbative radiative corrections in the expressions for the two-point correlators tend to cancel in the sum rule (6.22), explaining the almost equal value of $\chi'(0)$ obtained at leading order and the one including the perturbative α_s corrections. This is reassuring in view of the unknown higher order radiative corrections. In order to study the convergence of the perturbative series, we have estimated the α_s^2 corrections à la BNP [30] assuming that the coefficient of α_s grows geometrically, which, numerically, is about 430. This effect remains a small correction to the lowest order estimate.

We have also studied the effect of a $1/k^2$ correction due to the summation of the perturbative series, which we have parametrised here (see ref.[40]) through a phenomenological tachyonic gluon mass λ^2. We see that the presence of this term tends to shift the optimisation scale to smaller τ values, but affects only slightly the value of $\chi'(0)$.

The decay constant $f_{\eta'}$ defined in eq.(6.21) can be estimated in the same way using just the first (once-subtracted) sum rule in eq.(6.18). We find the result (see Fig. 2)

$$f_{\eta'} = (24.4 \pm 3.6)\ \text{MeV} \qquad (6.44)$$

where the different sources of error are again given in Table 1.

One can also derive a Finite Energy Sum Rule (FESR) for $\chi'(0)$. This can simply be found by taking the small τ limit of the Laplace transform sum rule. Including the radiative corrections, and neglecting the small λ^2 corrections, we obtain [12]

$$\chi'(0) \simeq \int_0^{t_c} \frac{dt}{t^2}\frac{1}{\pi}\mathrm{Im}\psi_5(t) - \left(\frac{\bar{\alpha}_s}{8\pi}\right)^2 \frac{2}{\pi^2} t_c\left[1+\left(\frac{\bar{\alpha}_s}{4\pi}\right)(83-4\beta_1)\right] \tag{6.45}$$

which confirms the consistency of the set of values of the parameters $\chi'(0)$, $f_{\eta'}$ and t_c obtained from the Laplace sum rules.

6.2 The sum rule for $\psi_5'(0)$ with massive quarks

In the case of massive quarks, $\psi_5(0)$ is non-zero. However, its value is known from the exact chiral Ward identities (2.9) or (2.11):

$$\psi_5(0) = -\frac{4}{(2n_f)^2} m_s\langle\bar{s}s\rangle \tag{6.46}$$

where we again set $m_u = m_d = 0$. As before, we then have two unknown physical quantities, viz. $\mathrm{Im}\psi_5(t)$ and $\psi_5'(0)$, to be determined from the two subtracted sum rules (6.18) and (6.19). (The unsubtracted sum rule[29], independent of $\psi_5(0)$, is more sensitive to the higher meson and gluonium mass than the subtracted sum rules, but is in any case not needed in this analysis.)

We now need the Laplace transforms of the quark-gluon and quark-quark correlators (see eqs.(6.31) and (6.32)). First, for the quark-gluon correlator, we have

$$\begin{aligned}\mathcal{L}(\mathcal{F}_{qg}) &= \tau^2\Bigg[\left(\frac{\bar{\alpha}_s}{\pi}\right)^2\frac{3m_s}{16\pi^2}\left(\frac{11}{6}\right)+\gamma_E\frac{\tau}{2}\left(\frac{\bar{\alpha}_s}{\pi}\right)^2\langle\bar{s}s\rangle \\ &\quad + \left(\frac{\bar{\alpha}_s}{\pi}\right)\frac{m_s}{8\pi}\langle\alpha_s G^2\rangle(1-\gamma_E)\tau^2\Bigg]\left(1-e^{-t_c\tau}\right)+\left(\frac{\bar{\alpha}_s}{\pi}\right)\frac{\tau^2}{2}M_0^2\langle\bar{s}s\rangle\end{aligned} \tag{6.47}$$

and

$$\begin{aligned}\mathcal{L}(\mathcal{G}_{qg}) &= \tau^2\Bigg[\left(\frac{\bar{\alpha}_s}{\pi}\right)^2\frac{3m_s}{16\pi^2}\left(\frac{11}{6}-\frac{17}{3}\gamma_E+3\gamma_E^2+\zeta(2)\right)+(1-\gamma_E)\frac{\tau}{2}\left(\frac{\bar{\alpha}_s}{\pi}\right)^2\langle\bar{s}s\rangle \\ &\quad + \left(\frac{\bar{\alpha}_s}{\pi}\right)\frac{m_s}{8\pi}\langle\alpha_s G^2\rangle\left(\gamma_E-\frac{3}{2}\right)\frac{\tau^2}{2}\Bigg]\left(1-e^{-t_c\tau}\right)-\left(\frac{\bar{\alpha}_s}{\pi}\right)\frac{\tau^2}{4}M_0^2\langle\bar{s}s\rangle\end{aligned} \tag{6.48}$$

The Laplace transform of the perturbative part of the quark-quark correlator including the $O(\alpha_s)$ corrections has a non-trivial analytic expression in terms of the Riemann ζ functions. It is more convenient to express it in a numerical form:

$$\begin{aligned}\mathcal{L}(\mathcal{F}_{qq}^{PT}) &= \frac{3}{8\pi^2}\tau^2\left[1+\left(\frac{17}{3}+2\gamma_E\right)\left(\frac{\bar{\alpha}_s}{\pi}\right)+O(\alpha_s^2)\right]\left(1-e^{-t_c\tau}\right) \\ \mathcal{L}(\mathcal{G}_{qq}^{PT}) &= -\frac{3}{8\pi^2}\tau^2\left[2+\gamma_E+13.298\left(\frac{\bar{\alpha}_s}{\pi}\right)+O(\alpha_s^2)\right]\left(1-e^{-t_c\tau}\right)\end{aligned} \tag{6.49}$$

The Laplace transforms of the m_s^2 and λ^2 corrections are

$$\mathcal{L}(\mathcal{F}_{qq}^{(2)}) = \frac{3}{8\pi^2}\tau^3\Big[\bar{m}_s^2\Big[2\gamma_E - 12.868\Big(\frac{\bar{\alpha}_s}{\pi}\Big)\Big] - 4\gamma_E\Big(\frac{\bar{\alpha}_s}{\pi}\Big)\lambda^2\Big]$$
$$\mathcal{L}(\mathcal{G}_{qq}^{(2)}) = \frac{3}{8\pi^2}\tau^3\Big[\bar{m}_s^2\Big[2(1-\gamma_E) + 12.152\Big(\frac{\bar{\alpha}_s}{\pi}\Big)\Big] + 4(\gamma_E - 1)\Big(\frac{\bar{\alpha}_s}{\pi}\Big)\lambda^2\Big] \qquad (6.50)$$

and the Laplace transforms of its non-perturbative part are

$$\begin{aligned}\mathcal{L}(\mathcal{F}_{qq}^{NP}) &= -\tau^4\Big[\frac{3}{8\pi^2}\bar{m}_s^4(1+2\gamma_E) + \Big(\frac{1}{8\pi}\langle\alpha_s G^2\rangle - m_s\langle\bar{s}s\rangle\Big) \\ &\quad + \frac{\tau}{2}\Big[-M_0^2 m_s\langle\bar{s}s\rangle + \frac{112}{27}\pi\rho\alpha_s\langle\bar{s}s\rangle^2\Big]\Big] \\ \mathcal{L}(\mathcal{G}_{qq}^{NP}) &= \tau^4\Big[\frac{3}{8\pi^2}\bar{m}_s^4\gamma_E + \frac{1}{2}\Big(\frac{1}{8\pi}\langle\alpha_s G^2\rangle - m_s\langle\bar{s}s\rangle\Big) \\ &\quad - \frac{\tau}{6}\Big[-M_0^2 m_s\langle\bar{s}s\rangle + \frac{112}{27}\pi\rho\alpha_s\langle\bar{s}s\rangle^2\Big]\Big] \end{aligned} \qquad (6.51)$$

Finally, collecting all these expressions in the combination (6.40), we deduce the Laplace sum rule for the complete correlation function $\psi_5'(0)$ with $m_s \neq 0$. Our result is shown in Fig. 1. We find

$$\sqrt{\psi_5'(0)} = (33.5 \pm 3.9)\ \text{MeV} \qquad (6.52)$$

for the range of stability in $\tau = (0.2 - 0.4)$ GeV^{-2}. The result obtained with $\lambda^2 = 0$ is very similar, though the stability in τ occurs at a slightly larger value of $\tau \sim 0.6$ GeV^{-2}.

Similarly, we find the value for the decay constant $f_{\eta'}$ for non-zero strange quark mass (see Fig. 2):

$$f_{\eta'} = (27.4 \pm 3.7)\ \text{MeV} \qquad (6.53)$$

Comparing these results with those obtained above in the chiral limit, we find that the effect of the $SU(3)$ breaking quark mass is to increase the values of $f_{\eta'}$ and $\sqrt{\psi_5'(0)}$ by approx. 10% and 20% respectively. This is a reasonable conclusion. The $SU(3)$ breaking effects are not negligible, but they are of the order expected in relatively smooth quantities such as decay constants which, as explained in section 5, are expected to be only weakly dependent on the quark masses.

Certainly we find no evidence of the huge $SU(3)$ breakings advertised in ref.[19], which were taken as an indication of the failure of the spectral sum rule method in the flavour singlet channel. The main reason for our different conclusion is that the τ stability region in our calculation is found to be much lower than that used in ref.[19], and so the $SU(3)$ breaking terms of $O(m_s^2\tau)$ are much smaller implying a much better convergence of the corresponding OPE. A more detailed comparision of our work with ref.[19] is given in appendix D.

6.3 Flavour non-singlet correlation functions

For the full unified Goldberger-Treiman relations, we also need the corresponding results for the octet current. These results are immediately obtained from the formulae presented above, with the obvious changes of m_η for $m_{\eta'}$ etc. In the derivation, we find it convenient to use the normalisations:

$$\langle 0|\partial^\mu J^8_{\mu 5}|\eta\rangle = \frac{2n_f}{\sqrt{3}}\ \sqrt{2}\ \tilde{f}_\eta m_\eta^2, \tag{6.54}$$

$$\psi_5^{88}(k^2) = \frac{3}{(2n_f)^2}\ i\int d^4x\ e^{ik.x}\ \langle 0|T\ D^8(x)\ D^8(0)|0\rangle \tag{6.55}$$

and:

$$\psi_5^{08}(k^2) = \frac{\sqrt{3}}{2n_f}\ i\int d^4x\ e^{ik.x}\ \langle 0|T\ D^0(x)\ D^8(0)|0\rangle \tag{6.56}$$

where D^a is normalised as in eq.(2.10). With these normalisation factors, the quark correlator ψ_{ss} occurs with the same coefficient in the sum rules for ψ_5, ψ_5^{88} and ψ_5^{08}. The octet decay constant is related to the conventionally normalised f_η by

$$f_\eta = 2\sqrt{6}\ \tilde{f}_\eta \tag{6.57}$$

so that $f_\eta = f_\pi = 93.3$ MeV for exact SU(3). We find:

$$\sqrt{\psi_5'^{88}(0)} = (43.8 \pm 5.0)\ \text{MeV} \tag{6.58}$$

and

$$\tilde{f}_\eta = (30.0 \pm 3.4)\ \text{MeV} \tag{6.59}$$

which corresponds to

$$f_\eta = (147 \pm 17)\ \text{MeV} \tag{6.60}$$

The sources of the errors are again tabulated in Table 1.

In order to quantify the systematic errors of the approach, we have re-estimated the value of f_π using the same inputs, approximations and methods (for different estimates of f_π from sum rules, see e.g. [29]) as used above for f_η, by using obvious changes of the parameters (quark masses, meson mass, continuum threshold). In this way, one obtains:

$$f_\pi = (107 \pm 12)\ \text{MeV} \tag{6.61}$$

Taking into account the slight deviation of the central value from the experimental number, we can consider as a final result:

$$f_\eta/f_\pi = 1.37 \pm 0.16 \tag{6.62}$$

where we expect that the error quoted here has been over-estimated. This ratio is in line with our expectations, since phenomenologically $f_K \simeq 1.2 f_\pi$, and we would expect $SU(3)$ breaking to be stronger for the η than the K [23,24].

As a by-product, we have checked that a systematic rescaling of the value of the decay constants f_η and $f_{\eta'}$ will affect similarly the value of the slope of both the non-singlet $\psi_5'^{88}(0)$ and singlet $\psi_5'(0)$ correlators, such that the ratios of correlators and decay constants which we use are not affected by this change.

Together with good t_c and τ stability, these results therefore confirm the general reliability of the spectral sum rules in this channel.

ΔO[MeV]	$t_c = 6 \pm 2$	Λ	$\bar{m}_s$	$\tau = 0.3 \pm 0.1$	$\langle \alpha_s G^2 \rangle$	Total
$f_{\eta'}\vert_{m_s=0}$	2.5	2.3	–	0.9	0.8	3.6
$\sqrt{\chi'(0)}$	3.3	2.2	–	0.1	0.8	4.1
$f_{\eta'}$	2.7	2	1.3	0.5	0.8	3.7
$\sqrt{\psi_5'(0)}$	2.1	1.9	2.6	–	0.8	3.9
$\tilde{f}_\eta$	0.9	1.3	2.9	–	0.8	3.4
$\sqrt{\psi_5'^{88}(0)}$	1.3	2	4.3	0.3	0.8	5.0
$f_{\eta'}/\tilde{f}_\eta$	0.030	0.025	0.045	–	–	0.060
$\frac{\sqrt{\psi_5'(0)}}{\sqrt{\psi_5'^{88}(0)}}$	0.022	0.008	0.015	–	–	0.028

Table 1: Error estimates in MeV for the different observables.
The sources of errors are in [GeV]^d where d is the corresponding dimension.

As already mentioned in sections 3 and 4, the calculation of the off-diagonal correlator $\psi_5'^{08}$ is much more delicate, since the contributions of both the η and η' to the spectral function must be taken into account. These tend to cancel because of the relative signs of the decay constants after flavour mixing, and the sum rule prediction for $\psi_5'^{08}$ should then be relatively small. This is confirmed by preliminary estimates. However, a complete calculation including the effects of flavour mixing for both the off-diagonal $\psi_5'^{08}$ and diagonal ψ_5' and $\psi_5'^{88}$ correlators requires significant further analysis and is beyond the scope of the present work.

We conclude that the QCD spectral sum rule method is indeed giving reliable results for the decay constants and susceptibilities in both the flavour singlet and non-singlet channels. Although the pattern of cancellations of quark mass effects observed in the effective lagrangian, or pole dominance, analysis in section 5 is not manifest in the more precise sum rule method, the essential observation that the slope at $k=0$ of the correlation functions $W_{S_D^a S_D^b}$ is relatively insensitive to the quark masses is confirmed by the numerical results found here.

7. Quantitative Analysis of the Unified GT Relation

In this section, we discuss the implications of these numerical results for the unified Goldberger-Treiman relations and the 'proton spin' suppression.

Collecting the results of the previous section and re-converting to the normalisations in sections 2-5, we have found

$$\left(FF^T\right)_{ab} \;=\; \lim_{k=0} \frac{d}{dk^2}\, W_{S_D^a S_D^b} \;=\; \begin{pmatrix} (201 \;\pm\; 23)^2 & \\ & (152 \;\pm\; 17)^2 \end{pmatrix} \mathrm{MeV}^2 \tag{7.1}$$

in the $a, b = 0, 8$ sector, within an approximation where we have kept only the η', or η, in the spectral functions for the correlators $\langle 0|T\; D^0\; D^0|0\rangle$, or $\langle 0|T\; D^8\; D^8|0\rangle$, respectively.

Within this approximation, neglecting $SU(3)$ flavour mixing in the unified GT formula, the generalisation beyond the chiral limit of the suppression formula for the singlet axial charge is (see eq.(4.10)):

$$\frac{a^0}{a^8} \;=\; \frac{1}{\sqrt{6}}\,\frac{F_{00}}{F_{88}} \;=\; \frac{1}{\sqrt{2}}\frac{\sqrt{\psi_5'(0)}}{\sqrt{\psi_5'^{88}(0)}} \;=\; 0.55 \;\pm\; 0.02 \tag{7.2}$$

This should be compared with the corresponding result in the chiral limit, using our new determination (6.43) of $\chi'(0)$ and using the sum rule estimate (6.61) for f_π:

$$\frac{a^0}{a^8} \;=\; \frac{\sqrt{6}}{f_\pi}\,\sqrt{\chi'(0)} \;=\; 0.60 \;\pm\; 0.12 \tag{7.3}$$

The relatively small error in eq.(7.2) is due to the cancellation of the systematic errors in the ratio (see Table 1), which was not taken into account in eq.(7.3). Running these results from the scale $\tau^{-1} \simeq 3$ GeV^2 to the SMC scale of $Q^2 = 10$ GeV^2, and substituting $a^8 = 3F - D = 0.58 \pm 0.03$, we find

$$\begin{aligned} a^0(Q^2 = 10\mathrm{GeV}^2) &= 0.31 \pm 0.02 \\ \Gamma_1^p(Q^2 = 10\mathrm{GeV}^2) &= 0.141 \pm 0.005 \end{aligned} \tag{7.4}$$

compared with

$$\begin{aligned} a^0(Q^2 = 10\mathrm{GeV}^2) &= 0.33 \pm 0.05 \\ \Gamma_1^p(Q^2 = 10\mathrm{GeV}^2) &= 0.144 \pm 0.009 \end{aligned} \tag{7.5}$$

in the chiral limit.

We therefore find very good agreement between the final prediction for the singlet axial charge in the presence of quark masses and in the chiral limit. This confirms our theoretical expectation that a^0 is relatively insensitive to the quark masses. Moreover, our new prediction for the 'proton spin' suppression remains, notwithstanding the large errors on the experimental data, in good agreement with the experimental results quoted in section 4.

8. Conclusions

In this paper, we have extended our previous analysis of the 'proton spin' problem in the chiral limit by considering the effects of chiral $SU(3)$ symmetry breaking and flavour mixing due to the quark masses.

The formal basis of our analysis is the derivation of the new, unified Goldberger-Treiman relations:

$$G_A^a = \frac{1}{2m_N} F_{ab} \hat{\Gamma}_{\eta^b NN} \tag{8.1}$$

where F is determined from

$$F_{ac}F_{cb}^T = \lim_{k=0} \frac{d}{dk^2} i \int dx\, e^{ikx} \langle 0|T\ \partial^\mu J_{\mu 5}^a(x)\ \partial^\nu J_{\nu 5}^b(0)|0\rangle \tag{8.2}$$

Apart from the mixing between the flavour singlet and octet channels induced by the non-vanishing strange quark mass, the most significant change is the generalisation of the slope of the topological susceptibility $\chi'(0)$ to the equivalent correlation function involving the *total* divergence of the singlet axial current, viz. $\frac{d}{dk^2}\langle 0|T\ \partial^\mu J_{\mu 5}^0\ \partial^\nu J_{\nu 5}^0|0\rangle\big|_{k=0}$. This is the quantity which displays the smoothest approach to the chiral limit, with the explicit quark mass dependence present in the individual correlators (section 5) cancelling in the sum. This observation may have important implications for attempts to calculate the topological susceptibility using lattice methods[53], where it is notoriously difficult to approach the chiral limit too closely.

We emphasise again that the unified GT relations are new results and are *exact* in QCD. The familiar PCAC forms (in the flavour non-singlet channels) are obtained by approximating the 1PI vertices by the corresponding low-energy meson-nucleon coupling constants and by approximating the slopes of the current correlation functions by decay constants. Away from the chiral limit, both approximations assume pole-dominance of the matrix elements and correlation functions by the pseudo-Goldstone bosons.

The relevant correlation functions were then evaluated using QCD spectral sum rules. In the singlet as well as octet channel, very good stability was obtained with respect to the parameter τ. The optimum value of $\tau^{-1} = 2.5 - 5\ \mathrm{GeV}^2$ is in line with general arguments for the appropriate scale in the gluon-rich $U_A(1)$ channel. Specific criticisms[16-20] of the applicability of spectral sum rules to the $U_A(1)$ channel were shown to be incorrect.

Our final numerical results agree with our earlier findings[12]. The suppression in the flavour singlet axial charge, driven by the mechanism of topological charge screening, is confirmed. The reduction in the predicted value of $a^0(Q^2)$ compared to its chiral limit is slight (less than 10%), in agreement with our general theory, although it should be emphasised that our results still neglect flavour mixing. Translated into a prediction for the first moment of g_1^p, under the assumption that the RG-invariant vertices in eq.(8.1) are well approximated by their OZI values, our final result:

$$\begin{aligned} a^0(Q^2 = 10\mathrm{GeV}^2) &= 0.31 \pm 0.02 \\ \Gamma_1^p(Q^2 = 10\mathrm{GeV}^2) &= 0.141 \pm 0.005 \end{aligned} \tag{8.3}$$

remains in good agreement with experiment, and confirms our proposal that the 'proton spin' suppression is a target-independent effect due to the screening of topological charge by the QCD vacuum.

Appendix A: Partial Legendre transforms

We derive here the relations between the Green functions and vertices, defined as functional derivatives of the generating functionals W and Γ respectively, used in the derivation of the GT relations[11].

For generality, we derive these results for a set of fields Φ^a and 'currents' J^r, with sources S^a and V^r, where the partial Legendre transform is made wrt the sources S^a only. That is,

$$W[V,S] = \Gamma[V,\Phi] + S^a\Phi^a \tag{A.1}$$

We adopt a compact notation where any Lorentz indices are implicit and a spacetime integration is assumed in the sum over repeated indices. As in the text, functional differentiation is indicated by subscripts. Thus, e.g., W_S denotes $\frac{\delta W}{\delta S}$ at fixed V, etc.

By definition,

$$\Phi^a = W_{S^a} \tag{A.2}$$

while

$$\Gamma_{\Phi^a} = -S^a \qquad\qquad \Gamma_{V^r} = W_{V^r} \tag{A.3}$$

From

$$\begin{aligned}\delta^a_b \;&=\; \frac{\delta}{\delta\Phi^a}\Phi^b \;=\; \frac{\delta V^r}{\delta\Phi^a}\,W_{V^rS^b} \;+\; \frac{\delta S^c}{\delta\Phi^a}\,W_{S^cS^b} \\ &=\; -\Gamma_{\Phi^a\Phi^c}\,W_{S^cS^b}\end{aligned} \tag{A.4}$$

we recover the usual result that the 2-point vertex matrix is just the inverse of the propagator matrix, but in this case restricted to the S^a,Φ^a sector.

Similarly, from

$$\begin{aligned}0 \;&=\; \frac{\delta}{\delta V^r}\Phi^b \;=\; \frac{\delta V^t}{\delta V^r}\,W_{V^tS^b} \;+\; \frac{\delta S^c}{\delta V^r}\,W_{S^cS^b} \\ &=\; W_{V^rS^b} \;-\; \Gamma_{V^r\Phi^c}\,W_{S^cS^b}\end{aligned} \tag{A.5}$$

we find

$$\Gamma_{V^r\Phi^b} = W_{V^rS^c}\,W^{-1}_{S^cS^b} \tag{A.6}$$

which can therefore be identified as the matrix element $\langle 0|J^r|\Phi^b\rangle$.

Taking this further,

$$\begin{aligned}0 \;&=\; \frac{\delta}{\delta V^r}\Big(W_{S^aS^c}\Gamma_{\Phi^c\Phi^b}\Big) \\ &=\; W_{V^rS^aS^c}\,\Gamma_{\Phi^c\Phi^b} + W_{S^aS^c}\,\Big(\Gamma_{V^r\Phi^c\Phi^b} \;+\; W_{V^rS^d}\,\Gamma_{\Phi^d\Phi^c\Phi^b}\Big)\end{aligned} \tag{A.7}$$

from which we find

$$\Gamma_{V^r\Phi^c\Phi^b} \;+\; W_{V^rS^d}\,\Gamma_{\Phi^d\Phi^c\Phi^b} \;=\; W^{-1}_{S^aS^c}\,W_{V^rS^cS^d}\,W^{-1}_{S^dS^b} \tag{A.8}$$

which is identified as $\langle \Phi^a | J^r | \Phi^b \rangle$.

As a final example, we derive the crucial identity (3.11) used in our derivation of the GT relations:

$$\begin{aligned}
\Gamma_{V^r V^s} \;&=\; \frac{\delta}{\delta V^r} W_{V^s} \;=\; \frac{\delta V^t}{\delta V^r} W_{V^t V^s} \;+\; \frac{\delta S^d}{\delta V^r} W_{S^d V^s} \\
&=\; W_{V^r V^s} \;+\; \Gamma_{V^r \Phi^d} W_{S^d V^s} \\
&=\; W_{V^r V^s} \;-\; W_{V^r S^c}\, W^{-1}_{S^c S^d}\, W_{S^d V^s} \qquad (A.9)
\end{aligned}$$

the last line following from eq.(A.6).

Appendix B: Current algebra, Dashen's formula and the GT relation

As an illustration of how standard current algebra (PCAC) relations arise from our formalism, we give here a short derivation of the Dashen formula for the masses of the pseudo-Goldstone bosons.

The starting point is the identification (see eq.(A.6))

$$\Gamma_{V^a_{\mu 5} \eta^b} = \langle 0 | J^a_{\mu 5} | \eta^b \rangle = i k_\mu f^{ab}(k^2) \qquad (B.1)$$

where the on-shell function $f^{ab}(m^2_\eta)$ is the decay constant matrix for the pseudo-Goldstone bosons η^a. In terms of the normalised fields $\eta^a = B_{ab}\phi^b_5$, the Ward identity (2.14) is written as

$$i k_\mu \Gamma_{V^a_{\mu 5} \eta^b} + \Phi_{ac} B^T_{cd}\, \Gamma_{\eta^d \eta^b} - M_{ac} B^{-1}_{cb} = 0 \qquad (B.2)$$

Now take $\frac{d}{dk^2}\Big|_{k=0}$ of this equation. Using the normalisation condition (3.7), we find immediately

$$f_{ab}(0) = \Phi_{ac} B^T_{cb} \qquad (B.3)$$

The assumption that f_{ab} is only a slowly-varying function of k^2 then allows (B.3) to be identified with the decay constant matrix. This is (as explained in detail in ref.[11]) the standard PCAC approximation, equivalent to pole dominance of correlation functions by pseudo-Goldstone bosons.

In the same approximation, we can write

$$\Gamma_{\eta^a \eta^b} = k^2 \delta_{ab} - (m^2_\eta)_{ab} \qquad (B.4)$$

Neglecting the mixing with Q, this would produce a pole in the propagator matrix with the corresponding mass matrix obtained from the zero-momentum limit of the Ward identity (B.2). In matrix notation, this means that

$$0 = -\Phi B^T m^2_\eta - M B^{-1} \qquad (B.5)$$

and so

$$\Phi B^T m_\eta^2 B \Phi^T = -M B^{-1} B \Phi^T \tag{B.6}$$

Using the identification (B.3) of the decay constant, we therefore have (recall $\Phi^T = \Phi$),

$$f_{ac}\ (m_\eta^2)_{cd}\ f_{db}^T = -M_{ac}\Phi_{cb} \tag{B.7}$$

This is Dashen's formula for the pseudo-Goldstone bosons, which for the $n_f = 2$ chiral symmetry breaking pattern $SU(2)_L \times SU(2)_R \rangle SU(2)_V$ is simply

$$f_\pi^2\ m_\pi^2 = -(m_u + m_d)\langle \bar{q}q\rangle \tag{B.8}$$

Mixing with the glueball field Q in general shifts the masses of the physical pseudo-Goldstone bosons. However, in the simple case where $\Phi_{a0} \equiv 2\langle\phi^a\rangle$ is zero for $a \neq 0$, this is only relevant in the singlet sector. There, the formula (B.7) refers to the unphysical η^0, *not* to the η'. The corresponding formula for the physical η' including mixing with the glueball field Q, and involving a different identification of the η' decay constant, is derived (in the chiral limit) in ref.[11].

We can also relate the generalised GT relations in the text to the standard formula using pole dominance. For $n_f = 2$, eq.(3.18) reduces to

$$m_N\ g_A = F\ g_{\pi NN} \tag{B.9}$$

where $g_A \equiv 2G_A^3$ in our notation. Evaluating F from eq.(3.20) using pole dominance, we find

$$F^2 = \frac{d}{dk^2}\Big(\big|\langle 0|\partial^\mu J_{\mu 5}^3|\pi\rangle\big|^2 \frac{(-1)}{k^2 - m_\pi^2}\Big)\Big|_{k=0} = f_\pi^2 \tag{B.10}$$

recovering the standard GT formula and confirming the interpretation of F in eq.(3.18) as a decay constant matrix. Notice that since this derivation assumes pole dominance, it is an approximation. Unlike the new relation (3.18), the standard GT relation becomes exact only in the chiral limit.

Appendix C: Renormalisation Group

The renormalisation group equations (RGEs) for the various quantities arising in the derivation of the unified GT relations can be derived using the same methods developed in ref.[11]. In this appendix, we summarise the most important identities.

The starting point is the definition of the renormalised composite operators[54]. For QCD, with non-zero quark masses, we have (denoting bare operators with the label 'B' and renormalised operators with no label for simplicity)

$$\begin{aligned} &J_{\mu 5}^0 = Z J_{\mu 5}^{0B} \qquad\qquad J_{\mu 5}^{a\neq 0} = J_{\mu 5}^{a\neq 0B} \\ &Q = Q^B - \frac{1}{2n_f}(1-Z)\partial^\mu J_{\mu 5}^{0B} \\ &\phi_5^a = Z_\phi \phi_5^{aB} \qquad\qquad \phi^a = Z_\phi \phi^{aB} \end{aligned} \tag{C.1}$$

where Z_ϕ is the inverse of the mass renormalisation, $Z_\phi = Z_m^{-1}$. The anomalous dimensions associated with Z and Z_ϕ are denoted γ and γ_ϕ respectively. These definitions ensure that the combinations $\partial^\mu J^0_{\mu 5} - 2n_f Q$ and $m_q[\bar{q}\gamma_5 q]$ occurring in the $U_A(1)$ anomaly equation (e.g. eq.(6.2)) are RG invariant.

The fundamental RGE for the generating functional W is therefore (in the notation of section 2, where suffices on W denote functional differentiation):

$$\mathcal{D}W = \gamma\Big(V^0_{\mu 5} - \frac{1}{2n_f}\partial_\mu \theta\Big)W_{V^0_{\mu 5}} + \gamma_\phi\Big(S^a_5 W_{S^a_5} + S^a W_{S^a}\Big) + \ldots \qquad (C.2)$$

where $\mathcal{D} = \Big(\mu\frac{\partial}{\partial\mu} + \beta\frac{\partial}{\partial g} - \gamma_m \sum_q m_q \frac{\partial}{\partial m_q}\Big)\Big|_{V,\theta,S_5,S}$ and a spacetime integration is assumed in the sum over repeated indices. The notation $+\ldots$ refers to the additional terms which are required to produce the contact term contributions to the RGEs for n-point Green functions of composite operators. These are discussed fully in ref.[11], but will be omitted here for simplicity. They vanish at zero momentum.

The RGEs for Green functions are found simply by differentiating eq.(C.2) wrt the sources. Simplifying the results using the chiral Ward identities (2.5), we find a complete set of RGEs for the 2-point functions. These are:

$$\mathcal{D}W_{V^0_{\mu 5}V^0_{\nu 5}} = 2\gamma W_{V^0_{\mu 5}V^0_{\nu 5}} + \ldots \qquad \mathcal{D}W_{V^0_{\mu 5}V^b_{\nu 5}} = \gamma W_{V^0_{\mu 5}V^b_{\nu 5}} + \ldots \qquad \mathcal{D}W_{V^a_{\mu 5}V^b_{\nu 5}} = 0 + \ldots$$
$$\mathcal{D}W_{V^0_{\mu 5}\theta} = 2\gamma W_{V^0_{\mu 5}\theta} + \gamma\frac{1}{2n_f}M_{0b}W_{V^0_{\mu 5}S^b_5} + \ldots$$
$$\mathcal{D}W_{V^a_{\mu 5}\theta} = \gamma W_{V^a_{\mu 5}\theta} + \gamma\frac{1}{2n_f}M_{0b}W_{V^0_{\mu 5}S^b_5} + \ldots$$
$$\mathcal{D}W_{V^0_{\mu 5}S^b_5} = (\gamma+\gamma_\phi)W_{V^0_{\mu 5}S^b_5} + \ldots \qquad \mathcal{D}W_{V^a_{\mu 5}S^b_5} = \gamma_\phi W_{V^a_{\mu 5}S^b_5} + \ldots$$
$$\mathcal{D}W_{\theta\theta} = 2\gamma W_{\theta\theta} + 2\gamma\frac{1}{2n_f}M_{0b}W_{\theta S^b_5} + \ldots$$
$$\mathcal{D}W_{\theta S^b_5} = (\gamma+\gamma_\phi)W_{\theta S^b_5} + \gamma\frac{1}{2n_f}\big(M_{0c}W_{S^c_5 S^b_5} + \Phi_{0b}\big) + \ldots$$
$$\mathcal{D}W_{S^a_5 S^b_5} = 2\gamma_\phi W_{S^a_5 S^b_5} + \ldots \qquad (C.3)$$

It is straightforward to check the self-consistency of these RGEs with the Ward identities (2.5) and (2.11). The pattern of cancellations which ensures this is nevertheless quite intricate.

Next, we need the RGE for the generating functional of the 1PI vertices. This follows immediately from its definition in eq.(2.12) and the RGE (C.2) for W:

$$\tilde{\mathcal{D}}\Gamma = \gamma\Big(V^0_{\mu 5} - \frac{1}{2n_f}\Gamma_Q\partial_\mu\Big)\Gamma_{V^0_{\mu 5}} - \gamma_\phi\Big(\phi^a_5\Gamma_{\phi^a_5} + \phi^a\Gamma_{\phi^a}\Big) + \ldots \qquad (C.4)$$

where $\tilde{\mathcal{D}} = \Big(\mu\frac{\partial}{\partial\mu} + \beta\frac{\partial}{\partial g} - \gamma_m \sum_q m_q \frac{\partial}{\partial m_q}\Big)\Big|_{V,Q,\phi_5,\phi}$.

The RGEs for the 1PI vertices are found by differentiation and, using the Ward identities (2.14) to simplify the results, we find in particular:

$$\mathcal{D}\hat{\Gamma}_{QNN} = -\gamma\hat{\Gamma}_{QNN} + \gamma\frac{1}{2n_f}\Phi_{0b}\Big(\Gamma_{Q\phi_5^b}\hat{\Gamma}_{QNN} + \Gamma_{QQ}\hat{\Gamma}_{\phi_5^b NN}\Big) + \ldots$$
$$\mathcal{D}\hat{\Gamma}_{\phi_5^a NN} = -\gamma_\phi\hat{\Gamma}_{\phi_5^a NN} + \gamma\frac{1}{2n_f}\Phi_{0b}\Big(\Gamma_{\phi_5^a\phi_5^b}\hat{\Gamma}_{QNN} + \Gamma_{\phi_5^a Q}\hat{\Gamma}_{\phi_5^b NN}\Big) - \gamma\frac{1}{2n_f}M_{0a}\hat{\Gamma}_{QNN} + \ldots \tag{C.5}$$

Here, $\mathcal{D} = \tilde{\mathcal{D}} + \gamma_\phi\langle\phi^a\rangle\frac{\delta}{\delta\phi^a}$. As explained in ref.[11], this is identical to the RG operator $\mathcal{D}$ defined above (acting on W) when the sources are set to zero and the fields to their VEVs. With some calculation, the consistency of the GT formulae (3.4) and (3.5) can now be shown using the RGEs (C.3) and (C.5). Again, a very intricate pattern of cancellations occurs to ensure this.

The RGEs for the 2-point vertices occurring in the Ward identities (2.14) are easily found by differentiating eq.(C.4). The most important is

$$\mathcal{D}\Gamma_{\phi_5^a\phi_5^b} = -2\gamma_\phi\Gamma_{\phi_5^a\phi_5^b} + \gamma\frac{1}{2n_f}\Big(\Gamma_{\phi_5^a Q}\big(\Phi_{0c}\Gamma_{\phi_5^c\phi_5^b} - M_{0b}\big) + \ a\leftrightarrow b\ \Big) + \ldots \tag{C.6}$$

This allows us to deduce the RGE for the matrix B_{ab} which relates the ϕ_5^a fields to the canonically normalised η^a fields by $\eta^a = B_{ab}\phi_5^b$. Recall the definition (3.9):

$$\frac{d}{dk^2}\Gamma_{\phi_5^a\phi_5^b}\big|_{k=0} = B^T_{ac}\ \frac{d}{dk^2}\Gamma_{\eta^c\eta^d}\big|_{k=0}\ B_{db} = B^T_{ac}B_{cb} \tag{C.7}$$

From eq.(C.6) and the zero-momentum limit of the Ward identities (2.14), we deduce

$$\mathcal{D}B_{ab} = -\gamma_\phi B_{ab} + \gamma B_{ac}\Phi_{c0}\Phi^{-1}_{0b} \tag{C.8}$$

The RGE for F_{ab} now follows immediately from its definition $F = \Phi B^T$ and the RGE $\mathcal{D}\Phi = \gamma_\phi\Phi$. It is simply

$$\mathcal{D}F_{ab} = \gamma\delta_{a0}F_{0b} \tag{C.9}$$

that is,

$$\begin{aligned} \mathcal{D}F_{0b} &= \gamma F_{0b} \qquad &&\text{for all } b \\ \mathcal{D}F_{ab} &= 0 && a\neq 0 \end{aligned} \tag{C.10}$$

The final step in proving RG consistency of the unified GT formulae is to show that the vertices $\hat{\Gamma}_{\eta^a NN}$ (at $k=0$) are RG invariant. Eq.(C.10) then ensures the required RGE for the axial charges, viz.

$$\mathcal{D}G^a_A = \gamma\delta_{a0}G^a_A \tag{C.11}$$

To check this explicitly, notice that eq.(C.5) for $\hat{\Gamma}_{\phi_5^a NN}$ simplifies at $k=0$. The contact terms vanish and using the zero-momentum Ward identities (see eq.(2.14)) we find

$$\mathcal{D}\hat{\Gamma}_{\phi_5^a NN}\big|_{k=0} = -\gamma_\phi\hat{\Gamma}_{\phi_5^a NN}\big|_{k=0} + \gamma\Phi^{-1}_{a0}\Phi_{0b}\hat{\Gamma}_{\phi_5^b NN}\big|_{k=0} \tag{C.12}$$

Since $\hat{\Gamma}_{\phi_5^a NN}\big|_{k=0} = B^T_{ab}\hat{\Gamma}_{\eta^b NN}\big|_{k=0}$, and comparing eq.(C.12) with the RGE (C.8) for B, we confirm

$$\mathcal{D}\hat{\Gamma}_{\eta^a NN}\big|_{k=0} = 0 \qquad \text{for all } a \qquad (C.13)$$

Appendix D: Comparison with the literature

In a number of papers and lectures (see e.g. refs.[16,17]), Ioffe has criticised our earlier work on the 'proton spin', expressing his view that our formal theory is "not justifiable" and claiming that the spectral sum rule technique we use is not valid for calculating the topological susceptibility or decay constants in the flavour singlet channel.

These criticisms are made explicit in the recent paper [17]. Describing our derivation of the $U_A(1)$ Goldberger-Treiman relation (in the chiral limit) for G_A^0, Ioffe states that "the matrix element $\langle p|Q|p\rangle$ was saturated by contribution of two operators Q and singlet pseudoscalar operator ϕ_5 – and the result was obtained by orthogonalisation of the corresponding matrix." This simply reflects a failure to understand our theoretical method. As we have repeatedly emphasised, no approximation is involved in the decomposition of the matrix element into composite propagators and 1PI vertices, as e.g. in eq.(3.5) here. If a different basis of operators is chosen, the definition of the vertices changes too – they become 1PI with respect to the new basis. The basis of operators chosen for the decomposition is in no sense required to be 'complete' – the procedure is *not* the familiar quantum mechanical one of inserting a complete set of states. The matrix element is *not* being saturated with a restricted number of operators chosen from some complete set. The only approximation comes in our subsequent conjecture that the vertices, defined specifically as we have defined them, obey the OZI rule. The motivations and *a posteriori* justifications for this conjecture are explained carefully and at length in our papers.

Still referring to our work[12], Ioffe continues, "the calculation of $\chi'(0)$ by QCD sum rules is not correct, because as shown in ref.[19] by considering the same problem with account of higher order terms of OPE than it was done in [12], the OPE breaks down at the scales characteristic of this problem." This refers to ref.[19], where Ioffe and Khodzhamiryan suggested that the extent of $SU(3)$ breaking which occurs in the Laplace sum rule approach is unrealistically large, and concluded that QCD spectral sum rules were unreliable in the $U_A(1)$ channel. In the rest of this appendix, we show explicitly how their calculation is related to ours and point out a number of problems (errors in the QCD expressions, inconsistencies of the input and stability parameters, etc.) in their approach which are responsible for this false conclusion.

We consider the current correlation function

$$\begin{aligned}\Pi^{0q}_{\mu\nu}(k) &= i\int d^4x\, e^{ik.x}\, \langle 0|T\ J^0_{\mu 5}(x)\ J^q_{\nu 5}(0)|0\rangle \\ &= \Pi^{0q}_T(k^2)(g_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}) + \Pi^{0q}_L(k^2)\frac{k_\mu k_\nu}{k^2} \qquad (D.1)\end{aligned}$$

where $J^{0q}_{\mu 5} = \bar{q}\gamma_\mu\gamma_5 q$ is the axial current for each flavour of quark $q = u, d, s$ separately. The notation follows our eq.(5.2). Comparing with the notation of ref.[19], the Π_L are the same up to a minus sign, whereas our Π_T is a linear combination of the form factors defined there. Only Π_L plays a role in what follows.

Taking the divergences, and using the chiral Ward identity (2.9), we have

$$k^\mu k^\nu \Pi^{0q}_{\mu\nu}(k) \;=\; k^2 \Pi^{0q}_L(k^2) \;=\; i\int d^4x\; e^{ik.x}\; \langle 0|T\; D^0(x)\; D^q(0)|0\rangle + 4m_q\langle\bar{q}q\rangle \qquad (D.2)$$

where

$$\begin{aligned} D^0 &= 2n_f Q + \sum_{q=u,d,s} 2m_q\bar{q}\gamma_5 q \\ D^q &= 2Q + 2m_q\bar{q}\gamma_5 q \end{aligned} \qquad (D.3)$$

The relation with the correlators studied in the text is therefore

$$\psi_5(k^2) - \psi_5(0) \;=\; \frac{1}{(2n_f)^2}k^2 \sum_{q=u,d,s} \Pi^{0q}_L(k^2) \qquad (D.4)$$

with the other $SU(3)$ combinations giving ψ_5^{03} and ψ_5^{08}. Taking the derivative wrt k^2 and evaluating at $k=0$, we find

$$\psi_5'(0) \;=\; \frac{1}{(2n_f)^2}\sum_{q=u,d,s} \Pi^{0q}_L(0) \qquad (D.5)$$

$\Pi^{0q}_L(k^2)$ obeys an unsubtracted dispersion relation

$$\Pi^{0q}_L(k^2) \;=\; \int_0^\infty \frac{dt}{t-k^2-i\epsilon}\frac{1}{\pi}\mathrm{Im}\Pi^{0q}_L(t) \qquad (D.6)$$

The corresponding Laplace sum rule is simply

$$\tau^{-3}\mathcal{L}(\mathcal{F}_\Pi) \;=\; \int_0^\infty dt e^{-t\tau}\frac{1}{\pi}\mathrm{Im}\Pi^{0q}_L(t) \qquad (D.7)$$

We can also write a once-subtracted sum rule, which enables us to calculate $\Pi^{0q}_L(0)$:

$$\tau^{-2}\mathcal{L}(\mathcal{G}_\Pi) + \Pi^{0q}_L(0) \;=\; \int_0^\infty \frac{dt}{t}e^{-t\tau}\frac{1}{\pi}\mathrm{Im}\Pi^{0q}_L(t) \qquad (D.8)$$

Here,

$$\mathcal{F}_\Pi \equiv \frac{d^2}{(dK^2)^2}\Pi^{0q}_L \qquad \mathcal{G}_\Pi \equiv \frac{d}{dK^2}\left(\frac{\Pi^{0q}_L}{K^2}\right) \qquad (D.9)$$

Taking the $SU(3)$ singlet combination of these sum rules for $q=u,d,s$ clearly gives just the Laplace sum rules (6.18) and (6.19) analysed in the text.

In ref.[19], Ioffe and Khodzhamiryan define the 'decay constants' for individual quark flavours as follows:

$$\langle 0|J^q_{\mu 5}|\eta'\rangle = ik_\mu g^q_{\eta'} \qquad (D.10)$$

and by saturating the r.h.s. of eq.(D.7) with the η', obtain sum rules for $f_{\eta'}g^q_{\eta'}$ for $q = u, d$ and $q = s$. Taking the ratio, they find an unrealistic $SU(3)$ breaking characterised by $g^s_{\eta'}/g^{u,d}_{\eta'} \sim 2.5$ and conclude that the Laplace sum rule for Π_L with the flavour singlet axial current does not work.

However, as we have shown in the text, a correct implementation of the sum rule method does indeed work, showing good stability over a range of appropriate τ and t_c values and giving results for the decay constants in both flavour singlet and non-singlet channels which show only the expected level of $SU(3)$ breaking. In the rest of this section, we shall therefore quote the full formula for the sum rule (D.7) for Π^{0q}_L, correcting some mistakes and omissions in ref.[19], then briefly indicate some of the problems with their calculation.

From the results given in section 6, we can immediately read off the required sum rule:

$$\begin{aligned}
2n_f\sqrt{2}f_{\eta'}g^q_{\eta'}m^2_{\eta'}e^{-\tau m^2_{\eta'}} \ + \ \ldots \ = \ &\frac{3}{8\pi^2}\tau^{-2}\Big(\frac{\bar\alpha_s}{\pi}\Big)^2\big(1-(1+t_c\tau)e^{-t_c\tau}\big)(1+\delta^{PT}_{gg}) \\
&+\frac{3}{2}\Big(\frac{\bar\alpha_s}{\pi}\Big)\bigg[\frac{1}{2\pi}\langle\alpha_s G^2\rangle(1+\delta^{NP}_{gg}) + \Big(\frac{\bar\alpha_s}{\pi}\Big)\tau\langle gG^3\rangle\bigg] \\
&+\delta_{qs}\frac{3}{2\pi^2}\tau^{-1}m_s^2(1-e^{-t_c\tau})(1+\delta^{PT}_{qq}) \\
&-2(1+3\delta_{qs})\Big(\frac{\bar\alpha_s}{\pi}\Big)M_0^2\tau m_s\langle\bar s s\rangle - \delta_{qs}4m_s\langle\bar s s\rangle
\end{aligned} \qquad (D.11)$$

where (see also [35])

$$\begin{aligned}
\delta^{PT}_{gg} &= \Big(\frac{\bar\alpha_s}{\pi}\Big)\bigg[\frac{83}{4} + \beta_1(1-\gamma_E) + 6\Big(3m_s^2 + \frac{\pi}{\bar\alpha_s}\lambda^2\Big)\tau\bigg] \\
\delta^{NP}_{gg} &= -\Big(\frac{\bar\alpha_s}{\pi}\Big)\Big(\frac{9\pi}{8}\Big)(1-e^{-t_c\tau}) \\
\delta^{PT}_{qq} &= \Big(\frac{17}{3} + 2\gamma_E\Big)\Big(\frac{\bar\alpha_s}{\pi}\Big)
\end{aligned} \qquad (D.12)$$

The dots on the l.h.s. denote the presence of any further intermediate states (in particular the η) which might be required. The terms appearing with δ_{qs} are present only when q is chosen to be the s quark, and as usual we have assumed $m_u = m_d = 0$.

We now comment on some of the differences between the paper [19] and our work:

• It is *a priori* dangerous to use the sum rule for Π^{0q}_L with the individual quark flavours while only keeping the η' as an intermediate state in the sum rule. This would imply that only the η' and not the η would contribute in the mixed $SU(3)$ combination Π^{08}_L. It follows that the quantity $g^s_{\eta'}/g^{u,d}_{\eta'}$ used in ref.[19] is not the most reliable measure of the strength of $SU(3)$ breaking: while a value close to 1 would indicate self-consistently that $SU(3)$ symmetry is very accurate and the $\eta - \eta'$ mixing angle is very small, a large value would simply show that the initial hypothesis of η' saturation for the individual Π_L^{0q} is not self-consistent. (Ref.[19] refers to a further calculation taking $\eta - \eta'$ mixing into account, but the details are not given.)

• The formula (D.11) differs in a number of important ways from that used in ref.[19]. In (D.11), the coefficient of the term $4m_s\langle\bar{s}s\rangle$ coming from the zero-momentum Ward identities has been corrected compared to ref.[19]. We have included the leading-order radiative corrections, which in this example have a significant effect in inducing stability in τ and t_c. Notice that the radiative corrections have a far greater effect on this single sum rule than in the combined sum rule used in the text to calculate $\psi_5'(0)$, where they cancel between the $\mathcal{L}(\mathcal{F})$ and $\mathcal{L}(\mathcal{G})$ terms. We have also included the contribution of $O(m_s^2)$ arising from the correlator denoted by ψ_{qq} in the text, which was omitted in ref.[19] but is of the same order as the other principal terms for the values of τ used in [19].

• In our analysis of the sum rules, we find good stability at values of $t_c \simeq 6$ GeV^2 and τ in the range $(0.2 - 0.4)$ GeV^{-2}. In contrast, ref.[19] uses too low a value of $t_c \simeq 2.5$ GeV^2 and without finding stability takes an *ad hoc* τ value of about 1 GeV^{-2}. This is far too high and goes against the expectation [41,40] that the optimal scale τ should be comparatively low in the gluon-rich flavour singlet channels. For this value of τ, the convergence of the OPE for the terms of $O(m_s^2\tau)$ is also poor.

We can therefore conclude that the analysis of the sum rule for $\Pi_L(k^2)$ in ref.[19] (equivalent to our once-subtracted sum rule for $\psi_5(k^2)$) is unreliable and that their conclusion that the spectral sum rule method does not work in the flavour singlet channel is mistaken.

By taking the once-subtracted sum rule (D.8) for $\Pi_L^{00}(k^2)$ in combination with (D.7), we can write a Laplace sum rule for $\Pi_L^{00}(0)$, the quantity required for the generalised Goldberger-Treiman relations (and therefore the 'proton spin' effect). This sum rule is of course identical to that for $\psi_5'(0)$ analysed in the text. This is not discussed in ref.[19]. Alternatively, Ioffe and Khodzhamiryan use a finite energy sum rule (FESR), analogous to the one described in our eq.(6.45) but omitting the radiative corrections. However, the FESR should be used with great care due to its strong t_c dependence, and the fact that the result comes from a difference of large numbers. Indeed, it is unsurprising that by substituting their set of values of $f_{\eta'}$, $g_{\eta'}$, and t_c, which are inconsistent with the values we have obtained from the Laplace sum rule based on τ and t_c stabilities, they obtain an unreliable result.

Finally, in more recent papers[20], Ioffe and Oganesian extend the work of ref.[19] by combining it with a sum rule for G_A^0 itself, derived using a composite 3-quark operator with the quantum numbers of the proton. However, one can immediately notice that the choice of the interpolating nucleon currents used by the authors is far away from the optimised choice analysed in refs.[48,49]. Irrespective of the validity of this method, it is evident that the results of ref.[20] are as unreliable as those discussed above, and for the same reasons, since the results of ref.[19] are used as input parameters in the new sum rule.

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Figures

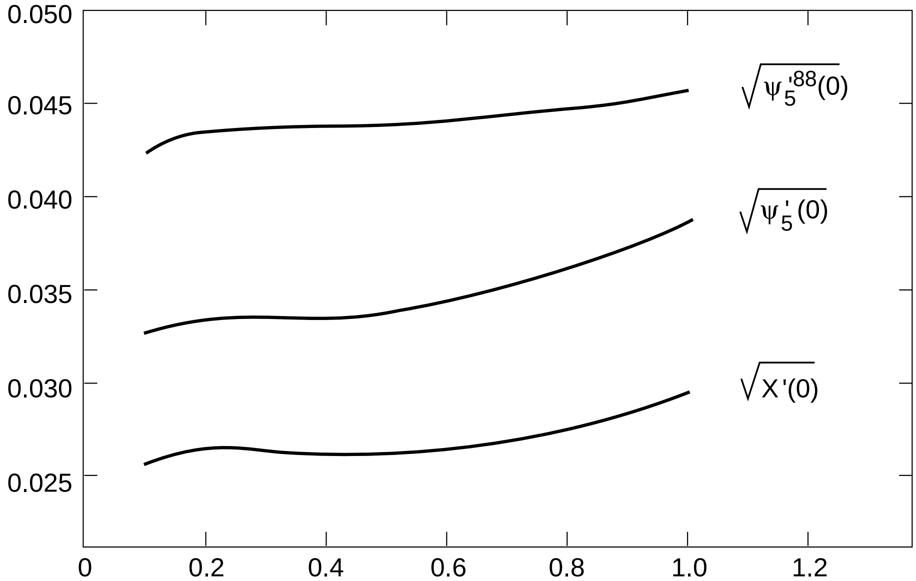


Fig. 1 The dependence of the correlation functions $\chi'(0)$, $\sqrt{\psi_5'(0)}$ and $\sqrt{\psi_5'^{88}(0)}$ (in GeV) on the Laplace sum rule parameter τ (in GeV^{-2}).

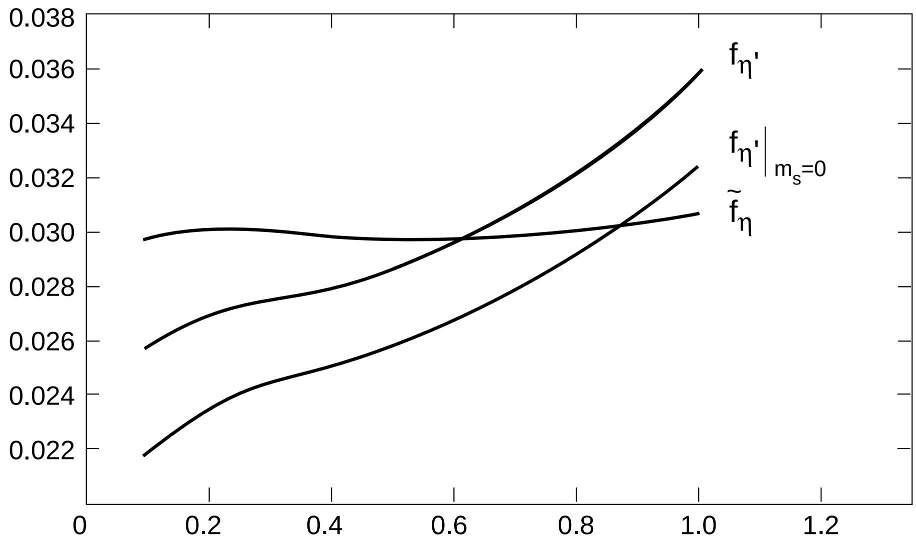
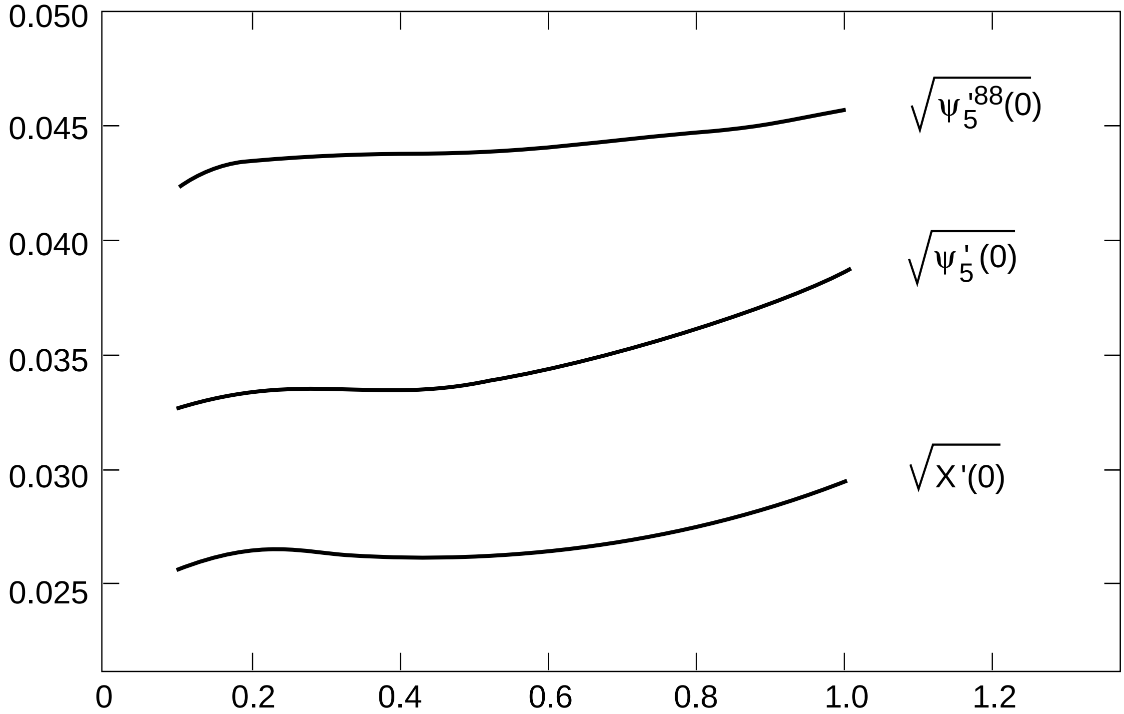


Fig. 2 The dependence of the decay constants $f_{\eta'}\big|_{m_s=0}$, $f_{\eta'}$ and $\tilde{f}_\eta$ (in GeV) on the Laplace sum rule parameter τ (in GeV^{-2}).


0.050
0.045
0.040
0.035
0.030
0.025
0
0.2
0.4
0.6
0.8
1.0
1.2
$\sqrt{\psi_5'^{88}(0)}$
$\sqrt{\psi_5'(0)}$
$\sqrt{X'(0)}$